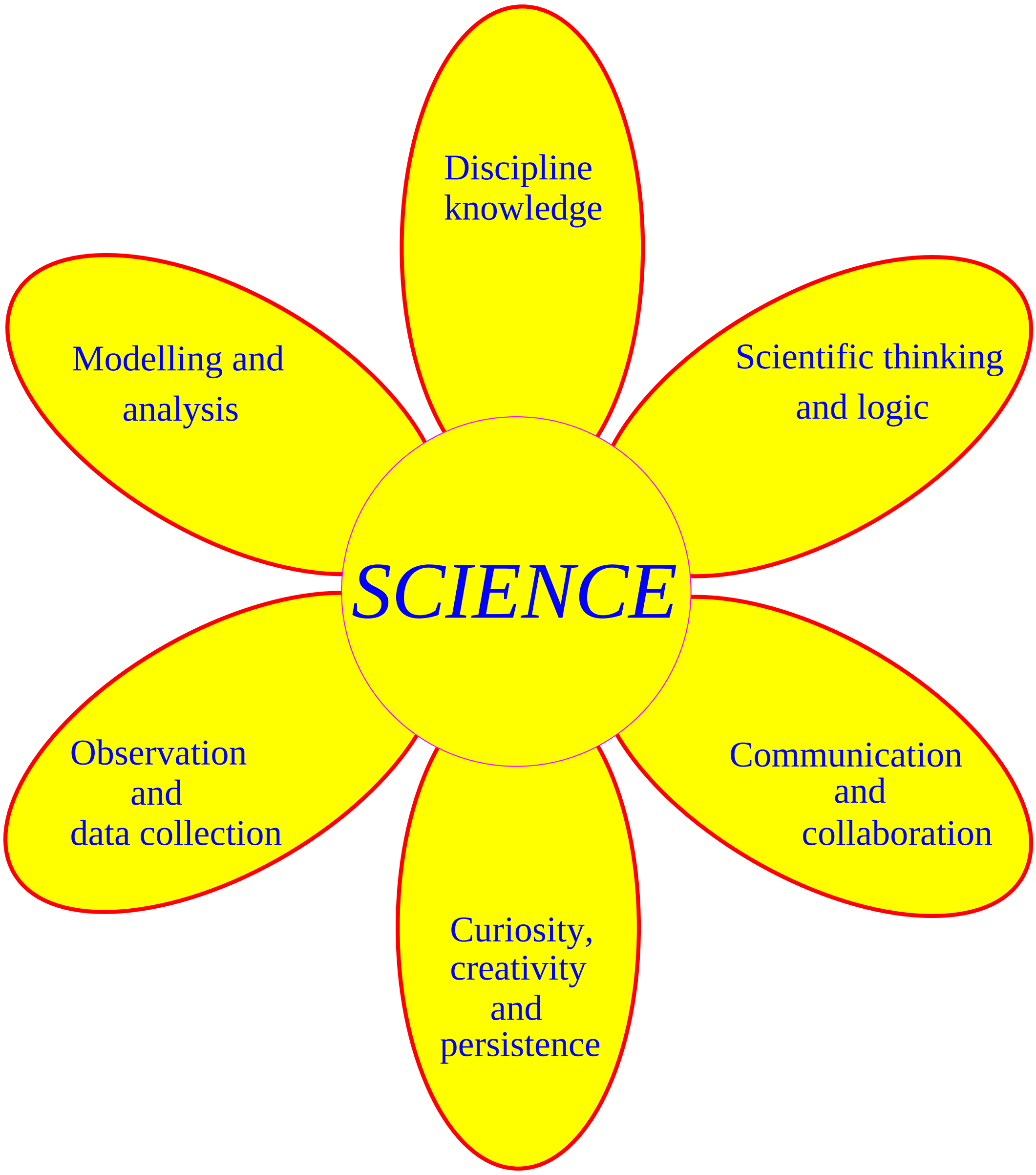
SCIE1000

Theory and Practice in Science



Course materials

Third edition, 2010

About these notes

This book contains the lecture notes and Python programming manual for SCIE1000.

We will use these notes extensively, so it is essential that you have your own copy. Details on how you can obtain a copy will be given in class during the first week of semester. Please note that there is no text book for SCIE1000, so these notes are your primary source of information. Do not try to re-use a copy from your friends or from a previous semester: the notes change from year to year, and it is very important for you to write things in your own words.

If you lose these notes then you will probably have big problems. You might like to write your name and some contact details on the bottom of this page just in case.

These notes have been prepared very carefully, but there will inevitably be some (hopefully minor) errors in them. We are continually trying to improve the notes; if you have any suggestions, please tell us. (Please note that attributions and web references are not given for some of the pictures in the lecture notes; a list of attributions is available from the course teaching team if you are interested.)

These important notes belong to: ______________________________

If you find them, please return them to me!

I can be contacted via: ____________________________________

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Table of contents.

1 SCIE1000 preliminaries

As deep as any ocean
As sweet as any harmony
She blinded me with science
And failed me in geometry

Artist: Thomas Dolby*

(www.youtube.com/watch?v=2IlHgbOWj4o)

*The School of Athens** (1510 – 1511), Raphael (1483 – 1520), Stanze di Raffaello, Apostolic Palace, Vatican.
(Image source: en.wikipedia.org/wiki/Image:Sanzio_01.jpg)

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* To emphasise that science and knowledge play fundamental roles in human history, culture and society, each section of the notes commences with two scientifically relevant cultural experiences, in the form of song lyrics and a work of art. Loosely, one could be regarded as low culture and the other as high culture; you can decide which is which. *The School of Athens* depicts some famous scientists, mathematicians and philosophers, including Plato, Aristotle, Euclid , Socrates and Pythagoras.

Introduction

SCIE1000 covers a wide range of topics. At first you might not see how all of these tie together, but the relationships are surprisingly close. The key areas covered include:

- specific problems and issues in a range of science disciplines;
- how to design, formulate and test models;
- mathematical techniques;
- computer programming;
- quantitative reasoning and critical evaluation; and
- the nature of science and scientific thinking.

It is likely that you will find some concepts harder than other concepts, and some areas will be of more immediate interest to you than others. Due to time constraints it is not possible to illustrate every concept with an example from each field of science; instead we illustrate concepts with a few important examples from one or two fields, and cover other fields elsewhere in the course. Rather than requiring memorisation of specific facts, the focus of SCIE1000 is to teach various scientific and mathematical techniques and concepts, and apply these to a wide range of disciplines.

Interestingly, almost every example and case study is either taken from a research paper or is a fairly accurate model of a realistic situation (so the examples are not contrived).

This section introduces the teaching team for SCIE1000, then discusses the course aims (including graduate attributes and learning goals) and different learning styles, and finishes with a brief description of how to use these notes.

1.1 Teaching staff

Here is some information about the members of the core teaching team for SCIE1000. (You will also encounter other staff members and tutors.)

Professor Peter Adams is Associate Dean (Academic) in the Faculty of Science. When he is not busy with administrative things he is a mathematician in the School of Mathematics and Physics. He studied mathematics, computer science and commerce at The University of Queensland, and completed a PhD in mathematics at UQ in 1995. He has worked as a computer system administrator, research officer and academic staff member at the University.

His area of research specialisation is combinatorial mathematics and computing. Combinatorial mathematics is concerned with selecting and arranging objects subject to constraints; problems involving this kind of activity arise in a range of practical applications. Thus his research work spans pure mathematics, computational algorithms and bioinformatics. Some of his recent research projects include using combinatorial methods for identifying drug lead molecules, and statistical methods for genome analysis. He has published over 90 scientific research papers, is an Associate Fellow of the Australian Learning and Teaching Council, and is Secretary of the Federation of Australian Scientific and Technological Societies.

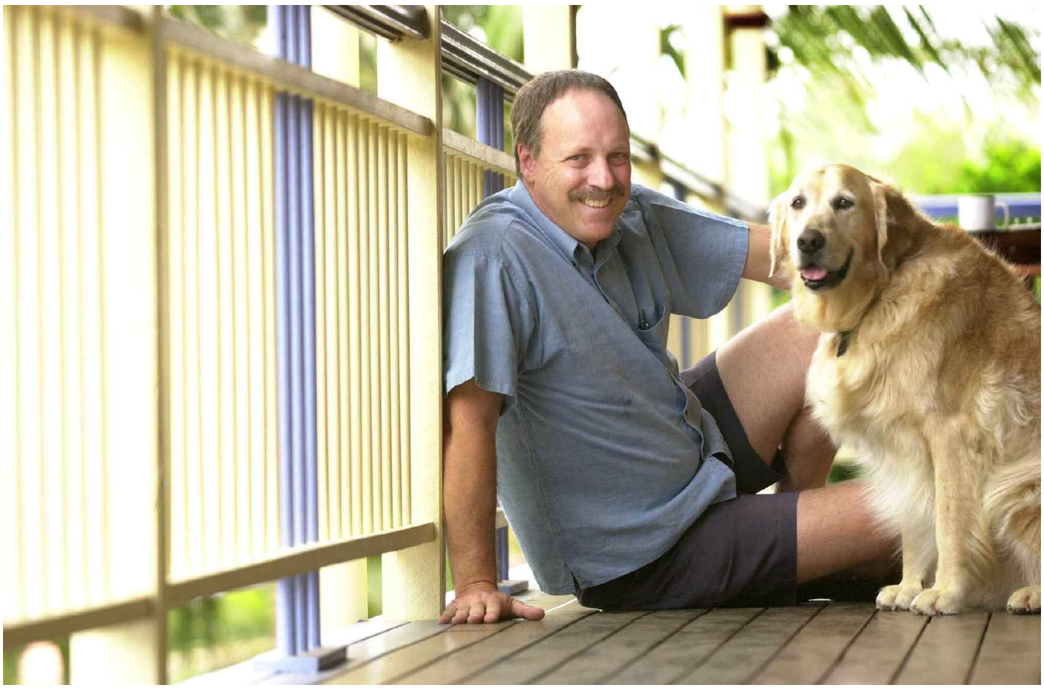
(-17 °C + tongue + metal pole = idiot)

Professor Peter O'Donoghue (POD) is one of the three resident parasitologists in the School of Chemistry and Molecular Biosciences in the Faculty of Science. He trained in cell biology at the University of Adelaide, medical parasitology at the University of Munich and veterinary parasitology at the Hannover Veterinary University. He worked at the Institute of Medical and Veterinary Science in Adelaide before moving to the University of Queensland in 1994.

His area of specialisation is clinical protozoology and he practices as a diagnostician; identifying protozoan parasites causing disease in vertebrate hosts. His goal is to characterise those species occurring in Australia, the last great unexplored bastion for micro-fauna. He conducts research on the morphology, biology, phylogeny and pathogenicity of protozoan species; including sporozoa, ciliates, flagellates and amoebae in the blood, gut and tissues of mammals, birds, reptiles and fish. He uses conventional and modern technologies to study organismal, cellular and molecular biology, including light and electron microscopy, immunoassays, biochemical profiles and nucleotide analyses. He has published over 150 scientific papers in five main areas of research: cyst-forming sporozoa in domestic animals; enteric coccidia and haemoprotozoa in wildlife; protozoa affecting aquaculture; endosymbiotic ciliates in herbivores; and protozoal biodiversity. He was recently awarded a Doctor of Science by the University of Queensland and was elected Fellow of the Australian Society for Parasitology.

Think small, become a protozoologist! Protozoa rule!

www.smms.uq.edu.au/pod



Associate Professor Phil Dowe is a Reader in Philosophy in the Faculty of Arts. He studied Physics, History and Philosophy of Science for a BSc at the University of New South Wales, and has a PhD in Philosophy from Sydney University.

He teaches *Introduction to Philosophy*, *Time Travel*, *Chance Coincidence and Chaos*, *Science and Religion*, *Philosophy of the Life Sciences* and *Advanced Philosophy of Science*. His main areas of research are philosophy of science and metaphysics. His books include *Physical Causation* (Cambridge 2000) and *Galileo, Darwin, Hawking* (Edinburgh, 2005). He has published papers on causation, chance and time.

When pushed to divulge something interesting about himself, after 3 weeks of deep thought he announced that he "likes good coffee and looking at lakes".

Dr Marcus Gallagher is a Senior Lecturer in the School of Information Technology and Electrical Engineering. He did his undergrad in computer science at the University of New England and completed a PhD in Computer Science and Electrical Engineering at the University of Queensland in 2000. Since then he has worked at UQ as a Researcher and Academic.

His area of research is Artificial Intelligence, more specifically in machine learning and nature-inspired optimization algorithms. Broadly speaking, these algorithms are techniques for solving hard computational problems. He has collaborated with other researchers in applying these techniques to problems in astronomy and the analysis of health-care data.

When he used to have spare time, he enjoyed appropriately geeky activities, including reading science fiction novels, playing computer games and listening to heavy metal.

1.2 SCIE1000 students

- SCIE1000 students come from many backgrounds, with diverse interests. Here is some information about the 546 students who took SCIE1000 in 2008; the cohort this year should be similar.

Backgrounds

- 88.9% of students completed high school in Queensland, 5.7% elsewhere in Australia and 5.4% overseas (in China, Japan, South Korea, Saudi Arabia, Mauritius, Vietnam, Singapore, India, Malaysia, France, Malaysia Sri Lanka, Vietnam, Hong Kong, Mexico, New Caledonia South Africa and Slovenia).
- 79.6% came directly from high school, 12.8% had a break of one year, and 7.6% longer.
- 30.7% had completed Maths C or equivalent, 68.8% Maths B and 0.5% Maths A.

Interests

- 62.2% of students were enrolled in a BSc, 21.9% in a BBiomedSc, 8.2% in a MBBS/BSc, 2.8% in a BBiotech, 2.4% in a BMarSt, 2.1% in a BSc/BA and 0.4% in a BSc/BEd.
- Students were asked to identify their primary area of scientific interest at the start and end of semester. The responses were:

Area	% at start	% at end
Biology	22.4%	29.0%
Biomedical Science	51.3%	39.2%
Chemistry	10.4%	7.0%
Computer Science	0.7%	0.6%
Earth Sciences	1.3%	1.5%
Geographical Sciences	0.7%	0.6%
Mathematics	2.4%	6.1%
Physics	4.1%	6.1%
Psychology	3%	4.6%
Other	3.7%	5.5%

Attitudes

- When asked to rate the importance of Mathematics to their area of science, on a scale of 5 (very important) to 1 (very unimportant), 30.7% of students responded 5, 49.6% responded 4, 11.3% responded 3, 2.8% responded 2 and 0.7% responded 1.
- When asked to rate the importance of Computing to their area of science on the same scale, 15.6% responded 5, 56.8% responded 4, 21.5% responded 3, 5.2% responded 2 and 0.9% responded 1.

Final grades

- The final grade distribution for SCIE1000 is shown in the following table. A grade of 7 is the highest grade, and any grade below 4 represents failure.

Grade	% students (2008)	% students (2009)
7	13.01%	8.96%
6	25.09%	21.88%
5	26.21%	28.33%
4	24.72%	26.04%
3	4.83%	7.50%
2	5.76%	4.79%
1	0.37%	2.50%

Course evaluations

- At the end of semester, UQ asks students to assign each course an overall "rating", ranging from 5 (Outstanding) to 1 (Very poor).
- Results from 2009 for BIOL1020 (twice), BIOL1030, BIOL1040, CHEM1020, CHEM1030, PHYS1002, PHYS1171, SCIE1000 and STAT1201, in decreasing numerical order (not course order) were 4.05, 3.98, 3.91, 3.81 (SCIE1000), 3.79, 3.64, 3.55, 3.45, 3.43, 3.22 and 3.18.
- Feedback from students identified ways to improve the course, including reducing the length and number of assignments, changing how Python is taught, linking tutorials and lectures more closely, and altering the Philosophy content. We have made these changes.

1.3 Mutual obligations

We believe that students and lecturers in a course incur a number of obligations, outlined below. Each party should inform the other if they believe that these obligations are not being met.

We will do our best to deliver a course that:

1. contains modern, interesting content from a range of science areas;
2. is relevant to your studies and future professions;
3. is intellectually challenging, accurate and correct;
4. is well-taught, by a team of engaging, professional experts;
5. respects your diverse backgrounds, aspirations and abilities;
6. helps you to improve both your technical knowledge and your generic learning skills;
7. includes assessment that is appropriate, challenging and identifies your level of skills, without being excessive; and
8. provides you with useful, appropriately timed feedback.

We expect that you will do your best to:

1. commit an appropriate amount of time, effort and intellectual engagement to your studies, and submit assessment on time;
2. attend lectures, tutorials and computer laboratory classes, and remain quiet and attentive in class;
3. respect your classmates, the teaching staff and the course content;
4. complete necessary pre-readings before lectures;
5. accept that at times we will cover content which you will find difficult, or of which you may not immediately see the relevance;
6. actively study all components of the course, including science, mathematics, computing and philosophy;
7. not plagiarise from classmates or other sources; and
8. seek help and advice in a timely manner.

1.4 Why have a special science course?

Many governments and industries have commented on the recent global decline in the numbers of career scientists. Collectively, they are looking to higher educational authorities to redress this situation by providing appropriate training. In Australia, state and federal governments are exploring incentive schemes and have initiated policy changes. The Queensland Department of Education, Training and the Arts has developed a comprehensive paper entitled *Towards a 10-year plan for science, technology, engineering and mathematics (STEM) education and skills in Queensland.* Amongst other things, this report states:

> *"The role of STEM cannot be underestimated in preparing Queenslanders for the challenges and opportunities of the future. The Queensland economy is booming. Strong demand for natural resources and the fastest-growing population in Australia are priming the rapid growth of Queensland's economy. However, our future prosperity cannot rely solely on the buoyancy of traditional industries and dynamic population growth. Global competition, market instabilities and changing trends in immigration are placing increasing pressures on the growth of the state's economy. To meet these challenges, Queensland needs to continue to encourage the emergence of new high-value, high-growth industries of the future and apply strategies to value-add to traditional industries. International experience demonstrates that high-growth economies are those that build upon strong foundations to move towards a knowledge-based economy. A workforce of scientifically and technologically literate people is key. With identified shortages across the engineering, science and medical professions, there is a growing need for students to specialise in STEM disciplines."*
>
> [www.education.qld.gov.au/projects/STEMplan]

Science is based on observation, hypothetico-deductive logic, experimentation, critical interpretation and reproducibility. Scientists are trained to be innovative, honest, precise, rigorous and critical. However, the training and attributes we look for in scientists are not always evident in science education programs. Many programs focus on content, especially theory, and graduating scientists may lack generic and specific scientific skills.

A recent review (2007) of the Bachelor of Science (BSc) program at UQ concluded that not enough foundational courses and too many specialist courses were being offered. The BSc program was revised to provide a stronger first-year focus on the enabling sciences (mathematics, chemistry, physics and biology), including quantitative skill development and computing, in keeping with modern technologies.

The course SCIE1000 was developed to focus on fundamental quantitative skills within the context of science. Mathematics is considered to be the primary enabling science as it is fundamental to all other sciences.

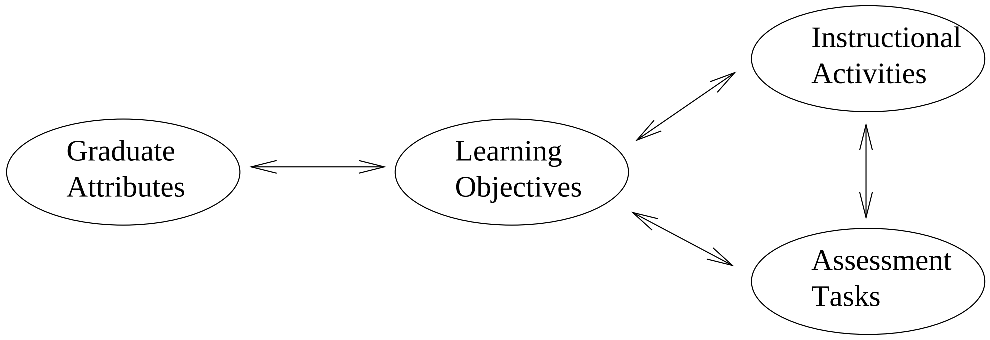
Conventional mathematics education seems to always generate the common lament from students: “When and where are we ever going to use this?” In this course we will show you that science and mathematics are intricately linked. Certainly, some science is non-mathematical, and some mathematics has no direct use in other sciences, but in many cases mathematics and science are identical (so an equation that describes population growth over time is both mathematics and science).

Globally, improving mathematics education has been identified as a common goal within scientific communities. For example, the US National Research Council wants to “Transform undergraduate education for future research biologists” and has published a booklet entitled *BIO2010* [National Academies Press, 2003. ISBN 0-309-08535-7]. They consider that the focus of educational programs in mathematics and computer science should be the acquisition and processing of data, quantitative analysis and display, modelling, prediction, program simulations, database access, search, retrieval, and *in silico* (computer) experiments.

Finally, scientific writing is an important component of SCIE1000. Professional scientists are called upon to write three main types of document: grant applications; scientific papers; and literature reviews. While the instructions given to authors by granting agencies, publishing houses and editors may differ, there are many common elements to these documents. All three are subject to peer review by independent referees to gauge integrity and quality, they generally adhere to a ‘scientific’ format, and they are mostly written in formal language (third person passive). Scientists conform to prescribed formats when publishing material, and they write for other scientists, rather than for the community at large. The growing demand to revise science communication has created jobs for science writers and knowledge brokers, third parties who are not science specialists but are trained communicators able to simplify and explain science to society.

1.5 Graduate attributes

UQ uses a teaching and learning paradigm called the *constructive alignment model*, whereby desirable graduate attributes are articulated within specific course learning objectives, which are achieved through relevant instructional activities and assessment tasks. It is also known as the CIA model, whereby Curriculum is linked to Instruction and Assessment. This approach ensures that all course components are interlinked and integrated.



Education authorities recognise three domains of learning (collectively known as the *SACK* model):

- psychomotor (about doing), involving skills (S);
- affective (about feeling), involving attitudes (A); and
- cognitive (about thinking), involving concepts (C) and knowledge (K).

UQ courses cannot include only content and technical procedures, but must also include generic skills applicable to vocation, employment, community and society. The BSc program identifies seventeen graduate attributes in five main categories. These are:

- **In-depth knowledge of field of study**, including knowledge, understanding and perspective.
- **Effective communication**, including interaction, written and spoken communication and IT competency.
- **Independence and creativity**, including the ability to work, learn, adapt, identify, create, innovate and solve.
- **Critical judgment**, including the ability to define, analyse, critique, evaluate, reason, decide and reflect.
- **Ethical and social understanding**, including responsibility, respect, appreciation and diversity.

Staff cannot simply pay lip-service to these graduate attributes, but have to demonstrate where and how they are embedded in each course. This information is available in the electronic course profile.

1.6 Learning objectives

The broad aims of this course are to instill an appreciation of the quantitative skills and fundamental philosophies required for the practice of modern science, provide interdisciplinary contextual relevance, improve the mathematical and computational skills and communication skills of students and engage them in the UQ 'science community'.

Students will learn to:

- **Analyse** the interdisciplinary nature of modern science;
- **Explain and demonstrate** the importance of modelling in science;
- **Apply** fundamental mathematical techniques to a range of scientific disciplines;
- **Design** and write simple computer programs in the language Python;
- **Interpret** the philosophy of science and scientific thought;
- **Evaluate** critically quantitative scientific information;
- **Communicate** scientific information in a logical and appropriate style; and
- **Describe and discuss** key issues in science, including social and ethical issues.

As you will notice, none of the learning objectives directly addresses specific content, neither scientific nor mathematical. For instance, they do not state that students will learn algebra, differential calculus, the laws of thermodynamics or the molecular structure of DNA. The learning objectives are more than content-driven, and also include process. To this end, all of the learning objectives commence with verbs such as analyse, explain, apply or design. SCIE1000 will combine theory with practice in all class activities.

The scope, sequence and schedule of course work has been built around a logical progression of principles which have been contextualised with real relevant scientific topics from a diverse array of disciplines. Mathematical principles covered will include models, functions, exponentials, logarithms, matrices, derivatives, optimisation, numerical methods for solving equations, integration and differential equations. Key scientific concepts will be drawn from chemical, physical, natural, earth, social and life science disciplines. Mathematically, the course can be likened to a fixed menu dinner, while scientifically, it is a smorgasbord. Hopefully, this framework will serve to reinforce our contention that mathematics underpins all the sciences.

1.7 Learning styles

Universities differ in many ways from secondary schools because they place the onus for learning firmly on the student as a responsible, independent adult learner. Even though there are many rules and regulations governing university courses and programs (and even professional codes of conduct), essentially the responsibility is on you, the student, to attend classes and examinations.

University staff schedule and conduct classes but usually they do not monitor attendance, although your failure to attend small group classes (such as tutorials and laboratory classes) will be conspicuous to your tutor. Students must exercise some self-discipline as independent learners and resist the temptation to miss classes. If you skip classes, you will be at a disadvantage compared to the rest of the class and will not perform as well.

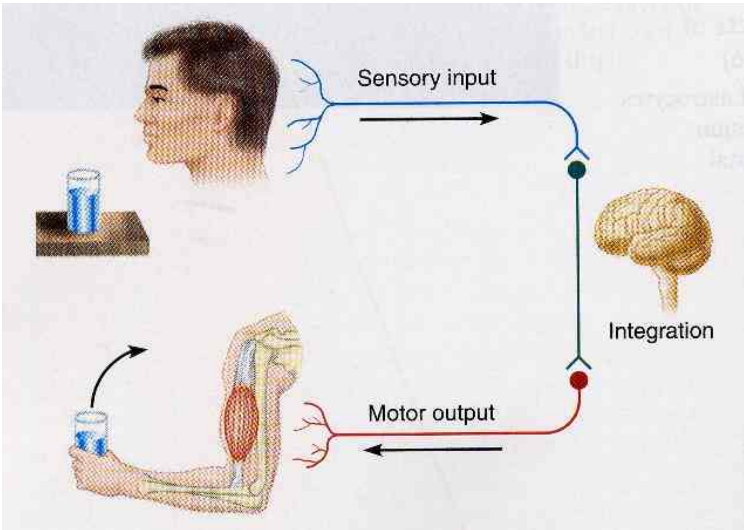
Many students have part-time employment to earn money for subsistence but they should not treat university as secondary to that employment. Full-time enrolment is exactly that. Although formal contact hours may only be 20 – 24 hours per week (5 – 6 hours per course for each of 4 courses), you are expected to undertake independent study (preview, review, extended readings, research and so on) on a matching basis (1 hour study for each hour of scheduled contact).

Your first substantial task will have been to organise your weekly schedule of classes. Ensure that you adhere to that schedule as it provides structure to the massive amount of content to which you will be exposed. In most cases, it will have been arranged for tutorials and practicals to follow-on from lectures so that small group activities have direction and focus.

During your degree, you will accumulate an extraordinarily large amount of material: reference texts, recommended readings, lecture booklets, tute notes, practical guides, and a huge assortment of electronic files (documents, power-points, spreadsheets and databases, accessed through intranet and internet servers (such as Blackboard and Google). You must be organised and develop appropriate systems to sort, store and retrieve these materials.

Clipart

You MUST take notes during your classes. Simply listening and observing classes does not guarantee data retention or understanding. Turning all that sensory input into motor output by taking notes ensures that your brain has been engaged. The very act of writing involves many neural pathways and cognitive functions that serve to enhance comprehension and memory. Short-term and long-term memories involve different parts of the brain and sorting occurs during sleep. Periodic review of material ensures information persists in long-term memory, so taking notes during study (preview and review) facilitates better retention and understanding. Get into the habit of taking notes at every possible opportunity!



Marieb et al. 2007, Fig. 11.1

There are many different modalities of education. All recognise the polarity of teaching (teacher-centred) and learning (student-centred) and attempt to reconcile these perspectives. Historically, teaching and learning occurred in small groups through question and discussion (the so-called Socratic method) and skilled trades were, and still are, taught through individual apprenticeships. With the Industrial revolution came an educational revolution. Class sizes grew and methods of teaching large groups were introduced, notably in the form of lectures. While primary and secondary schools have retained small class sizes to facilitate behaviour modification, tertiary institutions have embraced lecture formats as economical means for mass education. However, this does not mean lectures provide optimal learning opportunities for students.

Generally speaking, teaching and learning models form a continuum from what educational theorists call transmissivism (where knowledge is transmitted to students, such as in didactic lectures) to constructivism (where students construct meaning through dialogue). The former assumes the students' 'glass of knowledge" can be filled by the teacher, while the latter recognises that students already have some knowledge which must first be activated and validated before it can be built upon.

Students attend classes to learn, but what actually is learning? It is defined in many dictionaries simply as an increase in knowledge, but this covers many contexts, including acquisition, retention (memory), recognition (principles, ideas, concepts), cognition (making sense, understanding) and action (developing skills and competencies). Various strategies are used to avoid surface learning (atomistic in detail, isolated knowledge, limited understanding, quickly forgotten), foster deep learning (holistic in perspective, relational knowledge, good understanding, long-term retention) and develop and enhance student qualities (personal, social, philosophic, psychologic).

It is obvious that there is no single type of instructional activity that is universally suitable. Authorities recognise that a tailored teaching approach must be developed for each course, and even each cohort. In SCIE1000, classes have been scheduled for five hours each week during semester, ranging from didactic lectures (a lecturer speaking at the front of a room), dialectic lectorials (lectures with group discussions and activities), mauieutic tutorials (small-group discussion groups) and interactive computer laboratories (individual and small-group exercises). All classes will provide students with the opportunity to practice solving problems in the context of science, as befits contemporary workplace practices.

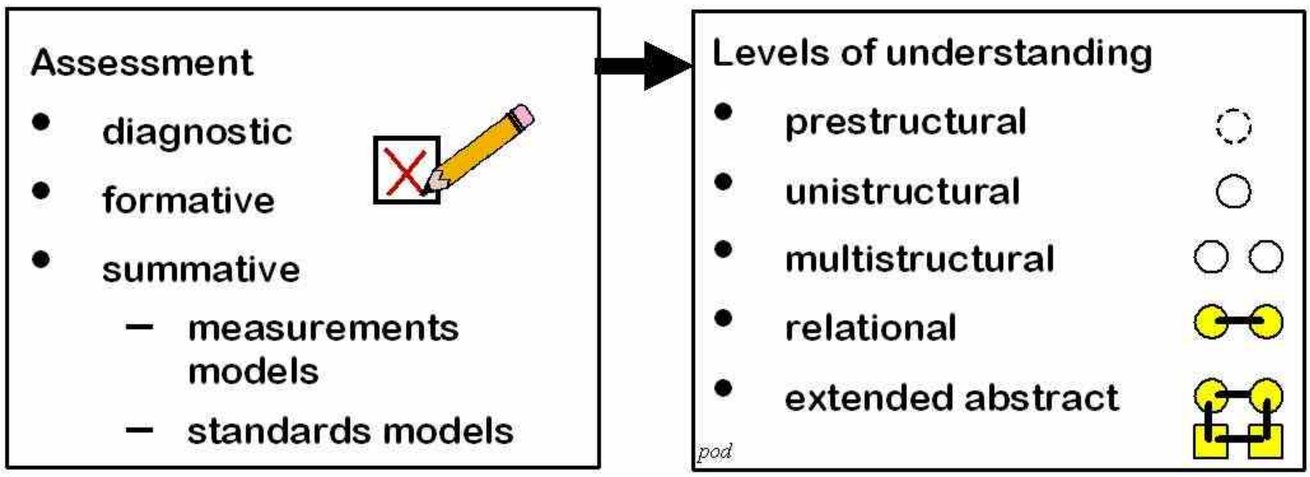
If you are interested in additional information on different learning styles, including an on-line survey to help identify what learning style most suits you, then you may like to visit the website:

www4.ncsu.edu/unity/lockers/users/f/felder/public/Learning_Styles.html

1.8 Assessment

While scientists concentrate on content and teachers on process, students typically focus on assessment. It has long been recognised that assessment drives learning. In the past, heavy emphasis has been placed on summative assessment tasks to measure learning rather than formative assessment to support learning. Assessment has traditionally been facilitated by *measurement* models which rate individual performance against population normal distributions rather than by *standards* models which rate performance against specific criteria. Courses should endeavour to *assess for understanding*. This involves defining what we mean by *understanding*.

Five hierarchical levels of understanding are recognised: prestructural (do not 'get it'); unistructural (identify single elements); multistructural (identify similar elements); relational (identify patterns); and extended abstract (generalise). Desirable learning outcomes should involve higher order understanding and assessment tools should evaluate cognitive, metacognitive and social competencies and affective dispositions. University courses should aim for at least multistructural pattern recognition and relational thinking (typified by compare/contrast questions).



The emphasis of any course on quantitative skill development must be on the demonstration of those skills through problem-solving. In SCIE1000, students will be guided through assessment requirements in classes and have the opportunity to work through examples and practice questions in their own time in addition to during class time. Lecturers and tutors are committed to providing timely and informed feedback to students, so that exam time will hold no surprises.

Details of assessment are in the course profile. Many questions will involve problem-solving and marks will be allocated not only for final answers but also for process logic (working out). You will be given ample instruction throughout the course, with practice questions given in classes and on the Blackboard website.

1.9 How to use these notes

This booklet contains many of the teaching materials required for SCIE1000. In lectures we will mostly focus on this material. You will need access to these notes in every lecture, as you will write additional notes and working directly on them. The lecture notes are organised into the following main components:

- *general notes*, which introduce new ideas and content;
- *key points*, which summarise key definitions and concepts;
- *examples*, which give fully-worked examples showing how to solve important problems;
- *questions*, through which we will work in class, and which you can try to solve yourself;
- *Python examples*, which show how to do something in Python;
- *case studies*, which illustrate several aspects of a large problem/issue and run for a number of pages;
- *extension materials*, which give some non-assessable extra material, often quoted from a media report or a scientific paper; and
- *blank space*, at the bottom of each page, in the margins, and at the end of each section, so you can write additional notes if you wish.

These components are all presented in different ways, to make them easier to find. A brief example of each one is:

- General notes (involving words and mathematical content) are often written with bullet points.

Key points

Key points are written in boxes with rounded corners, like this, with the title identifying the key point.

***Example** 1.9.1* How do worked examples look?

Answer: Worked examples are written in double boxes, like this.

***Question* 1.9.2** Questions are written like this, in bold boxes, with space to write the answers (including working). We will complete these questions in lectures, often with a mixture of individual work, group discussion and class discussion. These questions give a good idea of what will be on your exam.

Python Example 1.9.3

Examples involving Python programming are written like this. In each case there is some introductory text, followed by sample Python input and output, shown in `this font`, with numbered lines.

```
>>> 6+4
10
```

Case Study 0:
An example of a case study

Case studies look like this. The title summarises what the case study is covering, and this is followed by several pages of examples, questions, key points and so on. Each case study ends as follows.

End of Case Study 0.

***Extension* 1.9.4** (From (some attributed source))

Extension materials look like this, with the source identified. This material is not examinable.

Note that many of the examples and concepts in the SCIE1000 notes are worthy of additional exploration. If you are interested, you might like to look up more information about the topic, using web searches and other resources. In some cases the SCIE1000 website is a good place to start.

2 A short discussion of nearly everything

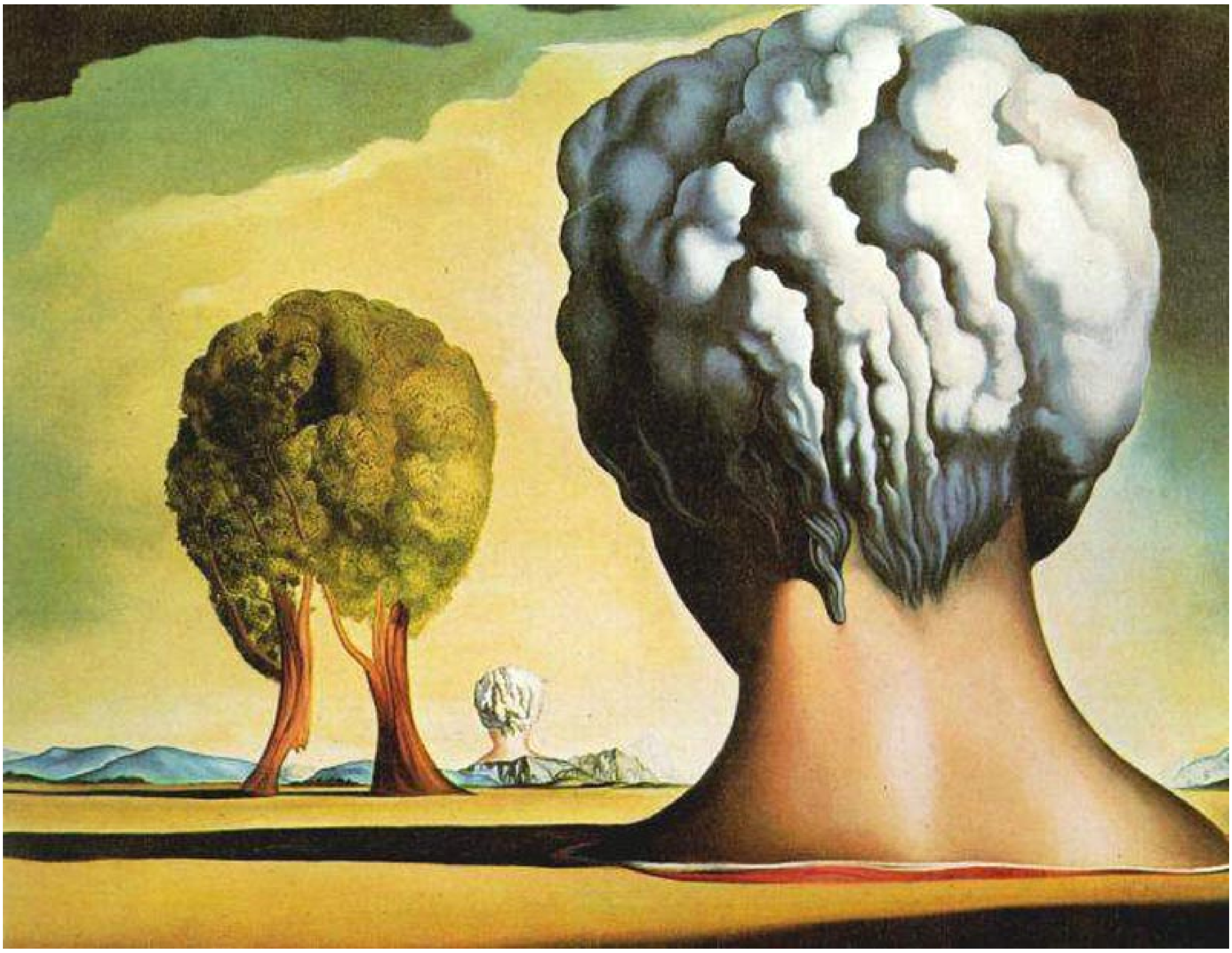
Gaudeamus igitur, Iuvenes dum sumus
Post iucundam iuventutem
Post molestam senectutem
Nos habebit humus, Nos habebit humus.

Vivat Academia, Vivant professores
Vivat membrum quodlibet
Vivant membra quaelibet
Semper sint in flore,
Semper sint in flore.

Artist: traditional

(www.youtube.com/watch?v=aLUKfU2AOBY)

(www.youtube.com/watch?v=kK2cAsXMn5w)
(slightly rude)



The Hands of God and Adam (1508 – 1512), Michelangelo (1475 – 1564), Sistine Chapel ceiling, Apostolic Palace, Vatican and *The Three Sphinxes of Bikini* (1947), Salvadore Dali (1904 – 1989), Morohashi Museum of Modern Art. (Image source: Museum publication.)

Introduction

Curiosity is an enduring human characteristic. For all of recorded history (and obviously for much longer – otherwise we would never have developed recorded history!), people have been asking questions such as "Why...", "What causes...", "What will happen if..." and "How can we...".

Curiosity has motivated people to explore Earth and space, to investigate a whole range of phenomena, and to seek new knowledge in the face of adversity or even great personal risk.

We all know that the universe is incredibly complex. Scientific investigation is undertaken in an attempt to make some sense of this complexity by enabling us to understand, explain, predict and (in some cases) influence phenomena.

Understanding and doing science requires a range of skills and knowledge, including: knowledge about the discipline area; an ability to think logically and creatively; an ability to observe, collect data and communicate; and an ability to formulate and apply models. The science courses you take at University (and at school) are largely aimed at improving your skills in these areas.

This chapter commences with a brief discussion on the nature of science (we will cover this in more detail in Chapter 6), then identifies six broad areas that are at the core of science, discusses why they are important, shows where they will be covered in your studies, and finishes with a specific description of the role SCIE1000 will play in developing your skills in these areas.

2.1 Science

***Question** 2.1.1* Consider the following quote from the American Physical Society (www.aps.org/policy/statements/99_6.cfm):

"Science extends and enriches our lives, expands our imagination and liberates us from the bonds of ignorance and superstition...

Science is the systematic enterprise of gathering knowledge about the universe and organising and condensing that knowledge into testable laws and theories.

The success and credibility of science are anchored in the willingness of scientists to:

- *Expose their ideas and results to independent testing and replication by others. This requires the open exchange of data, procedures and materials.*
- *Abandon or modify previously accepted conclusions when confronted with more complete or reliable experimental or observational evidence.*

Adherence to these principles provides a mechanism for self-correction that is the foundation of the credibility of science."

Briefly discuss the quote. Do you agree? Are any key points missing?

***Question** 2.1.2* Consider the following quote from the Federation of Australian Scientific and Technological Societies (www.fasts.org):

"*Science has evolved over thousands of years of human enquiry to provide a rational basis for understanding and predicting what happens in the world around us. We rely on science to enhance our standard of living, to keep us healthy, and to address the problems and challenges that we face.*

Over the last five hundred years humanity has developed a new way of systematically testing ideas against physical evidence. The modern world is a direct product of the growth of scientific knowledge sparked by that understanding.

Through scientific evaluation, we ensure that the knowledge we need is as reliable and as rigorously tested as we can make it. It is this process of scientific thought and examination that gives us confidence.

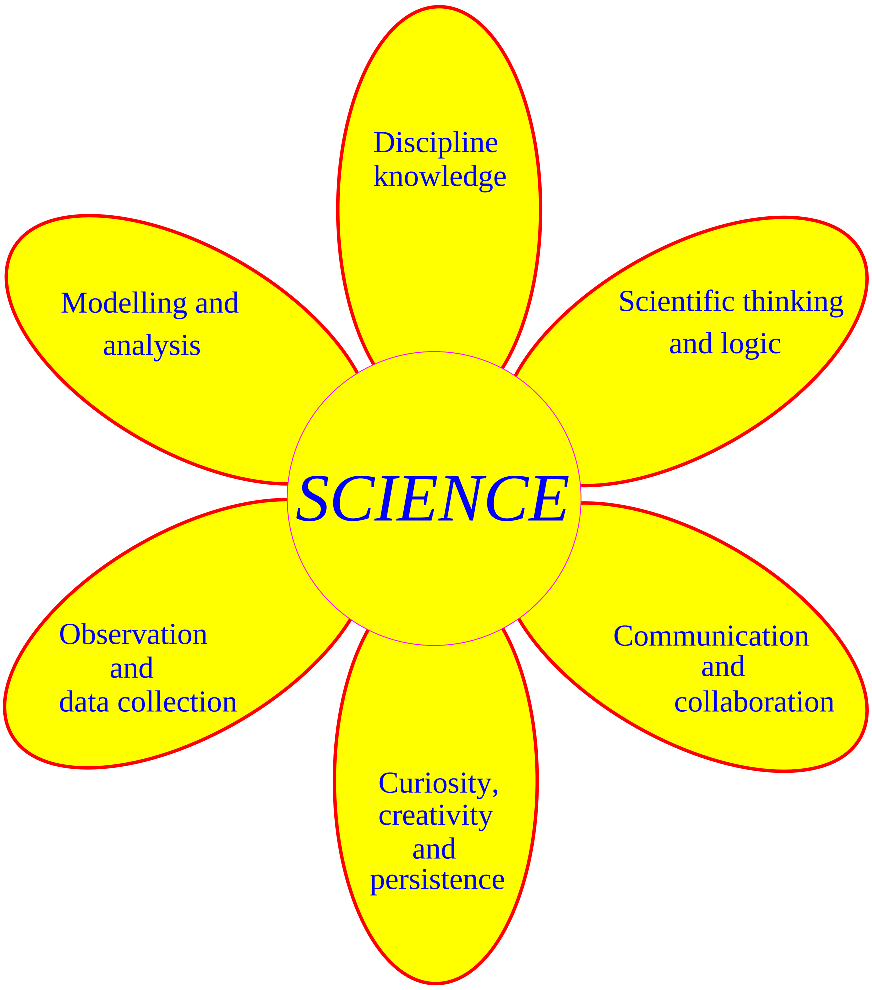
- *Science works by systematically testing ideas against the evidence.*
- *Evidence-based ideas are examined by peer review and published for further scrutiny in the scientific literature so that additional tests can be applied.*
- *Scientific ideas are adopted when they usefully describe the world.*
- *When scientific ideas are widely accepted they become mainstream, and are applied until replaced by the widespread adoption of an alternative idea that makes better sense of the evidence.*"

Briefly discuss the quote. Do you agree? Are any key points missing?

Science

Science aims to **understand**, **explain**, **predict** *and* **influence** *phenomena. Understanding and doing science requires:*

- *discipline knowledge and content;*
- *scientific thinking and logic;*
- *communication and collaboration;*
- *curiosity, creativity and persistence;*
- *observation and data collection; and*
- *modelling and analysis.*



- Most of your study and professional development will focus on enhancing your skills in these areas.
- The rest of this section shows *how* and *where* you will do so in some UQ courses, and specifically the role of SCIE1000.
- We also give tables showing how the coordinators of seven 1st year UQ science courses divide their courses into these categories.

2.2 Discipline knowledge

- *Discipline knowledge* (*DK*) describes the language, information and skills specific to each discipline area.
- *DK* includes such things as:
  - fundamental principles of the scientific area;
  - how to measure and record relevant data;
  - an appreciation of what is 'interesting';
  - the language and terminology of the discipline;
  - an understanding of relevant history, ethics and key milestones;
  - an understanding of what is known and what is not known; and
  - knowledge of the potential applications and the limitations of the discipline.
- Common sources of *DK* include:
  - research papers, journals, textbooks and online resources;
  - seminars, conferences and personal discussions; and
  - schools and universities, including courses such as BIOL, CHEM, ERTH, MATH, PHYS and PSYC.
- The role of SCIE1000:
  - SCIE1000 focuses much less on *DK* than most other courses.
  - We will define the terminology and concepts that you need, but if you are completing courses in (say) physics, chemistry, biology or mathematics, then you will acquire much more specific discipline knowledge in those courses.

***DK* % of various UQ science courses:**

SCIE 1000	BIOL 1030	MATH 1051	BIOL 1020	STAT 1201	CHEM 1030	CHEM 1020
5%	40%	35%	40%	20%	35%	25%

2.3 Scientific thinking and logic

- *Scientific thinking* and *logic* (*STL*) describes the approaches and thought processes associated with performing systematic investigations and making valid inferences.
- *STL* includes such things as:
  - hypothesis formulation and testing: the *scientific method*;
  - mounting valid, convincing arguments;
  - following logically defensible sequences of thoughts or steps; and
  - developing and applying a philosophy of rigour, precision and accuracy to all aspects of science.
- Common ways to increase skills in *STL* include:
  - exposure to written and verbal communications from experienced scientists;
  - undertaking substantial, open-ended, authentic experiments and projects;
  - studying philosophy, mathematics and formal logic; and
  - participation in learning activities at schools and universities.
- The role of SCIE1000:
  - SCIE1000 has a substantial focus on *STL*, with formal components on scientific thinking, the scientific method and the philosophy of science.

STL % of various UQ science courses:

SCIE 1000	BIOL 1030	MATH 1051	BIOL 1020	STAT 1201	CHEM 1030	CHEM 1020
15%	10%	20%	15%	10%	20%	30%

2.4 Communication and collaboration

- *Communication and collaboration* (*CC*) are the processes by which scientists use information from others, make their results available to others, and work together.
- *CC* includes such things as:
  - writing, reading, interpreting, speaking, listening, visualising and critically evaluating.
  - conciseness, precision, care and clarity of expression;
  - understanding electronic and other communication mechanisms;
  - familiarity with relevant information sources;
  - the ability to interact effectively with discipline experts;
  - the ability to work as a member of a team; and
  - the ability to collaborate in a cross-disciplinary manner.
- Common ways to increase your *CC* skills include:
  - practise in writing, reading and presenting scientific information;
  - undertaking group work; and
  - gaining familiarity with a range of scientific disciplines.
- The role of SCIE1000:
  - SCIE1000 has a substantial focus on *CC*.
  - You will be assessed on your scientific writing, quantitative reasoning, and ability to collect and synthesise information.
  - You will also cover a range of topics, increasing your ability to collaborate across disciplines.

***CC* % of various UQ science courses:**

SCIE 1000	BIOL 1030	MATH 1051	BIOL 1020	STAT 1201	CHEM 1030	CHEM 1020
15%	20%	10%	15%	10%	15%	10%

2.5 Curiosity, creativity and persistence

- *Curiosity, creativity and persistence* (*CCP*) describe relatively intangible characteristics which are commonly identified as drivers of success, particularly in research and knowledge discovery.
- *CCP* includes the ability to:
  - constantly ask "interesting" questions;
  - use lateral thinking to develop new approaches;
  - devise solutions to difficult problems;
  - apply knowledge in new ways and to different scenarios; and
  - develop hypotheses to explain unexpected observations.
- These skills are somewhat innate, but can be increased by:
  - practising on a range of problems;
  - attending seminars, classes and presentations;
  - observing and collaborating with creative people;
  - believing in the importance of what you do; and
  - working in an area that is of great interest to you.
- The role of SCIE1000:
  - SCIE1000 has a substantial focus on *CCP*.
  - We explore the role of creativity in science, and cover interesting, authentic examples from a wide range of disciplines.

***CCP* % of various UQ science courses:**

SCIE 1000	BIOL 1030	MATH 1051	BIOL 1020	STAT 1201	CHEM 1030	CHEM 1020
15%	15%	15%	5%	10%	10%	5%

2.6 Observation and data collection

- *Observation* and *data collection* (*ODC*) describes the processes and techniques used to collect data about particular phenomena.
- *ODC* includes such things as:
  - understanding which data is relevant;
  - knowing how to collect and record data;
  - knowing what levels of accuracy and precision are required; and
  - appreciating any ethical or related issues.
- Methods of developing skills in *ODC* include:
  - reading research papers and books, attending seminars and conferences, and engaging in personal discussions;
  - practising data collection in association with laboratory work and field trials; and
  - participating in experimental courses, such as BIOL, CHEM, ERTH, PHYS and PSYC.
- The role of SCIE1000:
  - For most students, SCIE1000 includes very little observation or data collection.
  - SCIE1000 focuses much more on how data can be *used* to develop models.

***ODC* % of various UQ science courses:**

SCIE 1000	BIOL 1030	MATH 1051	BIOL 1020	STAT 1201	CHEM 1030	CHEM 1020
0%	10%	0%	15%	10%	15%	15%

2.7 Modelling and analysis

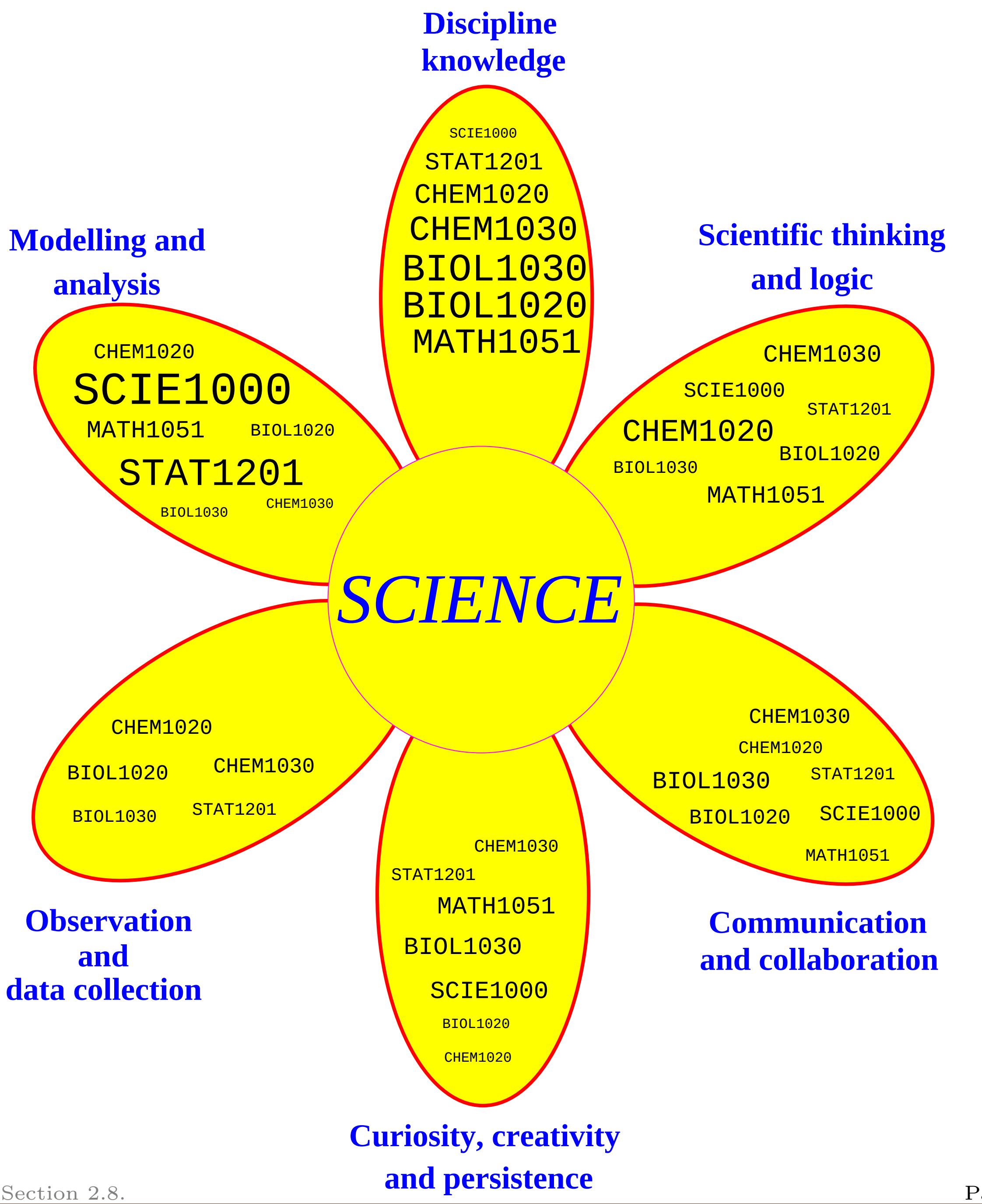
- *Modelling* and *analysis* (*MA*) describes the processes by which mathematics, statistics, computation and related techniques are used to represent phenomena approximately, and hence allow predictions to be made.
- *MA* includes such things as:
  - using statistics to allow for uncertainty and errors in measured data;
  - developing equations to approximately represent data;
  - using mathematical techniques to simplify or solve the equations; and
  - writing and executing computer models.
- Methods of developing skills in *MA* include:
  - reading research papers and books, attending seminars and conferences, and engaging in personal discussions; and
  - participating in courses on modelling, mathematics and statistics.
- The role of SCIE1000:
  - A key goal of SCIE1000 is to develop your *MA* skills; much of the course is devoted directly to this.
  - We will discuss the modelling process in detail, then explore a range of relevant mathematical techniques.
  - We will also learn how to write computer programs for modelling.

MA % of various UQ science courses:

SCIE 1000	BIOL 1030	MATH 1051	BIOL 1020	STAT 1201	CHEM 1030	CHEM 1020
50%	5%	20%	10%	40%	5%	15%

2.8 Some UQ science courses

- Through your studies, different courses will develop different aspects of your science skills, which together allow you to graduate with the range of skills and knowledge necessary to understand science and be a scientist (if you so choose).
- The following diagram demonstrates the relative balance of science skills covered by various first-year courses. Data from the tables on previous pages have been converted into relative font sizes.
- Make sure you appreciate what each course aims to achieve, and hence how your courses will fit together and how they differ.



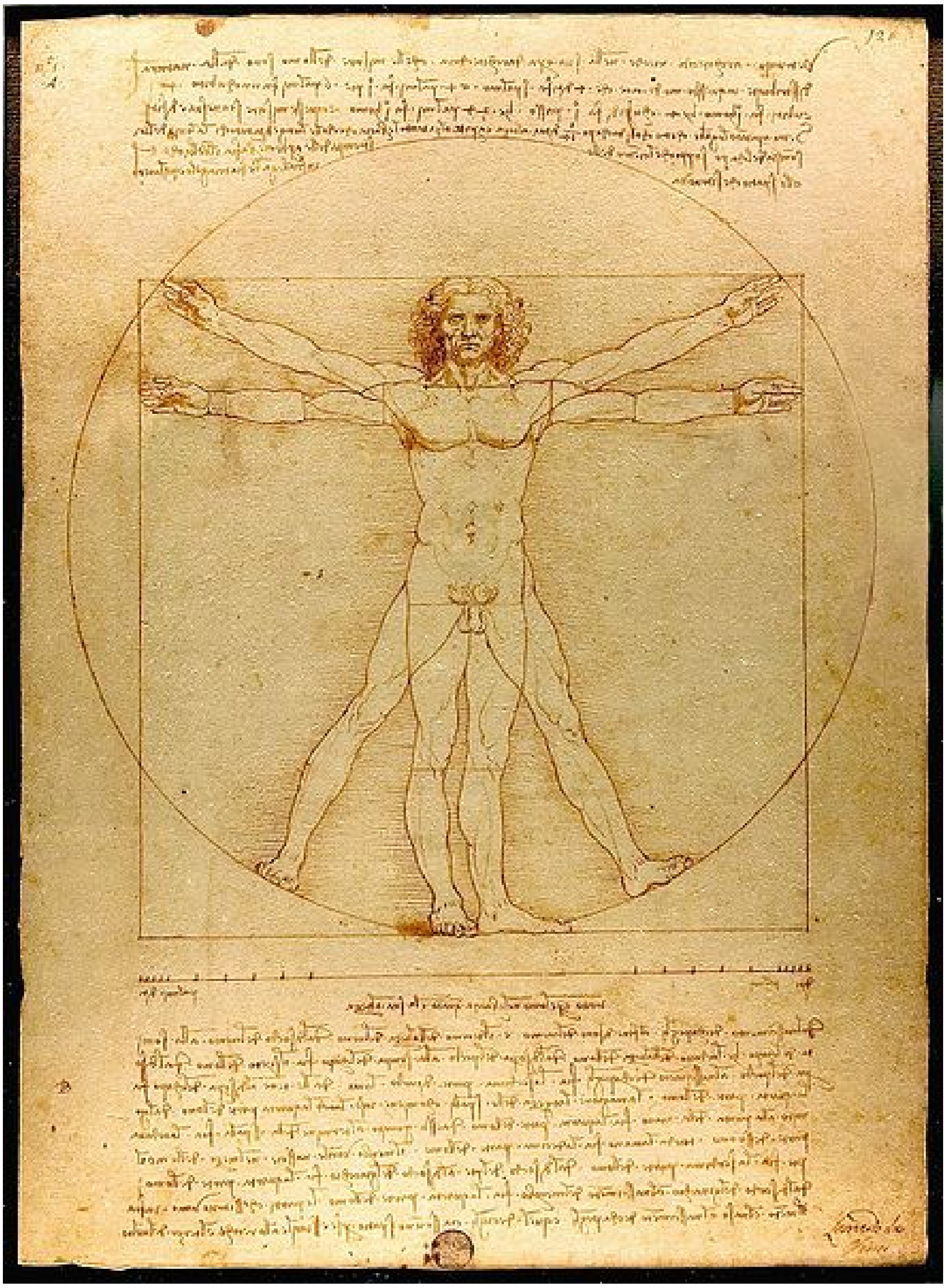
2.9 Space for additional notes

3 A career in modelling

I'm very well acquainted, too, with matters mathematical,
I understand equations, both the simple and quadratical,
About binomial theorem I'm teeming with a lot o' news,
With many cheerful facts about the square of the hypotenuse.
I'm very good at integral and differential calculus;
I know the scientific names of beings animalculous:
In short, in matters vegetable, animal, and mineral,
I am the very model of a modern Major-General.

Artist: Gilbert and Sullivan

(www.youtube.com/watch?v=iSloW2coCDQ)



The Vitruvian Man (c 1487), Leonardo da Vinci (1452 – 1519), Gallerie dell'Accademia, Venice, Italy. (Image source: en.wikipedia.org)

Introduction

We all know that the world is an incredibly complex place. It has been suggested that not only is the universe far more complex than we imagine, it may be more complex than we *can* imagine.

The primary goals of science are to understand, explain, predict and influence phenomena. To make this manageable, scientists regularly develop *models* of the phenomena. Models typically balance simplifying assumptions and approximations with accuracy and real-world applicability.

There are many different types of models. There are conceptual models which help to visualise what is happening, there are models containing systems of mathematical equations which aim to represent a phenomenon, and there are computer models which can be used for complex simulations. Many models include a hybrid of these components. However, all models are an approximation to the real world, and no model of a complex phenomenon will ever be completely accurate in every situation.

This section gives a brief introduction to different types of models, and some of the important background knowledge required for many models.

Some of the examples/contexts we will discuss are:

- Growth rates of tropical birds.
- Fluid flow.
- Cholesterol and heart disease.

Specific techniques and concepts we will cover include:

- How models, mathematics and computing are important in modern science.
- Different types of models and how they are developed.

3.1 Science's next top model

- Earlier we said that *science aims to understand, explain, predict and influence phenomena.*
- The concept of *change* (and the rate at which it occurs) is fundamental to science. (If we **know for certain** that something will not change then there is usually little interest in studying it.)
- Change can be naturally occurring or man-made, and desirable or undesirable.
- Most science is fundamentally quantitative, because quantifying phenomena allows us to measure, describe and compare variations in an efficient and precise manner.
- Science often involves observing and measuring values, such as the amount, frequency, magnitude, duration or rate of some phenomenon, then answering predictive questions about that phenomenon, such as
  - "What will happen if ...?"
  - "What causes ...?"
  - "How can we ...?"
  - "Why does ...?"
- A common approach is to use a *model,* based on the observed, measured data. This is a simplification of the real world which allow us to:
  - make predictions about likely future events;
  - evaluate the possible impacts of interventions; and
  - investigate the robustness and stability of a phenomenon.
- Statistics is fundamental to this process, allowing development of a theoretical model based on uncertain, imprecise data.

Models

All models aim to simplify reality sufficiently to allow approximations to be made and calculations to be done, while at the same time being convenient and easy to use, and providing a sufficiently accurate reflection of the true values to enable useful and meaningful conclusions to be drawn.

The process of modelling

The process of modelling typically involves:

- **observing** *some phenomenon;*
- **thinking** *about what relationships or patterns are important;*
- **measuring** *and recording data;*
- **using** *statistics to address uncertainty, imprecision and errors;*
- **developing** *equations to approximately represent the data;*
- **using** *mathematical techniques to simplify the equations;*
- **writing** *and executing computer models;*
- **interpreting** *results and relating them to the phenomenon;*
- **comparing** *modelled outcomes with actual outcomes;*
- **refining** *the model as required;*
- **applying** *the model using various conditions and assumptions;*
- **predicting** *possible future outcomes; and*
- **communicating** *results to an appropriate audience.*

- Ways of selecting 'appropriate' models include:
  - using "common sense";
  - using logical deduction;
  - using existing knowledge of similar phenomena; and
  - observing the measured data and seeing what it "looks like".

- Many phenomena in nature change according to a small number of underlying patterns (such as at a constant rate or at a rate proportional to the current value).

***Question** 3.1.1* List some strengths and weaknesses of each of the five common ways of presenting quantitative models:

(a) Words

(b) Values (such as weight/height/age tables)

(c) Pictures (such as graphs)

(d) Equations

(e) Computer programs

- Note that there is nothing "right" or "wrong" about each approach: each is suited to different uses and/or target audiences. Most models can be developed and presented in **all** of these ways.

- In SCIE1000 we will use all five methods, but will focus on the final two: equations and computer programs.

3.2 Mathematics and models

- Some people believe that mathematics is an abstract process and is separate from science and the 'real world', unlike disciplines such as biology or chemistry which directly relate to the real world.
- These perceptions of mathematics and science are incorrect.
- Certainly, scientists use a combination of discipline knowledge and a special language to describe nature and the real world (for example, biologists use taxonomic categorisations, anatomical descriptions and medical terminology).
- Mathematicians also use a combination of discipline knowledge and a special language to describe nature and the real world (for example, exponential, linear and square root all describe relationships between observed values in natural phenomena).

Mathematics

Mathematics is a standardised formal language which allows us to:

- *develop models to represent reality;*
- *perform correct, logical deductions;*
- *communicate information without risk of ambiguity or misunderstanding; and*
- *draw conclusions and make predictions.*

- Whatever your area of science, you will need to learn the scientific language and knowledge that allows you to practise in that area.
- Similarly, because all areas of personal and professional life include quantitative concepts, everyone needs to learn the mathematical language and knowledge that allows them to live and work.
- Studying and working in more specialised areas (such as science) requires a higher level of mathematical knowledge and sophistication.

- SCIE1000 includes mathematical language and knowledge.
- However, we do not study mathematics for its own sake, or to develop new mathematical knowledge; if you wish to do that then enrol in discipline-based mathematics courses.
- Instead, we study mathematics **solely** for its fundamental role in describing and modelling the real world, and we will interpret mathematical language in this context.
- For example:
  - **Statistics** is the process of addressing uncertainty, imprecision and errors in data, allowing approximate patterns to be observed and deduced.
  - The mathematical **function** is the formal representation of a pattern in a collection of values.
  - **Logical deduction** describes the process of starting with a collection of facts, approximations and knowledge, and then following a sequence of logically defensible steps which lead to valid conclusions.
- Sometimes we cannot directly measure a phenomenon of interest (due to physical, ethical or financial limitations). Instead, we may be able to measure and model a related phenomenon.
- We can then model the (unmeasurable) quantity using analytical techniques such as:
  - **algebra**, which allows us to conduct logically valid manipulations, simplifications and transformations;
  - **differentiation**, which allows us to model an (unmeasurable) rate of change in a (measurable) phenomenon; and
  - **integration**, which allows us to model an (unmeasurable) phenomenon based on a (measurable) rate of change.
- In SCIE1000 you will mostly use mathematics from your previous study to develop models.

- The following example shows a medical application in which the phenomenon of interest is difficult to measure directly, but a related phenomenon can be measured and modelled, and mathematics is used to deduce information about the primary phenomenon.

***Example** 3.2.1* The *cardiac output* of a heart is the volume of blood pumped by the heart in a given time period; a typical value for an adult human is around 5 L per minute.

There are many reasons to measure cardiac output (for example, to identify contraction abnormalities due to the presence of heart muscle scar tissue), but it is physically difficult to measure directly.

By injecting a fluorescent dye into the right side of the heart, it is possible to use a probe to measure the dye concentration in blood which has passed through the heart, at various time intervals.

Thus, we **want** to measure the *cardiac output*, but instead can **only** measure the *concentration of the dye in blood* over time.

The problem is resolved using the *dye dilution method* as follows:

- Use the observed concentrations, statistics and mathematics to model the measured dye concentrations over time with a mathematical function, say $c(t)$. This is commonly called the *dye dilution curve*.
- Let the initial amount of dye injected be D, and let T be the time at which the observed concentration is (close to) zero.
- Then we can estimate the cardiac output C using some mathematical techniques, including a mathematical integral:

$$C = \frac{D}{\displaystyle\int_0^T c(t)\, dt}$$

Mathematics gives us a range of logical and valid techniques that allow us to deduce information that we cannot measure or obtain in other ways!

Case Study 1:
Growth rates of tropical birds

Question *3.2.2* Bill wants to model and investigate the growth rates of tropical birds. In each of the following, is he acting more as a scientist or as a mathematician (or are they the same thing)?

(a) Bill chooses a particular species of North-Queensland bird, the Yellow-bellied Sunbird *Nectarinia jugularis*, and decides to predict the expected sizes of hatchlings at various times. In order to identify impacts of various factors on growth rates, he needs a more precise description of the size than words like "small", "medium","big", "bigger", "huge", "gigantic" or "gargantuan".

(commons.wikimedia.org/wiki/File:Nectarinia_jugularis.jpg)

(b) Bill visits a number of nests between 6:30 am and 10 am each day for 14 days, weighs individually marked nestlings on an Ohaus triple beam balance (accurate to 0.1 g) and records the weights.

(c) Bill calculates the mean and standard deviation of the weights of the nestlings each day.

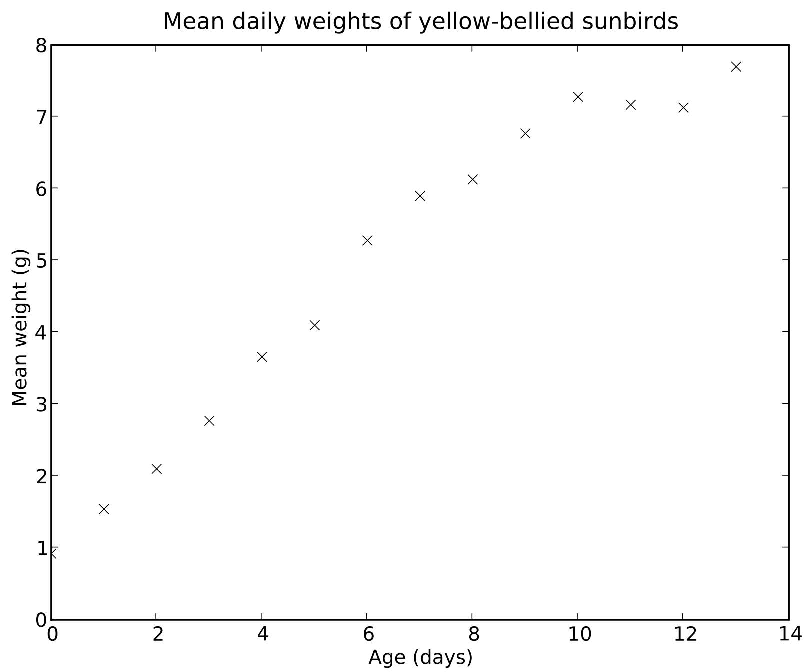
continued...

Question *3.2.2 (continued)*

(d) The data show that when sunbirds hatch, they:

- typically weigh around 0.92 ± 0.13 g;
- initially grow by about 0.62 g per day;
- have a rate of growth which generally increases for a few days, but then total weight starts to level off; and
- ultimately weigh around 8.92 ± 1.14 g (males) or 8.12 ± 1.11 g (females) as adults.

(e) Bill plots the average measured weights on a graph, as follows.



(f) Bill has read many research papers on the growth rates of birds. For example, in a paper[a] it was shown that the weights of most growing perching birds (passerines) follows the *logistic curve*, which is a curve with an elongated "S" shape.

continued...

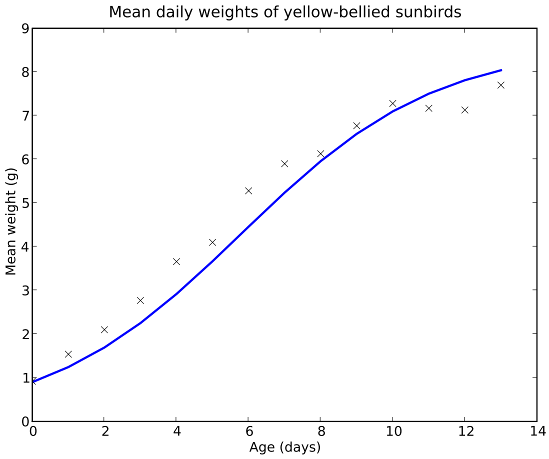
[a]Ricklefs, *Patterns of growth in birds*, Ibis **110** (1968) 421–451

***Question** 3.2.2 (continued)*

(g) The equation for the logistic curve is well-known, and previous researchers have shown how to use statistics to calculate the values for constants in the equation. Bill finds that a good model of the weight W (in g) of nestling sunbirds t days after birth is:

$$W = \frac{8.6}{1 + e^{-0.37(t-5.8)}}.$$

(h) Bill plots this equation and his data on a graph.



(i) Bill uses his model to show that (on average) sunbirds grow 25% more slowly than comparable species from Brazil.

- The above results and procedures are factual. All data, descriptions and equations were taken from a paper[a]. The author was a biologist from the University of Saskatchewan, Canada.

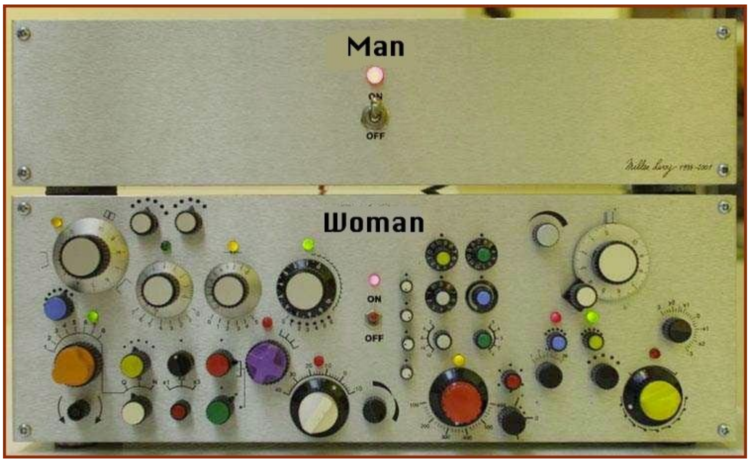
Science and mathematics are not separate areas, with mathematics *artificial* or *irrelevant*. Instead, they are often so closely interlinked that they are identical!

End of Case Study 1.

[a]Maher, *Growth and development of the Yellow-bellied Sunbird* Nectarinia jugularis *in North Queensland*, Emu **91** (1991) 58–61.

3.3 Developing models

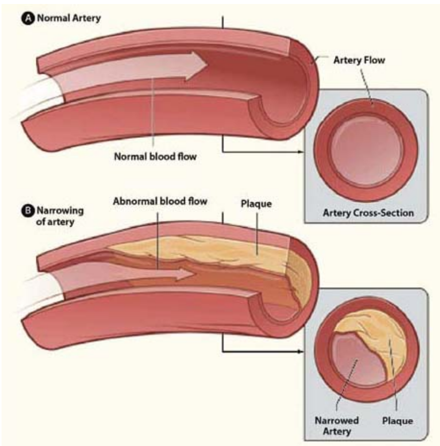
- All models are a trade-off between accuracy and complexity (and hence cost in terms of time, computational power and/or money).

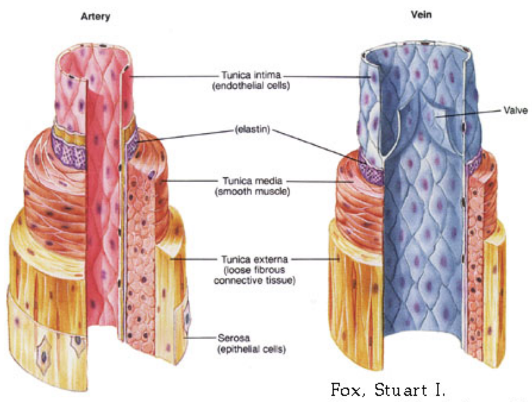


greggsutter.com/mt/archives/manWomanControlPanel.jpg

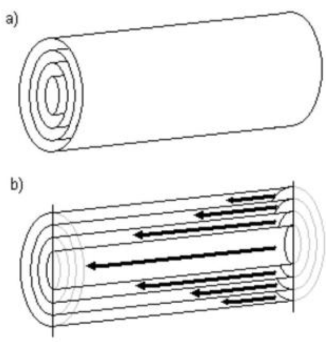
- When developing a model it is important to identify which physical factors and data are crucial, and what levels of accuracy and precision are required.

Case Study 2:
Modelling fluid flow





Fox, Stuart I.
Human Physiology 4th
Brown Publishers



- *Fluid dynamics* involves studying liquids and gases that are moving. This is important in many branches of science (particularly geology, environmental science and biomedical science) and engineering.
- There are various models in fluid dynamics, depending on the individual characteristics of the fluid and the nature of its movement.

***Question** 3.3.1* Develop a model of the flow rate of blood through a given blood vessel. (Hint: start by deciding which factors are important and whether they increase or decrease the flow rate.)

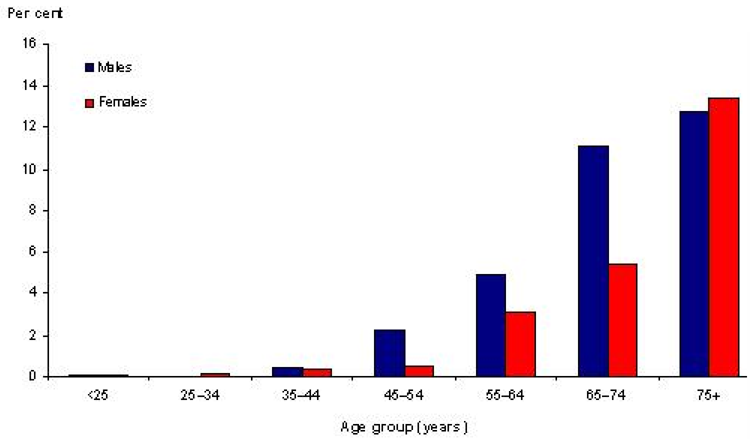
The following formula (called the *Hagen-Poiseuille equation*) is often used to estimate such flows:

Comment on the formula:

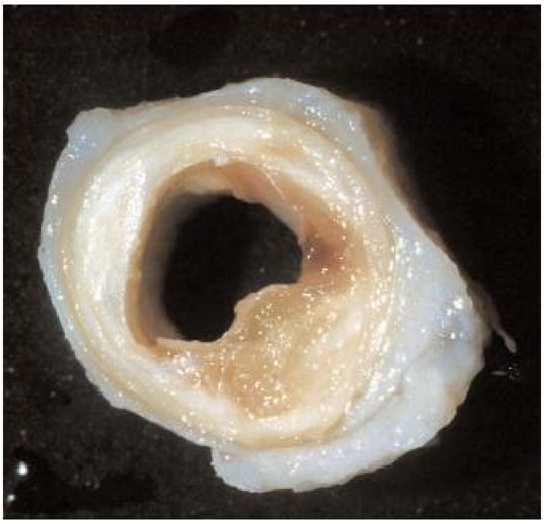
End of Case Study 2.

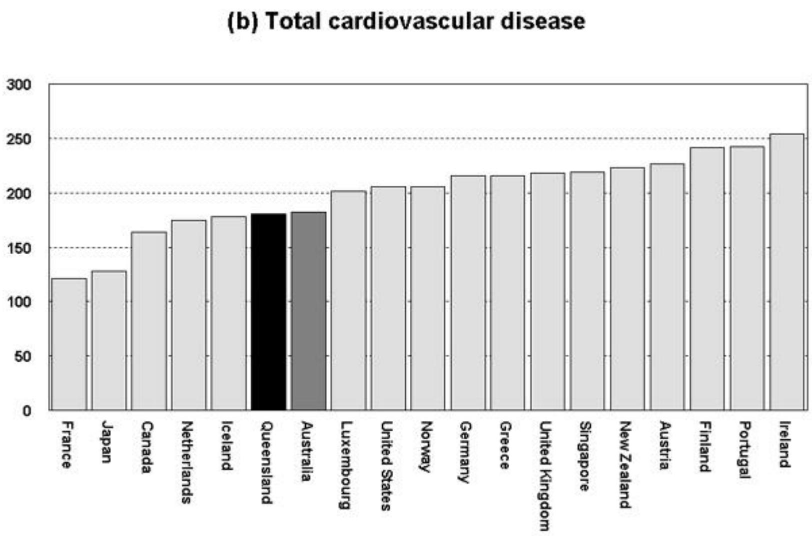
3.4 Models in action

Case Study 3:
Modelling the risk of heart disease



Age-specific prevalence of coronary heart disease, Australia, 2004-05





Top ten causes of death (QLD, 2005)	Number	percent
Diseases of the circulatory system (including ischaemic heart disease, stroke)	8479	36%
Neoplasms (cancer)	7148	30%
Diseases of the respiratory system	1963	8%
External causes (suicide, accidents, falls)	1556	7%
Endocrine, nutritional and metabolic diseases	917	4%
Diseases of the digestive system	803	3%
Diseases of the nervous system	750	3%
Diseases of the genitourinary system	508	2%
Mental and behavioural disorders	481	2%
Infectious and parasitic diseases	239	1%
Total all causes	23584	–

- Individuals, doctors and public health bodies all have an obvious interest in predicting who is at risk of suffering Cardiovascular Disease (CVD).
- The risk of suffering a certain medical event is often specified as a probability of the event occurring in a given time period.

***Question** 3.4.1* Shortly we will encounter a famous study into cardiovascular health, called the *Framingham* study. This study defines Coronary Heart Disease (CHD) as including:

- *angina pectoris*, which is severe chest pain caused by a lack of blood to heart muscle;
- *myocardial infarction*, commonly called a heart attack, arising from complete loss of blood supply to heart muscle; and
- death due to cardiac arrest.

When developing a model that allows estimation of the percentage likelihood that Peter will suffer CHD in the next 10 years, what information might be required and which factors are likely to be crucial? What is your "gut feeling" of his likelihood?

- The Framingham study has identified a number of risk factors for CHD, which have been included in a mathematical model for risk prediction. (We will see the specific equation on Page 60.)
- One of the key risk factors is associated with levels of different types of cholesterol in the blood.

***Extension** 3.4.2* (From www.csiro.au/resources/CholesterolFacts.html)

"Cholesterol is an essential type of fat that is carried in the blood. All cells in the body need cholesterol for internal and external membranes, and it is also needed to produce some hormones. High levels of cholesterol in the blood stream are a risk factor for coronary artery disease.

If your cholesterol level is 6.5 mmol/L or greater your risk of heart disease is about 4 times greater than that of a person with a cholesterol level of 4 mmol/L.

Cholesterol is carried in the blood stream in particles called lipoproteins. These are named according to how big they are:

- the very large particles are called Very Low Density Lipoproteins (VLDL)
- the intermediate size ones are called Low Density Lipoprotein (LDL) and these particles cause heart disease
- the smallest particles are called High Density Lipoproteins (HDL) and these particles protect against heart disease."

- Rather than simply measuring total cholesterol T, it is increasingly common for blood tests to measure the *ratio* of T to HDL.
- It is now widely accepted that the value of this ratio is a more accurate predictor of risk of suffering coronary artery disease than is the total cholesterol level (lower values have lower risks).
- Australian Heart Foundation guidelines suggest that for good health, the value of this ratio should be at most 4.

Modelling the risk of heart disease *(continued)*

- Until comparatively recently, little was known about the general causes of heart disease and stroke, although the rates of cardiovascular disease (CVD) had been rising for some time.
- In 1948, an ongoing study into heart disease was commenced in Framingham, Massachusetts. This has become one of the best-known longitudinal health studies.
- This study has monitored the cardiovascular health of the participants and identified a range of risk factors.

Extension *3.4.3* (From www.nhlbi.nih.gov)

"Since its inception, the study has produced approximately 1,200 articles in leading medical journals. The concept of CVD risk factors has become an integral part of the modern medical curriculum and has led to the development of effective treatment and preventive strategies in clinical practice."

Extension *3.4.4* (From www.framinghamheartstudy.org)

"Since our beginning in 1948, the Framingham Heart Study, under the direction of the National Heart, Lung and Blood Institute (NHLBI), formerly known as the National Heart Institute, has been committed to identifying the common factors or characteristics that contribute to cardiovascular disease (CVD). We have followed CVD development over a long period of time in three generations of participants.

Our Study began in 1948 by recruiting an Original Cohort of 5,209 men and women between the ages of 30 and 62 from the town of Framingham, Massachusetts, who had not yet developed overt symptoms of cardiovascular disease or suffered a heart attack or stroke. Since that time the Study has added an Offspring Cohort in 1971, the Omni Cohort in 1994, a Third Generation Cohort in 2002, a New Offspring Spouse Cohort in 2003, and a Second Generation Omni Cohort in 2003."

Extension 3.4.5 (From www.framinghamheartstudy.org)

"Over the years, careful monitoring of the Framingham Study population has led to the identification of major CVD risk factors, as well as valuable information on the effects of these factors such as blood pressure, blood triglyceride and cholesterol levels, age, gender, and psychosocial issues. Risk factors for other physiological conditions such as dementia have been and continue to be investigated....

Research milestones from the study include:

- 1960: Cigarette smoking found to increase the risk of heart disease
- 1961: Cholesterol level, blood pressure, and electrocardiogram abnormalities found to increase the risk of heart disease
- 1967: Physical activity found to reduce the risk of heart disease and obesity to increase the risk of heart disease
- 1970: High blood pressure found to increase the risk of stroke
- 1976: Menopause found to increase the risk of heart disease
- 1978: Psychosocial factors found to affect heart disease
- 1988: High levels of HDL cholesterol found to reduce risk of death
- 1994: Enlarged left ventricle (one of two lower chambers of the heart) shown to increase the risk of stroke
- 1996: Progression from hypertension to heart failure described
- 1998: Development of simple coronary disease prediction algorithm involving risk factor categories to allow physicians to predict multivariate coronary heart disease risk in patients without overt CVD
- 1999: Lifetime risk at age 40 years of developing coronary heart disease is one in two for men and one in three for women
- 2001: High-normal blood pressure is associated with an increased risk of cardiovascular disease, emphasising the need to determine whether lowering high-normal blood pressure can reduce the risk of CVD.
- 2002: Lifetime risk of developing high blood pressure in middle-aged adults is 9 in 10.
- 2002: Obesity is a risk factor for heart failure.
- 2004: Serum aldosterone levels predict future risk of hypertension in non-hypertensive individuals.
- 2005: Lifetime risk of becoming overweight exceeds 70 percent, that for obesity approximates 1 in 2."

Modelling the risk of heart disease *(continued)*

- One of the resources produced from the Framingham Study is a Coronary Heart Disease Risk Prediction score sheet, which is a table-based representation of the model they derived.

***Question** 3.4.6* Estimate the probability that Peter will suffer CHD within 10 years. Compare with your answer to Question 3.4.1.

Coronary Disease Risk Prediction Score Sheet for Men Based on LDL Cholesterol Level

Step 1

Age	
Years	Points
30-34	-1
35-39	0
40-44	1
45-49	2
50-54	3
55-59	4
60-64	5
65-69	6
70-74	7

Step 2

LDL - Cholesterol		
(mg/dl)	(mmol/L)	Points
<100	≤2.59	-3
100-129	2.60-3.36	0
130-159	3.37-4.14	0
160-189	4.15-4.91	1
≥190	≥4.92	2

Key	
Color	Risk
green	Very low
white	Low
yellow	Moderate
rose	High
red	Very high

Step 3

HDL - Cholesterol		
(mg/dl)	(mmol/L)	Points
<35	≤0.90	2
35-44	0.91-1.16	1
45-49	1.17-1.29	0
50-59	1.30-1.55	0
≥60	≥1.56	-1

Step 4

Blood Pressure					
Systolic	Diastolic (mmHg)				
(mmHg)	<80	80-84	85-89	90-99	≥100
<120	0				
120-129		0 pts			
130-139			1		
140-159				2	
≥160					3 pts

Note: When systolic and diastolic pressures provide different estimates for point scores, use the higher number

Step 5

Diabetes	
	Points
No	0
Yes	2

Step 6

Smoker	
	Points
No	0
Yes	2

Risk estimates were derived from the experience of the NHLBI's Framingham Heart Study, a predominantly Caucasian population in Massachusetts, USA

Step 7 (sum from steps 1-6)

Adding up the points	
Age	________
LDL Cholesterol	________
HDL Cholesterol	________
Blood Pressure	________
Diabetes	________
Smoker	________
Point Total	________

Step 8 (determine CHD risk from point total)

CHD Risk	
Point Total	10 Yr CHD Risk
≤-3	1%
-2	2%
-1	2%
0	3%
1	4%
2	4%
3	6%
4	7%
5	9%
6	11%
7	14%
8	18%
9	22%
10	27%
11	33%
12	40%
13	47%
≥14	≥56%

Step 9 (compare to man of the same age)

Comparative Risk		
Age (years)	Average 10 Yr CHD Risk	Low* 10 Yr CHD Risk
30-34	3%	2%
35-39	5%	3%
40-44	7%	4%
45-49	11%	4%
50-54	14%	6%
55-59	16%	7%
60-64	21%	9%
65-69	25%	11%
70-74	30%	14%

*Low risk was calculated for a man the same age, normal blood pressure, LDL cholesterol 100-129 mg/dL, HDL cholesterol 45 mg/dL, non-smoker, no diabetes

Modelling the risk of heart disease *(continued)*

For comparison with CHD risk for males, the risk sheet for females is:

Coronary Disease Risk Prediction Score Sheet for Women Based on LDL Cholesterol Level

Step 1

Age	
Years	Points
30-34	-9
35-39	-4
40-44	0
45-49	3
50-54	6
55-59	7
60-64	8
65-69	8
70-74	8

Step 2

LDL - Cholesterol		
(mg/dl)	(mmol/L)	Points
<100	≤2.59	-2
100-129	2.60-3.36	0
130-159	3.37-4.14	0
160-189	4.15-4.91	2
≥190	≥4.92	2

Key	
Color	Risk
green	Very low
white	Low
yellow	Moderate
rose	High
red	Very high

Step 3

HDL - Cholesterol		
(mg/dl)	(mmol/L)	Points
<35	≤0.90	5
35-44	0.91-1.16	2
45-49	1.17-1.29	1
50-59	1.30-1.55	0
≥60	≥1.56	-2

Step 4

Blood Pressure					
Systolic	Diastolic (mmHg)				
(mmHg)	<80	80-84	85-89	90-99	≥100
<120	-3 pts				
120-129		0 pts			
130-139			0 pts		
140-159				2 pts	
≥160					3 pts

Note: When systolic and diastolic pressures provide different estimates for point scores, use the higher number

Step 5

Diabetes	
	Points
No	0
Yes	4

Step 6

Smoker	
	Points
No	0
Yes	2

Risk estimates were derived from the experience of the NHLBI's Framingham Heart Study, a predominantly Caucasian population in Massachusetts, USA

Step 7 (sum from steps 1-6)

Adding up the points	
Age	________
LDL Cholesterol	________
HDL Cholesterol	________
Blood Pressure	________
Diabetes	________
Smoker	________
Point Total	________

Step 8 (determine CHD risk from point total)

CHD Risk	
Point Total	10 Yr CHD Risk
≤-2	1%
-1	2%
0	2%
1	2%
2	3%
3	3%
4	4%
5	5%
6	6%
7	7%
8	8%
9	9%
10	11%
11	13%
12	15%
13	17%
14	20%
15	24%
16	27%
≥17	≥32%

Step 9 (compare to women of the same age)

Comparative Risk		
Age (years)	Average 10 Yr CHD Risk	Low* 10 Yr CHD Risk
30-34	<1%	<1%
35-39	1%	<1%
40-44	2%	2%
45-49	5%	3%
50-54	8%	5%
55-59	12%	7%
60-64	12%	8%
65-69	13%	8%
70-74	14%	8%

*Low risk was calculated for a woman the same age, normal blood pressure, LDL cholesterol 100-129 mg/dL, HDL cholesterol 55 mg/dL, non-smoker, no diabetes

(Both risk sheets can be found at:
`www.nhlbi.nih.gov/about/framingham/riskabs.htm`)

***Question** 3.4.7* Briefly discuss some of the key points highlighted by the two coronary disease risk prediction sheets. (You may like to mention such things as the comparative impact of different risk factors, some 'risk factors' commonly mentioned in the media which are not included, and some differences between males and females.)

Extension 3.4.8 (From Brindle et al., *Predictive accuracy of the Framingham coronary risk score in British men: prospective cohort study*, British Medical Journal **327** (2003) 1267–1270.)

The Framingham researchers actually developed a mathematical model of the risk (shown below). The risk 'score' sheets are simply approximate table-based representations of the model.

Framingham risk equations for coronary heart disease death (B1) and coronary heart disease events (B2) in men over 10 years

Step 1

For coronary heart disease mortality calculate*

μ = 11.2889 – 0.588xln(systolic blood pressure) – 0.1367xsmoking – 0.3448xln(total/high density lipoprotein cholesterol) – 0.1237xelectrocardiographic left ventricular hypertrophy – 0.944xln(age) – 0.0474xdiabetes

σ= exp(2.9851 – 0.9142μ) (B1)

For coronary heart disease events calculate*

μ = 15.5303 – 0.9119xln(systolic blood pressure) – 0.2767xsmoking – 0.7181xln(total/high density lipoprotein cholesterol) – 0.5865xelectrocardiographic left ventricular hypertrophy – 1.4792xln(age) – 0.1759xdiabetes

σ= exp(– 0.3155 – 0.2784x(μ – 4.4181)) (B2)

Step 2

For both equations calculate:

u = (ln(10) – μ)/σ Length of follow up = 10 years

Step 3

The predicted probability is then given by:

p=1 – exp(– exp(u))

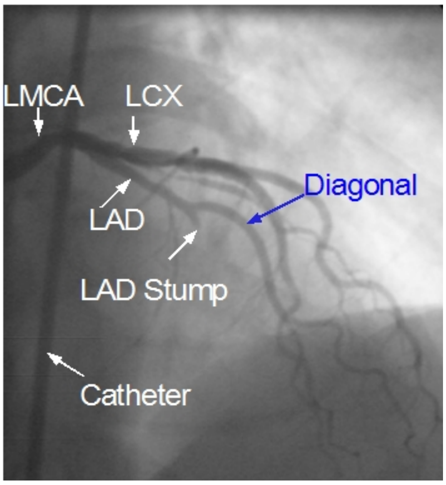
*Variables smoking, electrocardiographic left ventricular hypertrophy, and diabetes are set to 1 when present and 0 when absent. Systolic blood pressure measured in mm Hg and age in years

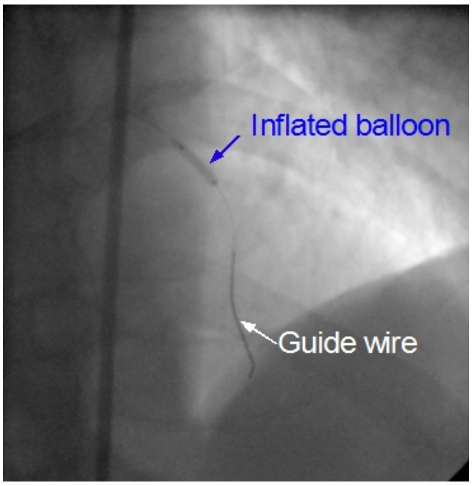
Question *3.4.9* When Peter underwent a blood test in August 2008, his total cholesterol was 4.7 mmol/L, with his HDL 0.9 mmol/L and his LDL 3.5 mmol/L. Medical advice was that he should try to raise his HDL level through lifestyle changes, including increased exercise, changed diet, less stress and giving fewer SCIE1000 lectures.

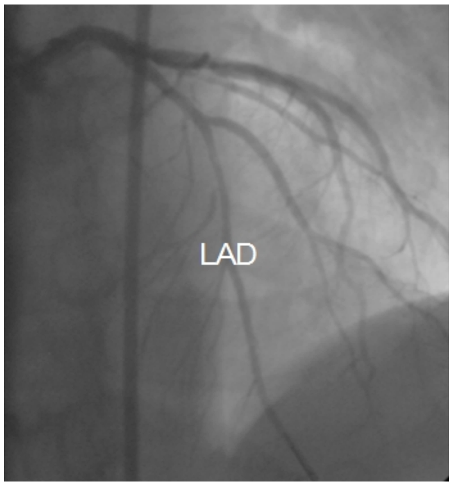
Assuming his lifestyle changes only have an impact on his HDL (so his other cholesterol levels remain unchanged), by what percent does Peter need to increase his HDL so that his ratio of total cholesterol to HDL equals 4?

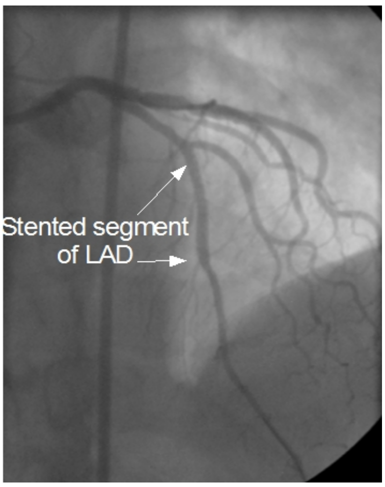
Modelling the risk of heart disease *(continued)*

- High levels of LDL cholesterol in the blood can lead to blockages in coronary arteries. One surgical method of increasing blood flow through partially blocked arteries is an *angioplasty*.
- In a coronary angioplasty, a balloon-tipped catheter is inserted into the body under local anaesthetic, typically through the groin or above the wrist. When in position in the coronary artery, the balloon is inflated to expand the blood vessel (and sometimes a metallic stent is inserted to maintain the expansion).
- An advantage of angioplasties over coronary artery bypass surgery is that the procedure is much simpler and less invasive, but a disadvantage is a higher rate of recurrence of the original occlusion.









('LAD' is the left anterior descending coronary artery)

cardiophile.org/wp-content/uploads/2008/10/lad-total-occulusion.jpg

Question *3.4.10* In an angioplasty operation, a patient has a 30% increase in the diameter of a partially occluded artery.

(a) Roughly estimate the resulting increase in blood flow through that artery.

(b) Explain how to calculate the increase more accurately, and do so.

End of Case Study 3.

3.5 Computer models

- Computation is important when formulating and applying models, particularly when dealing with complex phenomena.
- You almost certainly have already used computer models at some time, and may even have developed some of your own.
- Every computer program and computer model must be implemented in some computer *language*.
- A computer language is a collection of commands that can be interpreted by a computer, and instructs the computer to perform associated operations and calculations.
- There are many different computer languages, each suited to particular uses. In this course we use the language *Python*.
- We use Python because it is modern, freely available, fairly easy to learn, used in real science applications, and illustrates many important general computing concepts.
- (For interest, Python was named after *Monty Python's Flying Circus*.)

- Some well-known users of Python include Youtube, Google, Yahoo!, CERN and NASA.

Python in this course

You will encounter Python in this course in the following ways:

- *These lecture notes include some examples of Python programs and the output.*
- *You have a separate Python programming manual.*
- *You will write small Python programs in your computer lab classes and submit some of them for assessment.*

You will **not** *need to write programs in your exam. However, you will need to answer questions on general computing concepts, and also explain what given Python programs do.*

Python Example 3.5.1

Python examples appear in the notes like this.

```
# This is a comment.
print 6+4
print "Hello world!"
```

Note that

- The lines of Python code have a vertical line next to them and are numbered for ease of reference.
- The output from the above program is:

```
10
Hello world!
```

- The first step in writing a program (in Python or any language) is to specify **exactly** what the program should do: specifications should be precise, accurate and complete.
- The next step is to write the program; we study this in Chapter 7.
- In the next case study we will develop a mathematical model, and then give a computer representation of that model.

Case Study 4:
Blood Alcohol Concentration

- Blood Alcohol Concentration (BAC) is usually measured as the percentage of total blood volume which is alcohol.
- The following table shows some of the effects typically experienced at differing BACs.

Blood Alcohol Concentration *(continued)*

BAC (%)	Changes in Feelings/Personality	Physical/Mental Impairments
0.01 – 0.06	Relaxation Sense of Well-being Loss of Inhibition Lowered Alertness Joyous	Thought Judgement Coordination Concentration
0.06 – 0.10	Blunted Feelings Dis-inhibition Extroversion Impaired Sexual Pleasure	Reflexes Reasoning Depth Perception Distance Acuity Peripheral Vision Glare Recovery
0.11 – 0.20	Over-Expression Emotional Swings Angry or Sad Boisterous	Reaction Time Gross Motor Control Staggering Slurred Speech
0.21 – 0.29	Stupor Lose Understanding Impaired Sensations	Severe Motor Impairment Loss of Consciousness Memory Blackout
0.30 – 0.39	Severe Depression Unconsciousness Death Possible	Bladder Function Breathing Heart Rate
≥ 0.40	Unconsciousness Death	Breathing Heart Rate

(source: www.alcohol.vt.edu/Students/alcoholEffects/index.htm)

- Given these effects of alcohol, there are strict laws about driving and operating machinery after consuming alcohol.
- In Australia the maximum legal blood alcohol content for driving is 0.05%, or 0.5 g/L.
- It is important to be able to estimate the time taken for BAC to return to 0.
- This will vary somewhat between individuals, but governments and health bodies publish general guidelines.

Question 3.5.2 The following table estimates the number of hours required for the BAC of males of different weights to return to zero. (This is taken from an American government website; to approximately convert a weight from pounds to kg, divide by 2.2.)

num.	Weight (pounds)							
drinks	120	140	160	180	200	220	240	260
1	2	2	2	1.5	1	1	1	1
2	4	3.5	3	3	2.5	2	2	2
3	6	5	4.5	4	3.5	3.5	3	3
4	8	7	6	5.5	5	4.5	4	3.5
5	10	8.5	7.5	6.5	6	5.5	5	4.5

Derive a mathematical model for this data.

- This mathematical model can be implemented as a computer model.

Program specifications: Use the mathematical model to write a program which allows the user to:

(a) enter the weight of a male and a number of standard drinks, and calculates the approximate time for BAC to return to 0; and

(b) obtain an approximation to the given table of times.

Python Example 3.5.3

```
# A program to model the time for BAC to return to 0
# for male drinkers of different weights.

from __future__ import division
from pylab import *

choice = input("Type 1 to enter a man's details or 2 for
                                  the modelled table: ")

if choice == 1:
# Individual calculations
    weight = input("What is the man's weight in pounds? ")
    numDrinks = input("How many standard drinks does he have? ")
    approx = numDrinks * 240 / weight
    time = round(approx,1)
    print "His BAC should be 0 after about ",time," hours."
else:
# Table calculations
    print "   ",
    for weight in arange(120,280,20):
        print weight,"  ",
    print
    print "-------------------------------------------"

# Loop through the numbers of drinks and the weights.
    for numDrinks in arange(1,6):
        print numDrinks,"|",
        for weight in arange(120,280,20):
            time = numDrinks * 240 / weight
            print round(time,1),"  ",
        print
```

Blood Alcohol Concentration *(continued)*

Python Example 3.5.3 *(continued)*

Here is the output from running the above program twice:

```
Type 1 to enter a man's details or 2 for the modelled table: 1
What is the man's weight in pounds? 150
How many standard drinks does he have? 9
His BAC should be 0 after about  14.0  hours.

Type 1 to enter a man's details or 2 for the modelled table: 2
        120    140    160    180    200    220    240    260
    ----------------------------------------------------------
    1 | 2.0    1.7    1.5    1.3    1.2    1.1    1.0    0.9
    2 | 4.0    3.4    3.0    2.7    2.4    2.2    2.0    1.8
    3 | 6.0    5.1    4.5    4.0    3.6    3.3    3.0    2.8
    4 | 8.0    6.9    6.0    5.3    4.8    4.4    4.0    3.7
    5 | 10.0    8.6    7.5    6.7    6.0    5.5    5.0    4.6
```

***Question** 3.5.4* Briefly discuss the effectiveness and accuracy of the mathematical model.

End of Case Study 4.

3.6 Space for additional notes

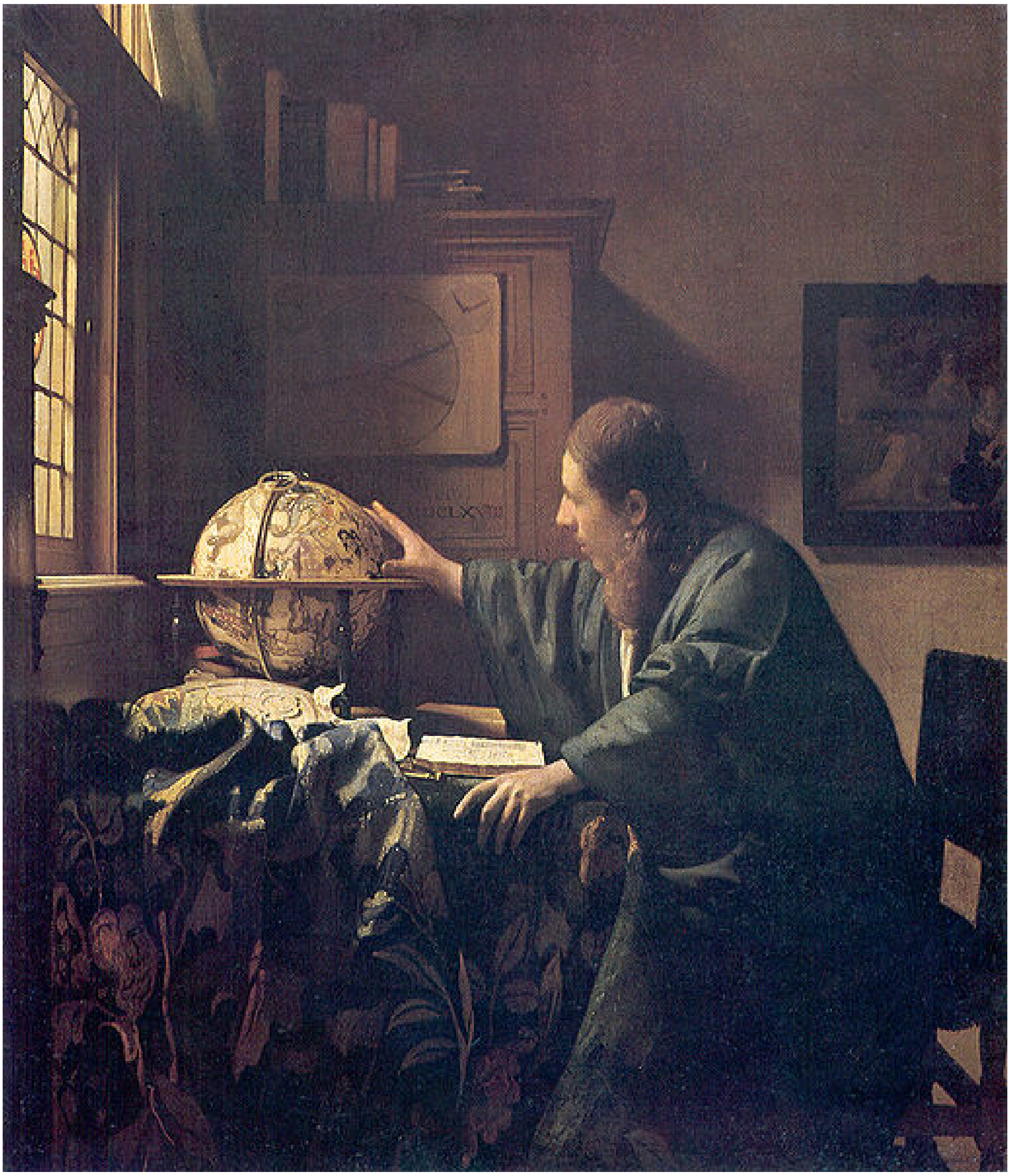
4 Some science

I see skies of blue, clouds of white
Bright blessed days, dark sacred nights
And I think to myself, what a wonderful world.
I hear babies cry, I watch them grow
They'll learn much more, than I'll never know
And I think to myself, what a wonderful world
Yes I think to myself, what a wonderful world

Artist: Louis Armstrong

(www.youtube.com/watch?v=fo-VDRvABkw)

(Take time to watch this.)



The Astronomer (1668), Jan Vermeer (1632 – 1675), Musee du Louvre, Paris. (Image source: en.wikipedia.org)

Introduction

Two of the goals of this course are to:

- demonstrate the importance of quantitative skills (including mathematics and computing) in science; and
- explore a breadth of scientific fields, showing some similarities and relationships between the diverse fields.

The examples and case studies have been deliberately chosen to represent different scientific disciplines, and in most cases no particular background knowledge is required to understand the content. However, some examples may require some knowledge of specific words or concepts.

This section of the notes is a very quick introduction to some fundamental concepts in physics, chemistry and biology. Of course, each of these areas represents a rich and extensive branch of human knowledge. All students enrolled in this course will be undertaking substantial studies in one or more of these areas, so the material in this section is designed primarily for those who have never studied a particular discipline before. Of necessity, the content here is very limited.

Some of the examples/contexts we will discuss are:

- Physics.
- Chemistry.
- Biology.

Specific techniques and concepts we will cover include:

- SI units.
- Dimensional analysis.
- Writing and solving equations.

4.1 Numbers and units

Some notation regarding numbers

You may see numbers written in **scientific notation**, *which is in the form* $a \times 10^b$, *where* a *and* b *are numbers.*

Computers and calculators often write numbers in scientific notation using "E" or "e" notation. Python uses the notation `ae+b` *or* `ae-b`. *For example, Python would print* 3×10^{17} *as* `3e+017`.

(Much of the following is sourced from the US National Institute of Standards, see *physics.nist.gov/cuu/Units/index.html.*)

- When measuring a physical quantity, modelling some phenomenon or communicating a result, it is essential to use a standard *unit of measurement.*
- There are famous examples of disasters arising from inconsistent use of units.

***Example** 4.1.1* The Mars Climate Orbiter was launched in 1998 as part of a $USD330 million project. In September 1999 the orbiter crashed into Mars.

It later transpired that the crash was caused by an inconsistency between units in the associated software.

One team of programmers had assumed a value was specified in imperial units, and another team assumed it was in metric.

- The most commonly used units of measurement are defined by the **International System of units**, and are called **SI** units.
- There are seven **SI base units**; each has a standard name and symbol.

SI units

The names and symbols of the seven **SI base units** *are:*

Base quantity	*SI base unit name*	*SI base unit symbol*
length	*metre*	*m*
mass	*kilogram*	*kg*
time	*second*	*s*
electric current	*ampere*	*A*
thermodynamic temperature	*kelvin*	*K*
amount of substance	*mole*	*mol*
luminous intensity	*candela*	*cd*

SI prefixes

The 20 **SI prefixes** *used to denote multiples of the SI units are as follows (each is a positive or negative power of 10).*

Multiple	*Name*	*Symbol*	*Multiple*	*Name*	*Symbol*
10^1	*deka*	*da*	10^{-1}	*deci*	*d*
10^2	*hecto*	*h*	10^{-2}	*centi*	*c*
10^3	*kilo*	*k*	10^{-3}	*milli*	*m*
10^6	*mega*	*M*	10^{-6}	*micro*	μ
10^9	*giga*	*G*	10^{-9}	*nano*	*n*
10^{12}	*tera*	*T*	10^{-12}	*pico*	*p*
10^{15}	*peta*	*P*	10^{-15}	*femto*	*f*
10^{18}	*exa*	*E*	10^{-18}	*atto*	*a*
10^{21}	*zetta*	*Z*	10^{-21}	*zepto*	*z*
10^{24}	*yotta*	*Y*	10^{-24}	*yocto*	*y*

Example *4.1.2* Some examples of using SI prefixes include:

- The SI base unit *kilogram*, denoted kg, is unusual because it already includes a prefix.
- One *kilometre*, denoted 1 km, is 10^3 m.
- A *nanosecond*, denoted 1 ns, is 10^{-9} s.

Derived units

Many natural and scientific quantities require more complex units than SI base units. These more complex units can **always** *be defined in terms of the seven base units, and are called* **SI derived units***.*

***Example** 4.1.3* Some examples of quantities with SI derived units are:

- Volume, measured in *cubic metres*;
- Velocity, measured in *metres per second*;
- Concentration, measured in *moles per cubic metre*.

  (In practice, concentration is often expressed as *moles per litre*. A *litre* is defined to be 1/1000 of a *cubic metre*, and is denoted L.)

- SI derived units can become lengthy to write, so it is usual to adopt a convenient mathematical shorthand.

Standard mathematical notation for SI derived units

Standard mathematical notation for SI derived units is based on the following principles:

- *if the quantity involves the "product" of two SI units then their SI symbols are separated by a space or a dot;*
- *mathematical power notation is used if the same SI unit occurs in a "product" more than once; and*
- *if the quantity involves the "quotient" of an SI unit then the derived unit either uses a quotient sign /, or (more often) mathematical power notation with a negative power.*

Example 4.1.4 The quantities from Example 4.1.3 rewritten with mathematical notation in their standard units are:

- Volume, measured in m^3 (or L, where 1 L is defined to be 10^{-3} m^3).
- Velocity, measured in m/s or $\mathrm{m\ s}^{-1}$ or $\mathrm{m} \cdot \mathrm{s}^{-1}$.
- Concentration, measured in mol/L or $\mathrm{mol\ L}^{-1}$ or $\mathrm{mol} \cdot \mathrm{L}^{-1}$.

Example 4.1.5 Some SI derived units are used very frequently, so they have been given special names and symbols. The following table shows some well-known examples.

Quantity	Name	Symbol	SI units	SI base units
frequency	hertz	Hz	-	s^{-1}
force	newton	N	-	$m \cdot kg \cdot s^{-2}$
pressure, stress	pascal	Pa	$N \cdot m^{-2}$	$m^{-1} \cdot kg \cdot s^{-2}$
energy, work, quantity of heat	joule	J	$N \cdot m$	$m^2 \cdot kg \cdot s^{-2}$
power, radiant flux	watt	W	$J \cdot s^{-1}$	$m^2 \cdot kg \cdot s^{-3}$
quantity of electricity, electric charge	coulomb	C	-	$s \cdot A$
electric potential difference, electromotive force	volt	V	$W \cdot A^{-1}$	$m^2 \cdot kg \cdot s^{-3} \cdot A^{-1}$
capacitance	farad	F	$C \cdot V^{-1}$	$m^{-2} \cdot kg^{-1} \cdot s^4 \cdot A^2$
electric resistance	ohm	Ω	$V \cdot A^{-1}$	$m^2 \cdot kg \cdot s^{-3} \cdot A^{-2}$
Celsius temperature	degree Celsius	$^\circ$ C	-	K

Example 4.1.6 The average daily energy intake of a reasonably active adult human male is around 10^7 J or 10 megajoules, written 10 MJ.

Dimensional analysis

A useful technique in science is **dimensional analysis**, *which is closely related to SI units. A full discussion of dimensional analysis is beyond this course, but some useful points are:*

- *Any equation describing a physical situation can only be true if it is* **dimensionally homogeneous**; *that is, both sides of the equation must have the same units.*
- *Units can be mathematically manipulated, including multiplied and cancelled.*
- *Quantities can be added or subtracted if and only if they have the same units.*

Dimensional analysis can very quickly give a rough check of whether a calculation is 'plausible': if the dimensions do not match, then there must be an error.

The importance of units

Every physical quantity must have units unless it is a pure number (such as 2 or π). Every length must be measured in m, km, inches, furlongs, or some other unit of length. So if $x = 3$ m then x is a length, but if $y = 3$ then y is just a number. **These two things are different.**

In scientific work, you should try to keep units on quantities. Sometimes when you are learning new mathematical concepts it can make things seem more complicated or harder to read if units are included. To keep things simpler in these notes, we have often defined variables to not require units. For example, if t is defined by saying "t is the time since the rocket was launched" then t needs a unit. If it is defined by saying "t is the number of seconds since the rocket was launched," it does not. We often use the latter terminology.

4.2 Science

The word *science* derives from the Latin *scientia*, meaning *knowledge*. In an historical sense, it refers to any systematic knowledge or practice. The modern use of the term refers to a system of acquiring knowledge based on the scientific method, as well as to the organised body of knowledge gained through such research.

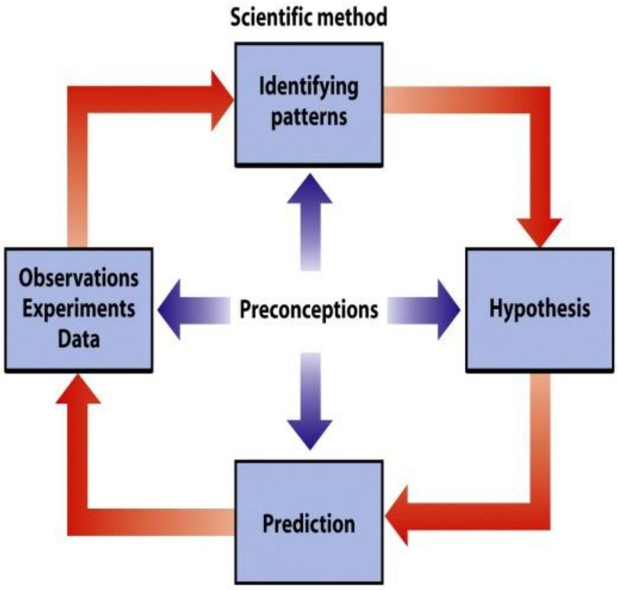
Fields of science are commonly classified into **natural sciences** (which study natural phenomena) and **social sciences** (which study human behaviour and societies). These are both *empirical sciences*, which means the knowledge must be based on observable phenomena and capable of being tested for validity by other researchers working under the same conditions.

Mathematics, which is sometimes classified within a third group of science called *formal science*, has both similarities and differences with the natural and social sciences. It is similar to empirical sciences in that it involves an objective, careful and systematic study of an area of knowledge; yet it is different because of its method of verifying its knowledge, using *a priori* rather than empirical methods. Major advances in formal science have often led to major advances in the physical and biological sciences. The formal sciences are essential to the formation of hypotheses, theories, and laws, both in discovering and describing how things work (natural sciences) and how people think and act (social sciences).

The history of science is marked by a chain of advances in technology and knowledge which have always complemented each other. Technological innovations are bred by other discoveries, and in turn give rise to new discoveries, inspiring new possibilities and approaches to long-standing science issues. Investing money, time, effort and education in science and technology is critical to ensuring long-term prosperity and a high quality of life. Scientists are at the forefront of developing scientific and technological innovations. Their primary objectives are to develop ideas and conduct novel research which can be used to solve problems for the private and public good. Although experimental science is often differentiated from applied science, which is the application of scientific research to specific human needs, the two are often interconnected.

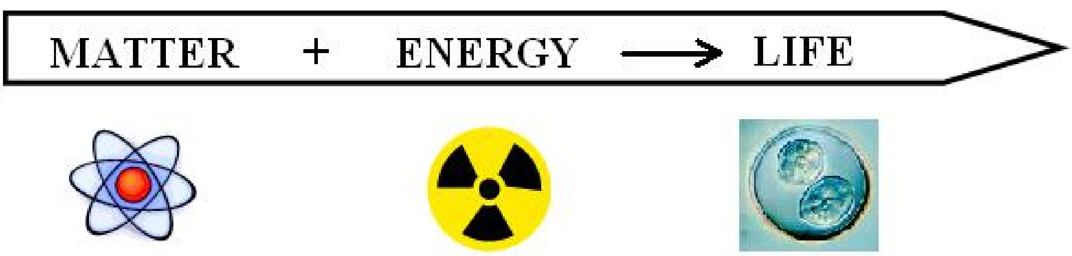
Science is both *content* and *process*. It is the collection of discovered knowledge as well as the processes used to discover knowledge. Science should not be taught as just a series of facts, but rather by explaining how materials were discovered and ideas developed over time. This approach provides an integrated and holistic appreciation as well as historical and contextual relevance for the scientific process.

The process of observing the physical universe, framing experimental questions (hypotheses), analysing and critically interpreting data, generating models and making predictions is considered to constitute the scientific method, based on hypothetico-deductive logic. This method should not be regarded as a rigid template, but rather as a natural, circular way of thinking, with no fixed start or end points.



The Enabling Sciences

There are many different ways to introduce fundamental and applied sciences. Most textbooks are dedicated to specific disciplines and therefore do not demonstrate how the sciences overlap and complement each other. They do not provide an *interdisciplinary* or *multidisciplinary* perspective or an *integrated* approach. The framework we have adopted covers the three fundamental enabling sciences of **chemistry**, **physics** and **biology**; the study of **matter**, **energy** and **life**.



Chemistry involves the study of *matter* - the *atoms* and *molecules* which interact to produce many different compounds. Fundamental concepts address the atomic and subatomic structure (periodic table), molecular structure (states, bonds, mixtures), reactions (types, energetics, equilibria, kinetics, dynamics), and analytical methods (mass spectrometry, magnetic resonance, diffraction).

Physics is the study of the *physical universe* - *energy*, *matter*, *motion*, *time* and *space*. It deals with celestial bodies, earthly objects, subatomic particles and various energy forms. Fundamental concepts address motion and force laws (velocity, acceleration, power, electro-magnetism); conservation laws (energy, momentum, thermodynamics); and wave laws (light, X-rays).

Biology is the study of *life* - the *structure*, *function* and *inter-relationships* of living organisms. Despite the extraordinary diversity amongst organisms, they show remarkable unity at the molecular and cellular levels, reflecting their common ancestry. Fundamental concepts address molecular biology (biochemical building blocks), cellular biology (membranes, organelles), organismal biology (biodiversity, species richness) and environmental biology (communities, populations, ecosystems).

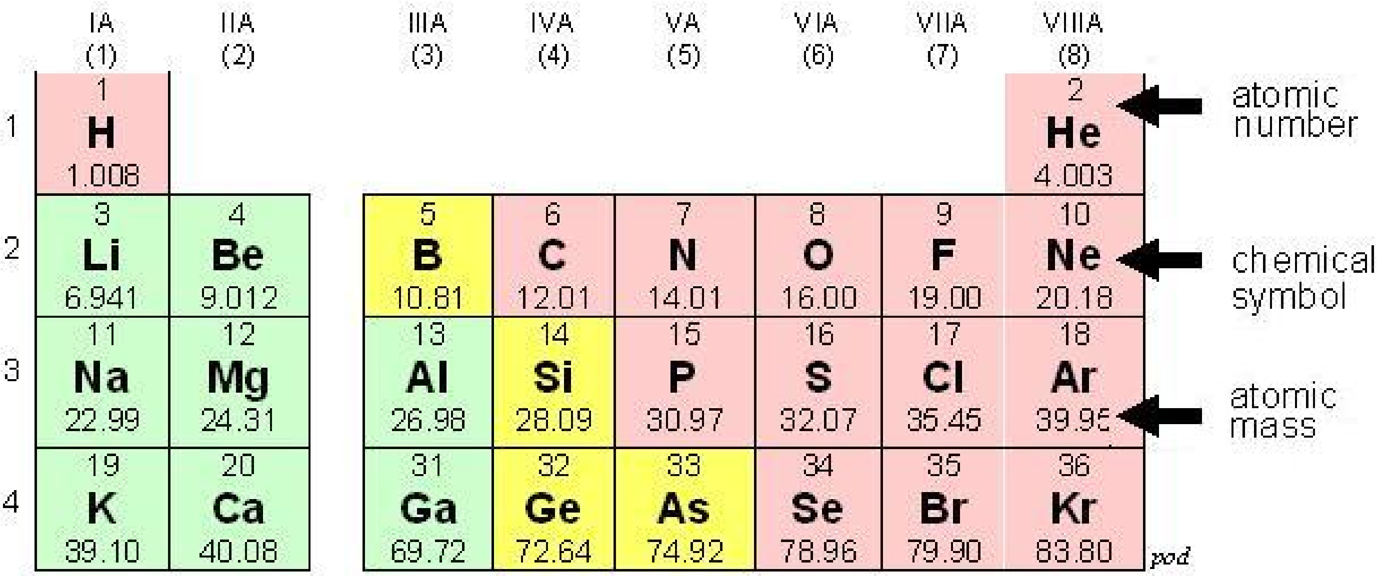
These fields of study are not mutually exclusive: they exhibit manifold inter-relationships. Scientists require an integrated knowledge of matter, energy and life in order to understand and practice *holistic science*. For example, the study of living things requires knowledge of their chemical composition and physical surroundings. Integrated knowledge is evident when considering some of the great fundamental and unifying themes in science:

- **Four fundamental forces hold everything together** - gravity, electromagnetism, the nuclear 'strong' force, and the decay 'weak' force (collectively called the unified field theory).
- **Energy is used to perform work** - it exists in many forms, can be converted from one form to another, and is conserved in closed systems.
- **Chemicals are the building blocks of life** - hydrocarbons dominate on Earth (consistent with carbon-based life forms on a water planet).
- **All life forms have a unique genetic code** which undergoes replication (essential for inheritance) and transcription and translation (essential for protein synthesis and metabolism).
- **Cells are the basic units of life** - all living organisms have microscopic membrane-bound cells containing the genetic material and various organelles for energy transduction.
- **Life-forms co-exist** - populations of organisms collect together in ecosystems where energy flows through while matter is recycled.

4.3 Chemistry: matter and molecules

Chemistry is the science concerned with the study of *matter* - anything that takes up *space* and has *mass*. Matter can exist in three different states: *solid*, *liquid* and *gas*. These states have markedly different characteristics: solids are generally denser than liquids, which in turn are denser than gases; solids have a fixed shape while liquids and gases do not; and solids and liquids have a fixed volume while gases do not. The relationship between *density* ρ, *mass* m and *volume* v is given by $\rho = m/v$ (with appropriate units).

All matter is composed of atoms which have a central *nucleus* (containing *protons* and *neutrons*) surrounded by *electrons*. The atoms of every element have a characteristic number of protons, given as the *atomic number* (shown as a superscript in the periodic table). Every atom also has mass, measured in atomic mass units (amu) (shown as a subscript in the periodic table).



Atomic mass units have been scaled against the carbon-12 (C-12) atom (which was arbitrarily selected as a common solid stable element on Earth), whereby 1 amu equals 1/12 of the mass of a carbon-12 atom. That is, 1 amu $= 1.66 \times 10^{-24}$ g. When this definition is reversed, we obtain 1 g $= 6.022 \times 10^{23}$ amu. As 1 amu $= 1/12$ of the mass of a carbon-12 atom, the number of atoms in 1 g of carbon-12 $= 1/12 \times (6.022 \times 10^{23})$ atoms. This means 12 g of carbon-12 contains 6.022×10^{23} atoms.

Moles

The SI unit for the amount of a substance is the **mole** (mol), which is defined as the amount of substance that contains the same number of specified entities as there are atoms in 12 g of carbon-12; that is, 6.022×10^{23}. This is called *Avogadro's number*; 1 mole of any substance contains this many entities. For example:

- one mole of lead (Pb) contains 6.022×10^{23} atoms of Pb; and
- one mole of carbon dioxide (CO_2) contains 6.022×10^{23} molecules of CO_2.

Obviously, the atomic masses of all these substances differ, but 1 mole of each contains the same number of entities (atoms or molecules). While this may appear cumbersome, it actually allows very simple calculations to be performed without having to revert to complex base units.

Moles can be converted to mass, and vice versa, using their relationship with molar mass (also called molecular mass, formula mass, and sometimes molecular weight). The *molar mass* of a substance is derived from its chemical formula and it equals the combined mass of all the constituent atoms. For example, the molecular formula for ethylene is C_2H_4, comprising 2 carbon and 4 hydrogen atoms. According to the periodic table, carbon atoms have an atomic mass of 12.01 g/mol and hydrogen atoms have an atomic mass of 1.008 g/mol, so the molar mass of ethylene equals

$$(2 \times 12.01) + (4 \times 1.008) = 28.05 \text{ g/mol}.$$

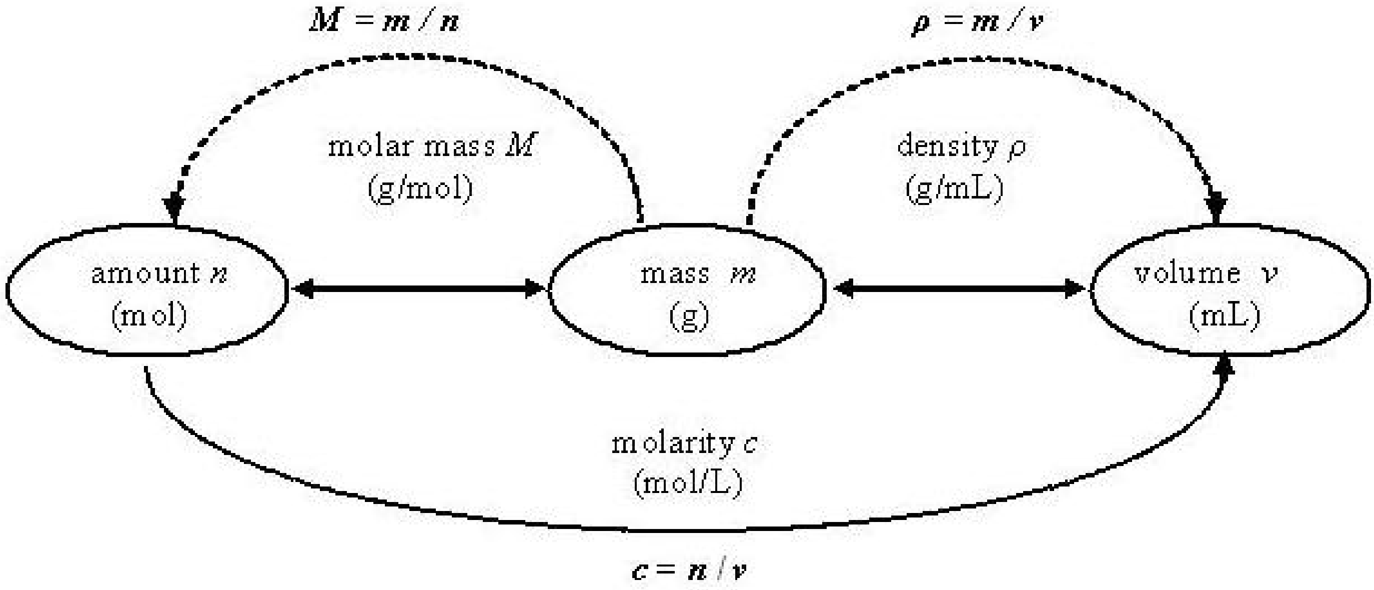
Thus, 1 mole of ethylene weighs 28.05 g. The relationship between number of moles n, mass m and molar mass M, is given by:

$$\text{molar mass (g/mol)} = \text{mass (g)} \ / \ \text{amount (mol)} \qquad (M = m/n)$$

Molarity (or molar concentration) is the unit of concentration used for aqueous solutions. It denotes the amount of substance in a particular volume of solution, expressed as the number of moles of solute per litre of solution (mol/L). For example, a one-molar (1 M) solution of sucrose ($C_{12}H_{22}O_{11}$, molar mass 342.3 g/mol) consists of 342.3 grams of sucrose dissolved in enough water to bring the final total volume to 1 litre. It is often convenient to think of molarity in terms of grams per litre (g/L) where the molar mass of a chemical (g/mol) gives the number of grams required in 1 litre of solution to give a 1 M solution. The formula for molarity is:

$$\text{molarity (mol/L)} = \text{amount (mol)} \ / \ \text{volume (L)} \qquad (c = n/v)$$

We can summarise the relationships between quantity, volume and mass as follows:



By knowing the values for some of these quantities, we can calculate missing values by simple algebraic substitution within the formulae.

Radioactive decay

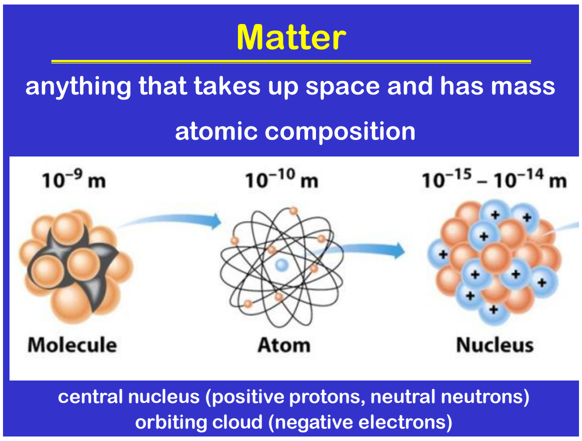
The periodic table lists more than 100 elements according to the number of protons in their nuclei; for example, hydrogen has 1 proton, carbon has 6, and oxygen has 8. However, different *isotopes* of each element can be produced depending on the number of *neutrons* present in the nucleus; for example, 'normal' carbon has 6 protons and 6 neutrons (giving a total 'mass number' of 12 and hence the name carbon-12) compared to carbon-14 which has two extra neutrons.

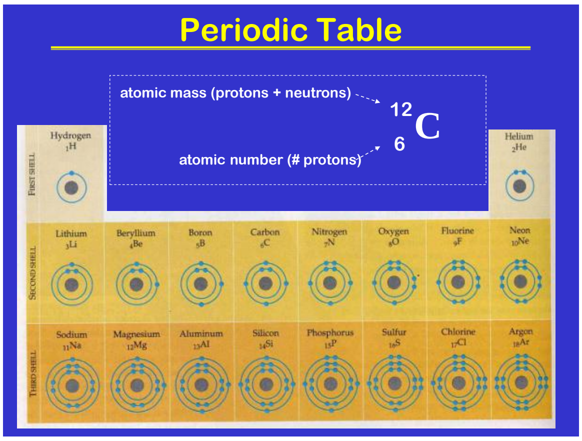
Not all isotopes are stable; many are unstable (*radioactive*) and their structure changes by various means (including neutron-proton replacement, electron capture, alpha decay, and beta decay). While it is impossible to predict exactly when the nucleus of an unstable isotope will change, the statistical likelihood can be calculated and expressed as an exponential decay rate, which gives rise to the notion of *half-life*. The half-life of strontium-90 (Sr-90) is 28.9 years, that of carbon-15 (C-15) is 2.4 seconds, and that of uranium-238 (U-238) is 4.5 billion years.

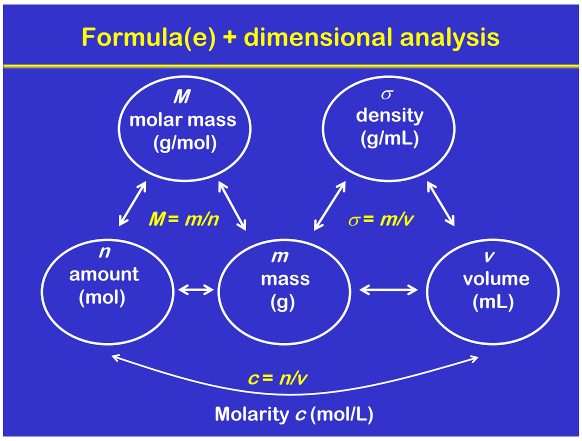
Radiological or *radiometric* dating is a technique which can be applied to determine the age of a geological deposit or an archaeological find. It is based on the rate of decay of radioactive isotopes contained within samples of various substances. Isotopes with long half-lives are used to date rocks and fossils of great antiquity while those with shorter half-lives are used to date younger materials.

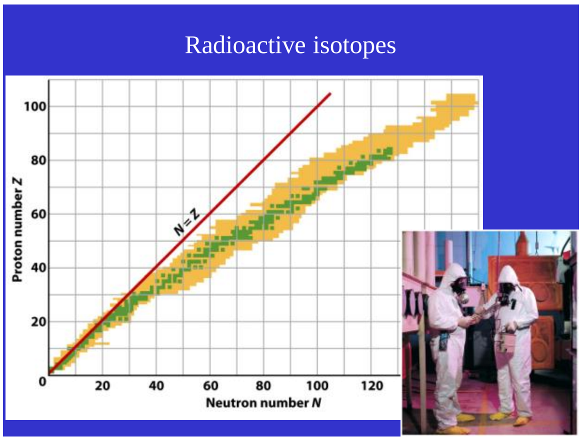
Volcanic rocks often contain potassium-40 (K-40) which decays to argon-40 (Ar-40) with a half-life of 1.25 billion years. From the moment of formation (crystallisation/solidification of molten lava), the parent isotope decays at a constant rate while the daughter isotope becomes trapped and accumulates in the crystal (it is freed only when the rock sample is melted). By determining the ratio of the two isotopes, the age of the rock can be calculated. If there are equal amounts of potassium-40 and argon-40, half the potassium-40 must have decayed so the age of the rock equals the half-life of the isotope (that is, 1.25 billion years). While dateable crystals are usually found in volcanic rock, fossils are usually found in sedimentary rocks. Fossils are therefore often dated indirectly by dating the volcanic rocks that sandwich their strata. Other isotopes used to date rocks include uranium-238 (U-238; half-life of 4.5 billion years) and rubidium-87 (Rb-87; half-life of 49 billion years).

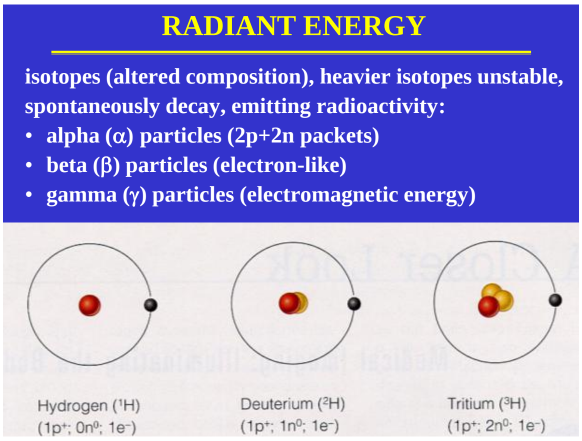
Carbon dating has frequently been used to estimate the ages of many organic relics of human civilisations (such as wooden items, clothing and tools) as well as fragments of biological specimens that are not fossilised (such as bones, hair and teeth). The technique has gained certain notoriety in television dramas about archaeology and forensics, and on shows devoted to investigating scientific 'myths'. The age of organic remains is calculated by comparing the ratio of carbon-14 to carbon-12 in the remains with the ratio in contemporary samples. Living organisms constantly take up carbon from their environments and use it as chemical building blocks. Plants take up carbon from the atmosphere for photosynthesis and animals ingest it as part of their food web. Most carbon consists of the stable isotope carbon-12 but a small amount consists of the unstable isotope carbon-14 which decays with a half-life of 5,730 years. When plants and animals die, they no longer take up fresh supplies of carbon. The amount of carbon-12 in the dead tissues will remain constant while the amount of carbon-14 will decline. Objects more than 50,000 years old, however, have too little carbon-14 left to measure accurately, so this dating scheme cannot be used to date older objects.

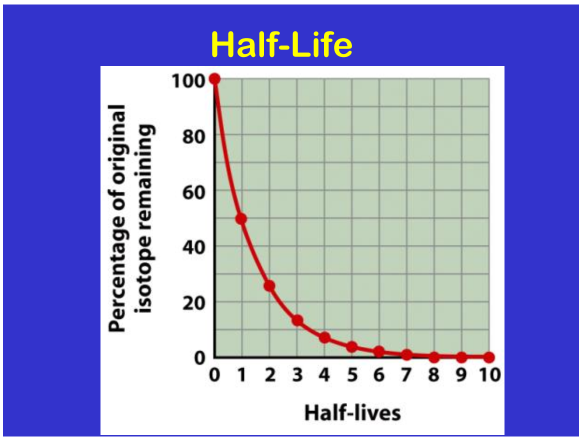

Matter
anything that takes up space and has mass
atomic composition
10^-9 m
10^-10 m
10^-15 – 10^-14 m
Molecule
Atom
Nucleus
central nucleus (positive protons, neutral neutrons)
orbiting cloud (negative electrons)


Periodic Table
atomic mass (protons + neutrons)
12
C
6
atomic number (# protons)
Hydrogen
Helium
Lithium
Beryllium
Boron
Carbon
Nitrogen
Oxygen
Fluorine
Neon
Sodium
Magnesium
Aluminum
Silicon
Phosphorus
Sulfur
Chlorine
Argon


Formula(e) + dimensional analysis
M
molar mass
(g/mol)
σ
density
(g/mL)
M = m/n
σ = m/v
n
amount
(mol)
m
mass
(g)
v
volume
(mL)
c = n/v
Molarity c (mol/L)


Radioactive isotopes
Proton number Z
Neutron number N
N = Z
0
20
40
60
80
100
120


RADIANT ENERGY
isotopes (altered composition), heavier isotopes unstable, spontaneously decay, emitting radioactivity:
• alpha (α) particles (2p+2n packets)
• beta (β) particles (electron-like)
• gamma (γ) particles (electromagnetic energy)
Hydrogen (¹H)
(1p⁺; 0n⁰; 1e⁻)
Deuterium (²H)
(1p⁺; 1n⁰; 1e⁻)
Tritium (³H)
(1p⁺; 2n⁰; 1e⁻)


Half-Life
Percentage of original isotope remaining
Half-lives
0
20
40
60
80
100
0 1 2 3 4 5 6 7 8 9 10

1

Question *4.3.1* The label of a bottle of a chemical such as concentrated hydrochloric acid (HCl) provides information relating to the contents, including the:

- *molar mass* of HCl, in g/mol (also called the *molecular mass* or the obsolete term *molecular weight*);
- *density* of the solution, in g/mL; and
- *concentration* of HCl in the solution, as a % weight/weight.

Laboratories often require solutions of a particular molarity (mol/L) so it is necessary to do a conversion from one unit (%) to another (molarity).

An example of a possible label from a bottle of concentrated HCl is shown below.

320331 Chem-Corp

Hydrochloric acid

Concentrated hydrochloric acid, 32%

Molecular Formula	HCl
Molecular Weight	36.46 g/mol
Density	1.16 g/mL at 25 °C

Note the following formulae:

$$\text{molarity } \; c = \frac{\text{moles of solute } \; n}{\text{litres of solution } \; v}$$

$$\text{molar mass } \; M = \frac{\text{mass of solute } \; m}{\text{moles of solute } \; n}$$

$$\text{density } \; \sigma = \frac{\text{mass } \; m}{\text{volume } \; v}$$

continued...

Question *4.3.1 (continued)* Using the above molar mass, density and concentration information for HCl, derive an equation (including units) to calculate the molarity of the HCl solution.

Question *4.3.2* An inorganic chemist[a] is preparing a solution for an experiment. She needs 750 mL of a 10% v/v (volume per volume) aqueous (water-based) solution of hydrochloric acid (HCl), and she has available 450 mL of 32% v/v aqueous solution of HCl. Write in a system of simultaneous equations the problem of calculating what volumes of 32% HCl and distilled water she needs to mix in order to make her required solution, then solve the equations. Ensure that your answer includes units correctly.

[a]that is, her profession is inorganic chemistry. As a life form, she is organic.

4.4 Physics: motion and energy

Physics is concerned with studying the *physical universe*, including energy, matter, forces, motion, heat, light, time and space. Core fields include astrophysics, classical mechanics, quantum mechanics, thermodynamics, electromagnetism and relativity. Theories hold true within these fields but sometimes not between fields. For example, classical mechanics describes the motion of objects in everyday experience, but breaks down at the atomic scale, where it is superseded by quantum mechanics, and at speeds approaching the speed of light, where relativistic effects become important.

Motion kinematics

Most objects move - they exhibit changes in position over time. This includes inanimate objects (ranging in size from specks of dust to stellar constellations) and animated life-forms (growing plants and motile animals). Movement may be barely perceptible (growing grass), apparently rapid (dragon-fly wingbeats), 'non-visibly' fast (fired bullet) or incomprehensibly astronomical (speed of light). Mankind has observed motion throughout history, and certain relationships have become apparent. The Italian scientist Galileo Galilei (1564-1642) studied moving objects and conducted a series of experiments that helped formalise our knowledge of motion into three concepts: *displacement*, *velocity* and *acceleration*.

Displacement: The relative positions of two objects can be measured using known reference points to create a scale. We commonly refer to the interval between objects as 'distance', measured in SI base units metres. A single object can also change its position or location, and we often refer to this as the distance traveled. However, it is more accurate to use the term *displacement* S, which refers to the *net* change in position.

Velocity: When time is taken into consideration, an object can be perceived to have travelled a specific distance in a particular time interval. We often refer to this as 'speed' and measure it as distance travelled divided by the time taken to travel (with SI derived units metres per second). However, scientists recognised that the *direction* of travel was also important, so they incorporated this into the definition of *velocity* which is the displacement of an object in a particular direction divided by the time taken.

Acceleration: When considering objects in motion, their velocity may also change over time; this change is called *acceleration*, which can be positive (increasing velocity) or negative (decreasing velocity). Acceleration is defined as the change in velocity over time taken. Because this is a rate of change of a rate of change, the units of acceleration are metres per second per second, or metres per second squared (m/s^2).

Newton's Laws

The English scientist Isaac Newton (1642–1727) synthesised the work of Galileo and others into statements of the basic principles that govern the motion of everything in the universe. He developed three fundamental Laws of Motion and one Law of Universal Gravitation.

First Law of Motion: *An object at rest will remain at rest, and an object in motion will remain in motion, unless acted upon by an external force.* This law recognises that things stay the same unless something disrupts that stasis. The tendency to stay unchanged is called *inertia*. It is necessary to apply force to get a stationary object to move, or to change its motion. This law recognises two types of motion: *uniform motion* (velocity), and *changing motion* (acceleration). The force required to produce a change in motion depends on the size of the object as well as its velocity. Objects are said to possess *momentum* p, which is defined as:

$$\text{Momentum (kg m s}^{-1}\text{)} = \text{mass (kg)} \times \text{velocity (m/s)} \qquad (p = mv)$$

Second Law of Motion: *The acceleration of an object is directly proportional to the force applied to it, and inversely proportional to its mass.* This law extends the concept of force being necessary to change motion. Applying force to an object causes acceleration; the greater the force, the greater the acceleration. However, greater force is required to accelerate larger objects because of their greater mass. These relationships are given in the definition of force as follows (note that the units are kilogram metres per second squared, where one kg m s^{-2} is called the *newton*, N):

$$\text{Force (newtons, N)} = \text{mass (kg)} \times \text{acceleration (m/s}^2\text{)} \qquad (F = ma)$$

Third Law of Motion: *For every action, there is an equal and opposite reaction.* This law may be less intuitive than the others. We tend to think of our world in terms of causes and effects rather than opposing reactions. We think of the forceful damage done to a car when it hits a tree, rather than the tree providing an opposing force to stop the car. Forces always act simultaneously in pairs. Your weight is exerting a force on your chair, while your chair is exerting an equal and opposite force to support you. Indeed, your weight is a measure of the force required to counter-balance the gravitational pull of the Earth on your body. At the surface of Earth, if an object is dropped and allowed to fall freely, it will accelerate at a rate known as *the acceleration due to gravity* g, with $g = 9.8$ m s^{-2}.

Newton's Law of Universal Gravitation: *The attractive force between any two objects, called* gravity, *is proportional to the product of their masses and inversely proportional to the square of the distance between them.* Gravitational forces are found throughout the universe between any two objects:

$$F = \frac{G \times m_1 \times m_2}{d^2}$$

The constant G is called the *universal gravitational constant*, and its units are m^3 s^{-2} kg^{-1} (or N m^2 kg^{-2}). In 1798, Henry Cavendish (1731–1810) first measured G in an experiment where he suspended small lead balls near large fixed lead spheres and measured the twisting force (torque) on the suspension wire. He obtained the value for $G = 6.67 \times 10^{-11}$ m^3 s^{-2} kg^{-1}.

Energy

Energy is defined as the *ability to do work.* It exists in several forms, as:

- *potential* energy (stored energy);
- *kinetic* energy (associated with movement);
- *radiant* energy (associated with light);
- *thermal* energy or *heat* (kinetic energy of atoms and molecules);
- *chemical* energy (stored in the bonds between atoms); and
- *nuclear* energy (bound within the nucleus of an atom).

Energy may be converted from one form to another, such as radiant energy from the sun being converted to heat, and the potential energy in a battery being converted to light in a torch. One of the most important laws of science is the *law of conservation of energy* (also called the *First Law of Thermodynamics*) which states that, *even though energy can be converted from one form to another, the total amount of energy in a closed system remains constant.*

Energy can be used to perform work. Muscles use chemical energy to enable movement, and domestic appliances use electrical energy to heat water and cook food. Work is defined as the application of energy over distance, according to the formula:

$$\text{Work (joules)} = \text{force (newtons)} \times \text{distance (m)} \qquad (W = Fd)$$

In the metric system, force is measured in newtons (N) and work is measured in newton metres (N m) or *joules*. One joule is defined as the *amount of work done when a force of one newton is exerted through a distance of one metre*.

The measurement of force conforms to Newton's second law of motion, which states that force is proportional to mass times acceleration:

$$\text{Force (newton)} = \text{mass (kg)} \times \text{acceleration (m s}^{-2}\text{)} \qquad (F = ma)$$

Another dimension is added to the concept of doing work (or utilising energy) when we introduce a temporal element, that is, the *time taken to do work*. The *rate at which energy is used* is called *power*, and is defined as the *amount of work done divided by time*:

$$\text{Power (watts)} = \text{work (joules) / time (s)} \qquad (P = W/t)$$

In the metric system, the unit of measurement for power is the *watt*, named after the inventor of the steam engine. One watt is defined as the *expenditure of one joule of energy in one second*. The formula for power can be restated as:

$$\text{work, or energy (joules)} = \text{power (watts)} \times \text{time (s)}$$

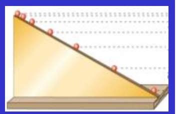
This equation is used by power companies to calculate and charge for energy consumption. They transform the units of power from watts to kilowatts and the units of time from seconds to hours, thus deriving units of kilowatt hours (kW h) which appear on electricity bills.

Galileo (1564-1642)

formalized motion kinematics

distance
[displacement, ΔS]
(m)

speed
[velocity, $\Delta S / \Delta t$]
(m/s)



acceleration
[rate of change in velocity, $\Delta v / \Delta t$]
(m/s^2)

Newton (1642-1727)

developed fundamental Laws of Motion

1. INERTIA: an object in motion will remain in motion, and an object at rest will stay at rest, unless acted upon by an external force
   [momentum = mass x velocity]
2. ACCELERATION: acceleration of an object is directly proportional to the force applied, and inversely proportional to its mass
   [force = mass x acceleration]
3. REACTION: for every action, there is an equal and opposite reaction
   [gravity = 9.8 $m.s^{-2}$]

Energy

defined as the ability to do work

- potential energy (stored)
- kinetic energy (of motion)
- thermal energy (heat)
- chemical energy (stored in bonds between atoms)
- nuclear energy (bound within nucleus of atom)
- electromagnetic energy (electricity, magnetism, light, X-rays, microwaves, radio waves, etc)

POWER (kW = kWh/d)

Does it make sense in terms of SI units?

FORCE: Newton's second law of motion
Force (newtons) = mass (kg) x acceleration ($m\ s^{-2}$) [1 kg m s^{-2} = 1 N]

WORK: application of energy over distance
Work, energy (joules) = force (N) x distance (m) [1 N m = 1 J]

POWER: rate of energy usage
Power (watts) = work, energy (J) / time (s) [1 J s^{-1} = 1 W]
[1 J = 1 Ws]

Energy is a quantity (measured in J or kWh) [1kWh = 3.6 million J]
Power is a rate (measured in W or kWh/d) [1 kW = 24 kWh/d]
[1 kWh/d = 1000 Wh / 24 h = 40 W]

Australian CO_2 emissions

World emission ~ 30 $GtCO_2$e/y
(population of 6 billion, ⇒ ~ 5 $tonsCO_2$e/y per person)

BUT, not all countries are equal

Australian emission ~ 0.5 $GtCO_2$e/y
(population of 20 million, ⇒ ~ 25 $tonsCO_2$e/y per person)

Regrettably, we are the champions!!!
Ranked fourth in world (behind Qatar, UAE & Kuwait)
(worse than USA & Canada)

WHY? Life-style, tyranny of distance, over-reliance of coal

Australian power consumption

Australians emit ~ 25 $tonsCO_2$e/y per person
Equates to:
Power consumption = rate of energy use
= 7.9 kW pp [1 kW = 24 kWh/d]
= 190 kWh/d pp

Sources:
- fossil fuels (coal, gas, oil)
- renewables (hydroelectricity, solar, wind)
- other (nuclear)

Consumption:
- most as electricity (domestic/industrial power)
- internal combustion engines (automotive power)

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Energy consumption (Australia)

TOTAL 190 kWh/d per person

Cars	
Planes	
Household	
Lighting	
Gadjets	
Food/farming	
Manufacturing	
Public services	

Energy consumption: cars

Consider average daily use of car

Fuel calorific value = 10 kWh/L

$$\text{Energy per day} = \frac{\text{distance travelled per day}}{\text{distance per unit fuel}} \times \text{energy per unit fuel}$$

$$= \frac{50 \text{ km/day}}{12 \text{ km/L}} \times 10 \text{ kWh/L}$$

$$= 40 \text{ kWh/d}$$

Energy consumption: planes

Boeing 747 uses 200,000 L fuel to carry 400 passengers a distance of 14,000 km [fuel calorific value = 10 kWh/L]

Energy used for single return flight once per year

$$= \frac{\text{distance travelled per day}}{\text{distance per unit fuel per person}} \times \text{energy per unit fuel}$$

$$= \frac{(2 \times 14{,}000 \text{ km}) / 365 \text{ days}}{(2 \times 14{,}000 \text{ km}) / [(2 \times 200{,}000 \text{ L}) / 400 \text{ persons}]} \times 10 \text{ kWh/L}$$

$= 27$ kWh/d per person

Energy consumption: household

$E_{hot\text{-}water}$ = heat capacity x volume x temperature difference

E_{shower} = 4200 J/L/°C x 30 L x (50-10)°C = 5 MJ (= 1.4 kWh)

Energy used for one 5 minute shower per day = 1.4/12 = 0.1 kWh/d]

Energy used by electric kettle per day = power x time used per day
= 3 kW x 0.5 h/d = 1.5 kWh/d

Cooking (stove, oven, microwave, kettle) (~3kW appliances) = 5 kWh/d
Cleaning (bathing, washer/dryer, dishwasher) (~2.5 kW) = 5 kWh/d
Cooling (refrigerator, freezer) (0.1 kW) = 2 kWh/d
Air-conditioning (heating/cooling) (1 kW) = 24 kWh/d

TOTAL = 36 kWh/d

Energy consumption: light

Average home uses ~ 20 globes for 6 hours per day
- 10 incandescent globes require 1 kW power
- 10 low-energy globes require 0.1 kW power

Energy used per day for:

household lighting = (power x time) / av. no. people per home
= (1.1 Kw x 6 h/d) / 2
= 3.3 kWh/d

workplace lighting = 1.6 kWh/d
street lighting = 0.1 kWh/d

TOTAL = 5 kWh/d

Energy consumption: gadjets

Appliance with power rating of 40 W = 1 kWh/d
but only used for fraction of each day

	quantity (no.)	x	rating (W)	=	sum (kW)	x	usage (h/d)	=	Power (kWh/d)
Computer/printer	2		100		0.2		4		0.8
TV/DVD/VCR	2		100		0.2		3		0.6
Xbox/PS/Wii	2		200		0.4		2		0.8
CD/stereo/radio	2		100		0.2		2		0.4
Chargers (phone,…)	4		5		0.02		24		0.5
Vacuum cleaner	1		1600		1.6		1		1.6
Lawn mower	1								0.3

TOTAL = 5 kWh/d

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Energy consumption: food/farming

One 65 kg person uses 2,600 Calories per day (= 2.6 million calories) ~ 3 kWh/d

Item	Consumption – Production	Power
milk, cheese	consume 0.75 L/d, 450 kg cow produces 16 L/d, uses 450 x 3/65 kWh/d (0.75/16 x 450 x 3/65)	1 kWh/d
eggs	eat 2 eggs/d, chicken lays 290 eggs/yr, eat 120 g/d @ 3.3 kWh/kg (2 x 365/290 x 0.12 x 3.3)	1 kWh/d
meat	eat 100 g/d each of chicken, beef and pork, (50, 1000 & 400 days nurture @ 3/65 kWh/d/kg)	7 kWh/d
fruit/vegies	eat 250 g/d, 200 days nurture @ 3/130 kWh/d/kg	1 kWh/d
pets	cats, dogs and horses, 1 per 10 persons	3 kWh/d
TOTAL		13 kWh/d

Energy consumption: manufacturing

Item	Consumption x embodied production cost	Power
drink containers (aluminum cans/bottles)	5 units/d @ 0.6 kWh/unit	3 kWh/d
packaging (glass/paper/plastic/steel)	0.4 kg/d @ 10 kWh/kg	4 kWh/d
computer (1 every 2 years)	1/(2x365) unit/d @ 1500kWh/unit	2 kWh/d
print (newspapers/magazines/junk mail)	0 .2 kg/d @ 10 kWh/kg	2 kWh/d
house (1 every 100 years, 2.3 persons)	1/(100x365x2.3) @ 84000	1 kWh/d
car (1 every 15 years)	1/(15x365) units/d @ 76000 kWh/unit	14 kWh/d
roads (building/upkeep over 50 yrs)	1/(50x365) m/d @ 36000 kWh/m	2 kWh/d
road transport	51billion t-km / (365 x 20 million pop) @ 1 kWh/t-km	7 kWh/d
shipping	2000billion t-km / (365 x 20million pop) @ 0.015kWh/t-km	4 kWh/d
water treatment	160 L/d @ 0.002 kWh/L	0.3 kWh/d
sewage treatment	100L/d @ 0.002 kWh/L	0.2 kWh/d
supermarkets	5000 units / (365 x 20 million) @ 3.6 GWh/unit	0.5 kWh/d
imports (55 million tonnes per yr)	2 kg/d @ 10 kWh/kg	20 kWh/d
TOTAL		60 kWh/d

Energy consumption: public services

Australian government annual budget $560 billion (GDP)

Energy consumption greatest in ADF

3.2% GDP spent on defence = $18 billion

25% spent on energy = $4.5 billion
@ 14.8cents/kWh = 30 billion kWh per year
= 83 million kWh per day

Population of 20 million
gives 4 kWh/d per person

Energy consumption (Oz)

	kWh/d per person
Cars	40
Planes	27
Household	36
Lighting	5
Gadjets	5
Food/farming	13
Manufacturing	60
Public services	4
TOTAL	190

Renewable power production (Aust.)

SOURCE		kWh/d per person
Fossil fuels	coal, gas, oil	6
Wind	onshore	20
	offshore shallow	15
	offshore deep	30
Solar	thermal	12
	photovoltaic	5
	biomass	33
Hydroelectricity	lowland	8
	highland	3
Wave	oceanic	5
Tide	coastal	15
Geothermal	crust	2
TOTAL		154

Power deficit

Total power production 154 kWh/d per person

Total power consumption 190 kWh/d per person

Deficit 36 kWh/d per person

Where will it come from?
What sources are left?

Nuclear energy (fission, fusion) 1-420

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Question *4.4.1* Later in semester we will study the HyShot rocket project, initiated by UQ scientists to help develop hypersonic flight. On one HyShot launch, a rocket reached a height of 330 km above the surface of Earth. Find the acceleration due to gravity at that height. (Hint: the mass of Earth is $M_e \approx 5.97 \times 10^{24}$ kg and the radius of Earth is $R_e \approx 6.37 \times 10^6$ m. Use units in your calculations.)

4.5 Biology: living organisms

Biology is the science concerned with the *study of life* - the structure, function and co-existence of living organisms. Matter and energy are both vitally important to living organisms, providing substance and sustenance. Living organisms are carbon- and water-based cellular forms, with complex organisation and heritable genetic information. They undergo metabolism, possess a capacity to grow, respond to stimuli, reproduce and, through natural selection, adapt to their environment in successive generations. Living organisms could be described as 'self-replicating, membrane-bound, microscopic bags of sugary, proteinaceous water'.

1. **Why bags?** Cells are the basic units of life. These bags preserve the structural integrity of the organism and maintain the boundary between the external and internal environments. Many life forms persist as unicellular organisms, while others exist as complex multicellular organisms with aggregates of cells forming specialised tissues and organs. All cells exhibit three basic features:
   - they are bound by cytoskeletal elements (to provide form, and sometimes motility);
   - they have internal organelle systems (to meet metabolic and developmental requirements); and
   - they have centralised genetic material (to process information).
2. **Why microscopic?** Living organisms exist as a wide range of sizes. Compare the sizes of giant redwoods, blue whales, dogs, mushrooms, plankton, algae, amoebas, and bacteria. They occur over 8 orders of magnitude, from 1 μm (10^{-6} m) to 100 m (10^{2} m). However, their constituent cells only range in size over 2 orders of magnitude, from 1 to 100 μm. Cells are limited to microscopic sizes in order to maintain high surface-to-volume ratios so that molecules can move throughout the whole cell. Even though molecular transport processes may involve *diffusion* (random movement down concentration gradients towards equilibrium), *passive transport* (facilitated diffusion through specific channels), or *active transport* (energy-dependent movement against concentration gradient using carrier protein/transporter/pump), they are only effective over microscopic distances.
3. **Why water?** Water is the fluid of life! Many cells are composed of 70–95% water. The molecule H_2O has many unique properties. Due to its nonlinear shape, it has a polar charge that contributes to its *cohesive* (binding) and *adhesive* (wetting) properties. It has three physical states under prevailing climatic conditions: gas (water vapour), liquid (oceans, lakes) and solid (ice).

Water has a high specific heat due to its kinetic energy and acts as a thermal bank to stabilise temperatures. Water has remarkable chemical properties which allow it to function as a reactant (able to hydrolyse chemical reactions) and as a universal solvent (able to dissolve salts, sugars, and many proteins).

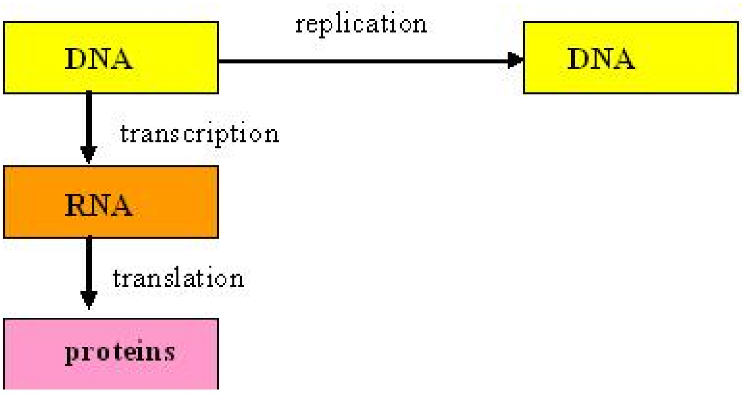
Atoms in water may occasionally lose or gain electrons, resulting in the dissociation of the molecule into positively charged hydrogen ions (H^+) and negatively charged hydroxide ions (OH^-). The relative ratio of these ions contributes to the acid-base balance of a solution. In any aqueous solution, the product of H^+ and OH^- concentrations is constant at 10^{-14}, written as the equation $[H^+]\,[OH^-] = 10^{-14}$, where square brackets indicate molar concentrations (mol L^{-1}). In a neutral solution, both $[H^+]$ and $[OH^-]$ equal 10^{-7}, so as expected the product is 10^{-14}. If acid is added to increase $[H^+]$ to 10^{-6}, then $[OH^-]$ will decrease proportionately to 10^{-8}. Because ion concentrations can vary by a factor of 10^{12} or more, scientists used logarithms to compress this variation into the pH scale, defined as the negative logarithm of the hydrogen ion concentration, so $\text{pH} = -\log[H^+]$. For a neutral solution, $[H^+]$ is 10^{-7} M, thus giving $\text{pH} = -\log 10^{-7} = -(-7) = 7$. Notice that pH decreases as $[H^+]$ increases, meaning acids have low pH whereas bases have high pH. Most biological fluids are in the range pH 6-8.

4. **Why membrane-bound?** Cells must be structurally bound by substances that are insoluble in water. Lipids (fats) provide those substances, as most lipids are insoluble. They are composed of long chain fatty acids attached to a glycerol core. In modern society, fats are perceived to be bad things, associated with obesity and chronic disease. However, lipids serve many essential functions: triglycerides and lipoproteins act as energy stores, cholesterol is the precursor of many steroid hormones, and phospholipids form membranes. They are essential building blocks, and all cell membranes are composed of phospholipid bilayers. These polar molecules have hydrophilic heads and hydrophobic tails, which become assembled into bilayered sheets, forming the core of all cell membranes.

5. **Why proteinaceous?** Cells require many chemicals for metabolic processes, development and multiplication. The basic building blocks are *proteins*, which are polymeric molecules composed of chains of amino acids. While the numbers of proteins found in a cell may run into the hundreds of thousands, they are all formed from the same set of 20 amino acids. Proteins vary extensively in structure, each type having a unique three-dimensional shape due to four levels of conformational complexity: amino acid sequence (primary), coiling (secondary), folding (tertiary) and combination (quaternary).

6. **Why sugary?** Carbohydrates include monosaccharides (simple sugars), disaccharides (double sugars) and polysaccharides (polymers). They are all rich sources of chemical energy (stored in their molecular bonds) and their carbon skeletons serve as raw materials for the synthesis of other molecules, including amino acids (proteins) and fatty acids (lipids). Glucose ($C_6H_{12}O_6$) is the most common sugar involved in the chemistry of life. It is produced as an energy source through photosynthesis by plants, and it is ingested by animals for glycolysis via *aerobic metabolism* (literally, burning sugar in the presence of oxygen to yield energy). It is therefore a vital fuel for many living organisms, and its cellular uptake is tightly regulated by various hormonal homeostatic mechanisms (insulin and glucagon in humans).

7. **Why self-replicating?** All life forms have limited life spans and ultimately die (their components effectively wear out). They must therefore replicate themselves in order for their species to survive. Whether cells multiply asexually (mitosis) or sexually (meiosis), they essentially copy their genetic codes spelt out by the nucleotide sequences of their DNA (deoxyribonucleic acid). DNA is a linear polymer composed of four nucleotides: the purines, adenine (A) and guanine (G), and the pyrimidines, cytosine (C) and thymine (T) (T is substituted by uracil (U) in RNA). Two strands of DNA are wound together in a double helix, such that only complementary bases are aligned (G aligns only with C, and A only with T). The central dogma of life is that of DNA replication, for it facilitates inheritance and metabolism (through DNA transcription to RNA and its translation to proteins).



Collective co-existence

There are many levels of biological organisation, from miniscule to majestic. We have examined molecules (building blocks of matter) and cells (basic units of life). We know living things range from single-celled organisms (simple, but by no means primitive) to multicellular organisms (with cellular specialisation to form complex tissues and organs).

We also recognise several levels of collective co-existence, where organisms live together in:

- **populations** (all the individuals of one species within a given area);
- **communities** (all species of living organisms within a given area);
- **ecosystems** (all living things within a given area, together with all the non-living components in that area with which life interacts); and the
- **biosphere** (all the environments on Earth inhabited by life).

The definitions of these collective concepts have elastic boundaries, so the area of study must be specified. For example, ecosystems can vary in size from an aquarium to a lake, meadow, mountain range or continent.

The dynamics of all ecosystems include two major processes: *nutrient cycling*; and *energy flow*. Nutrients are constantly recycled within ecosystems. They are used to build organic materials which subsequently degrade, releasing them back into the system. All chemical elements (such as carbon and nitrogen) pass through complex cycles which incorporate both living and nonliving parts of an ecosystem. In contrast, energy constantly flows into an ecosystem (usually as sunlight), where it is converted to chemical energy by *producers* (usually photosynthetic organisms) and utilised by *consumers* (herbivores and carnivores) and *decomposers* (microbes). Ecosystems are therefore said to *recycle matter while energy flows through*.

Ecology is the *study of interactions between organisms and their environments* - a holistic science involving many disciplines. Ecologists study organismal biodiversity, distribution and abundance (species richness, temporal and spatial variation) with respect to biotic and abiotic (environmental) influences. In particular, human activities can have profound ecological effects, whether accidental (like oil spills), deliberate (urban development) or unintended (acid rain, global warming). Key areas of ecological research include:

- **Ecosystem ecology**, emphasising energy flow and chemical cycling among the various biotic and abiotic components;
- **Community ecology**, dealing with the interactions between the whole array of species in a community, including competition, predation, herbivory, symbiosis, and disease; and
- **Population ecology**, concentrating mainly on factors that affect how many individuals of a particular species live in an area.

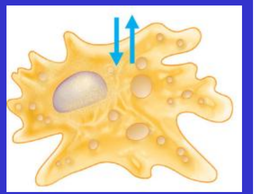
BIOLOGY

the study of life

molecular biology
cellular biology
organismal biology
population biology
environmental biology

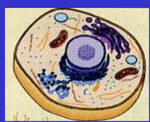
Living organisms are:

- self-replicating,
- membrane-bound,
- microscopic
- bags of
- sugary,
- proteinaceous
- water



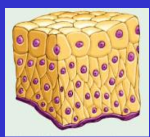
Why bags?

Cells are basic units of life
- preserve structural integrity
- maintain boundary between internal & external environments



unicellular

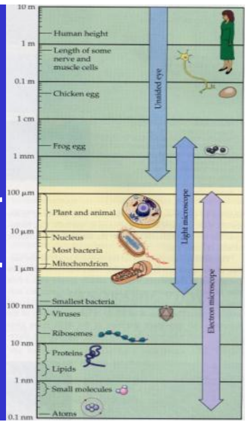
Cells possess:
- internal cytoskeletal elements
- internal organelle systems
- centralized genetic material



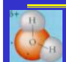
multicellular

Why microscopic?

- cells 1-100 μm (note log scale)
- need to preserve high surface-to-volume ratio (for efficient molecular transport)
- imagine cell as cube [double length involves 4-fold change in area and 8-fold change in volume]



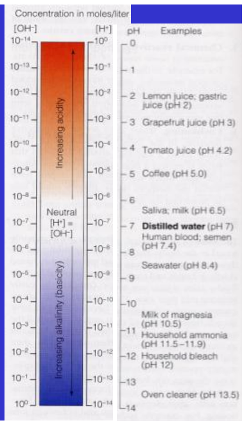
Why water?



fantastic molecule
- polar charge (adhesion/cohesion)
- universal solvent (dissolve electrolytes, sugars, proteins, etc)
- biochemical reactant (hydrolysis)

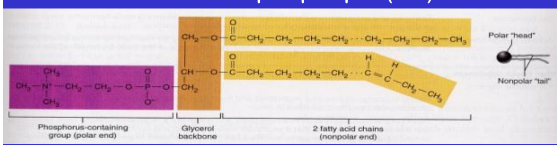
H_2O dissociation into ions
acid-base balance
$[H^+]\,[OH^-] = 10^{-14}$

cumbersome, so developed
pH scale = -log [H^+]
physiological saline pH 7.4

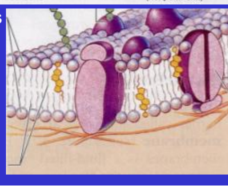


Why membrane-bound?

- membranes hold cells together
- made of insoluble phospholipids (fats)



polar heads
phospholipid bilayer
nonpolar tails



semipermeable membrane

plus embedded proteins, sugars, cholesterol, filaments

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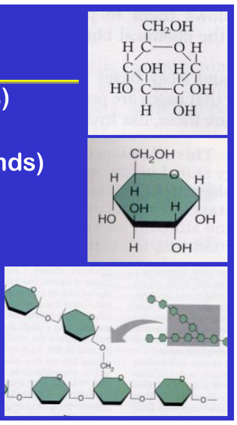
Why sugar?

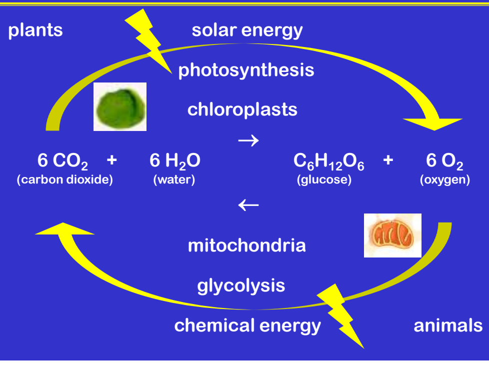
carbo-hydrates (sugars)
rich source of energy
(stored in molecular bonds)

glucose $C_6H_{12}O_6$

- produced by plants (photosynthesis)
- used by animals (glycolysis)
- stored as glycogen

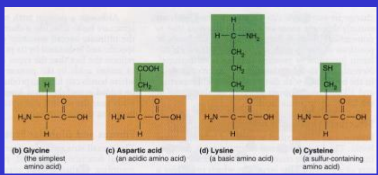


Energy flow (it's a plastid world)



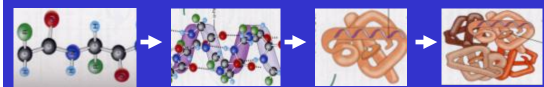
Why proteinaceous?

Building blocks of life (structural, functional)
polymers composed of chains of amino acids



20 amino acids produced

chains with 3D structure



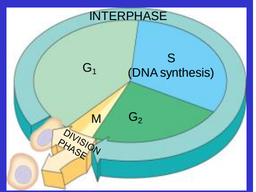
primary (chain) → secondary (coil) → tertiary (fold) → quaternary

Why self-replicating?

Cells not immortal (need to grow and divide)

Cell cycle

- interphase (G1, S, G2)
- division phase (M)



Type of division

- asexual (1 → 2)
  - mitosis, fission, budding, endogeny
- sexual (1+1 → 2)
  - meiosis (haploid gametes combine)

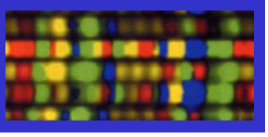
Cellular basis of life

Central dogma:

- flow of genetic information is unidirectional

$$\text{DNA} \xrightarrow{\text{transcription}} \text{RNA} \xrightarrow{\text{translation}} \text{Protein}$$

$$\text{DNA} \xrightarrow{\text{replication}} \text{DNA}$$



LIFE on Earth

- chemical basis (carbon-based life on water-planet)
  - proteins, sugars, fats, nucleotides
- genetic code (DNA)
  - replication, transcription, translation
  - four bases (2 bit (binary digit) code)
- cellular organization (membranes, organelles, nuclei)
  - basic units of life
- evolution (natural selection, survival of fittest)
  - mutation, recombination
- symbioses (living together)
  - organelles (SET)
  - organisms (life styles)

→ collective co-existence (ecology)

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***Question** 4.5.1* Cells are the basic units of all life-forms.

(a) Why are cells constrained to microscopic sizes? What would you predict about their surface area to volume ratio?

(b) Calculate algebraically the surface area to volume ratio of a (model) cell in the shape of a cube. What happens to this ratio if the side-length of the cell doubles? What happens with a 10-fold increase?

(c) What structural adaptations have cells adopted to maintain optimal ratios?

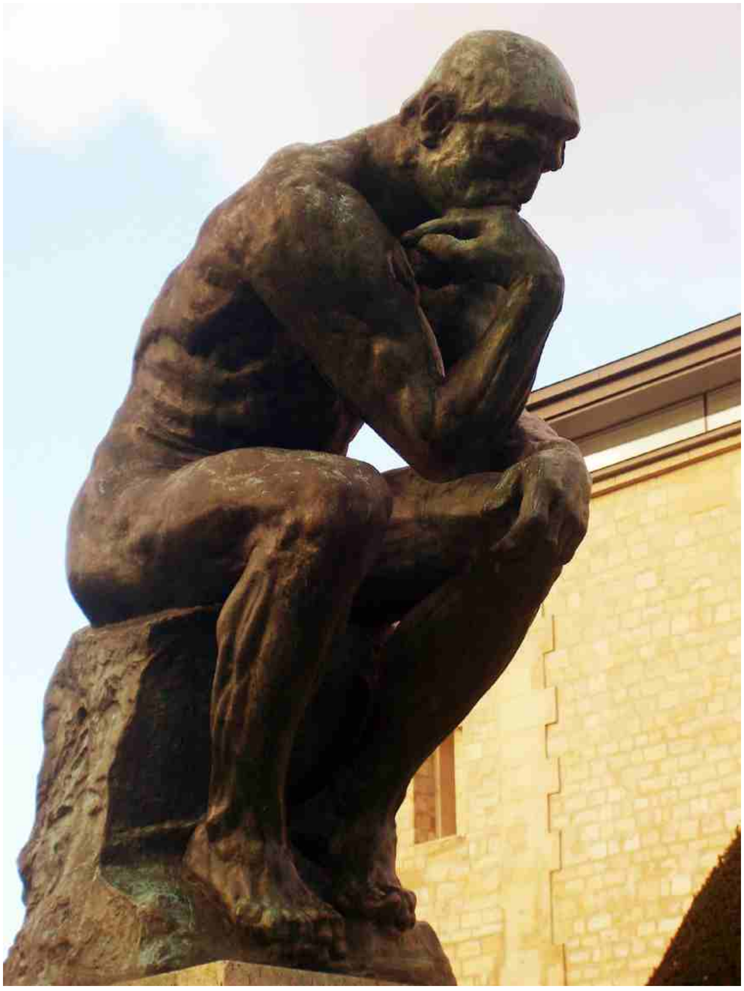
4.6 Space for additional notes

5 Quantitative reasoning

Our galaxy itself contains a hundred billion stars.
It's a hundred thousand light years side to side.
It bulges in the middle, sixteen thousand light years thick,
But out by us, it's just three thousand light years wide.
We're thirty thousand light years from galactic central point.
We go 'round every two hundred million years,
And our galaxy is only one of millions of billions
In this amazing and expanding universe.

The universe itself keeps on expanding and expanding
In all of the directions it can whizz
As fast as it can go, at the speed of light, you know,
Twelve million miles a minute, and that's the fastest speed there is.
So remember, when you're feeling very small and insecure,
How amazingly unlikely is your birth,
And pray that there's intelligent life somewhere up in space,
'Cause there's bugger all down here on Earth.

Artist: Monty Python
(www.youtube.com/watch?v=buqtdpuZxvk)



The Thinker (1879 – 1888), Auguste Rodin (1840 – 1917), Musee Rodin, Paris. (Image source: en.wikipedia.org/wiki/File:The_Thinker_close.jpg)

Introduction

One of the most important activities in almost every profession is communicating, both verbally and in written form. Clear and accurate communication is particularly important in science-based disciplines, whether you work in research, education or industry.

A large amount of science relies heavily on mathematics and statistics, and most scientific advances are based on quantitative evidence. For example, each time you visit a doctor (or see a patient if you are a doctor), it is almost certain that the conversation and recommendations will make direct or indirect use of quantitative facts and analysis. (For example, most people in this room either already have sought, or will in the future seek, answers to questions like: what are the chances of pregnancy if a sexually active woman uses an oral contraceptive; what is the likelihood of suffering a significant harmful side effect from the contraceptive; and what are the relative risks and benefits of choosing a longer-term contraceptive injection instead?)

As a producer of quantitative scientific communication, you should take care that your communication is honest, unambiguous and precise, and that you always use appropriate units. As a consumer of such information, you should always critically evaluate the content, maintaining a healthy scepticism (note that 'healthy' means questioning claims and statements, while at the same time accepting evidence even if it is counter to your beliefs or preconceptions).

Some of the examples/contexts we will discuss are:

- Health practitioners, patients and mathematics.
- Breast cancer.
- Media reports.

Specific techniques and concepts we will cover include:

- Estimation.
- Critical evaluation.

5.1 Quantitative communication

- In SCIE1000 we will investigate some of the fundamental skills and concepts that will help you to participate in effective scientific analysis and communication.
- We are all producers and consumers of quantitative scientific information:
  - we produce it (for example) in scientific papers, assignments, lecture notes, exam answers and professional communications such as doctor/patient discussions.
  - we consume it (for example) in scientific papers, the classroom, media reports and when we visit a doctor.
- As a *producer* of such information, we should aspire to be concise, precise, accurate, honest, logical, unambiguous, not excessively technical, use appropriate units and always mindful of the intended audience.
- As a *consumer* of such information, we should aspire to be thoughtful, reflective, sceptical, logical and analytical, while at the same time open-minded and accepting of evidence which may differ from our preconceptions or opinions.
- The media and internet provide a continual bombardment of facts, reports, summaries, interpretations and opinions, often covering sophisticated concepts but written and read by non-experts. In many cases there are errors (or deliberate falsities)in such communications.
- Two approaches to identifying errors or false claims are:
  - estimation and
  - critical evaluation.
- You should apply these when doing your own work, and also when using material from other sources.

5.2 Estimation

- **Estimation** (or *back-of-the-envelope calculations*, or *rough estimation*) is the process of calculating approximate values.
- Estimating relies on building rough, conceptual models which can either be evaluated mentally or using simple calculations.
- Estimating 'gives an idea' whether a particular value is plausible. Often, the aim is for the approximate value to be within an *order of magnitude* of the correct value (that is, within a factor of 10).
- Estimation problems are sometimes called *Fermi problems*.

***Question** 5.2.1* Develop approaches that allow you to **roughly** estimate answers to each of the following Fermi problems, then estimate the value.

(a) Each year, around 4×10^7 kg of space dust lands on earth. Roughly estimate the amount of space dust which lands on your head during your lifetime.

continued...

Question *5.2.1 (continued)*

(b) Measurements of various processes within the body are crucial health indicators. Estimate the total volume of blood pumped by your heart each day.

(c) Estimate the mass of a large storm cloud.

continued...

Question *5.2.1 (continued)*

(d) The change in a population size over a given time period equals

$$\text{births} - \text{deaths} + \text{immigration} - \text{emigration.}$$

If migration is ignored, the calculated quantity is called the *rate of natural increase* of the population. Estimate the number of births and deaths in Australia each year.

(e) After consuming alcohol, Blood Alcohol Concentration (BAC) is influenced by such factors as: volume of alcohol consumed, time since consumption and the water % of the body (because alcohol is water-soluble, but is not fat-soluble). Estimate the water % of a 'typical' human body. (Forensic science units need to do this.)

5.3 Critical evaluation

The Wikipedia[a] entry on **critical thinking** says:

"*Critical thinking is the purposeful and reflective judgment about what to believe or what to do in response to observations, experience, verbal or written expressions, or arguments. Critical thinking involves determining the meaning and significance of what is observed or expressed, or, concerning a given inference or argument, determining whether there is adequate justification to accept the conclusion as true... Parker and Moore define it more naturally as the careful, deliberate determination of whether one should accept, reject, or suspend judgment about a claim and the degree of confidence with which one accepts or rejects it.*

Critical thinking gives due consideration to the evidence, the context of judgment, the relevant criteria for making the judgment well, the applicable methods or techniques for forming the judgment, and the applicable theoretical constructs for understanding the problem and the question at hand. Critical thinking employs not only logic but broad intellectual criteria such as clarity, credibility, accuracy, precision, relevance, depth, breadth, significance and fairness."

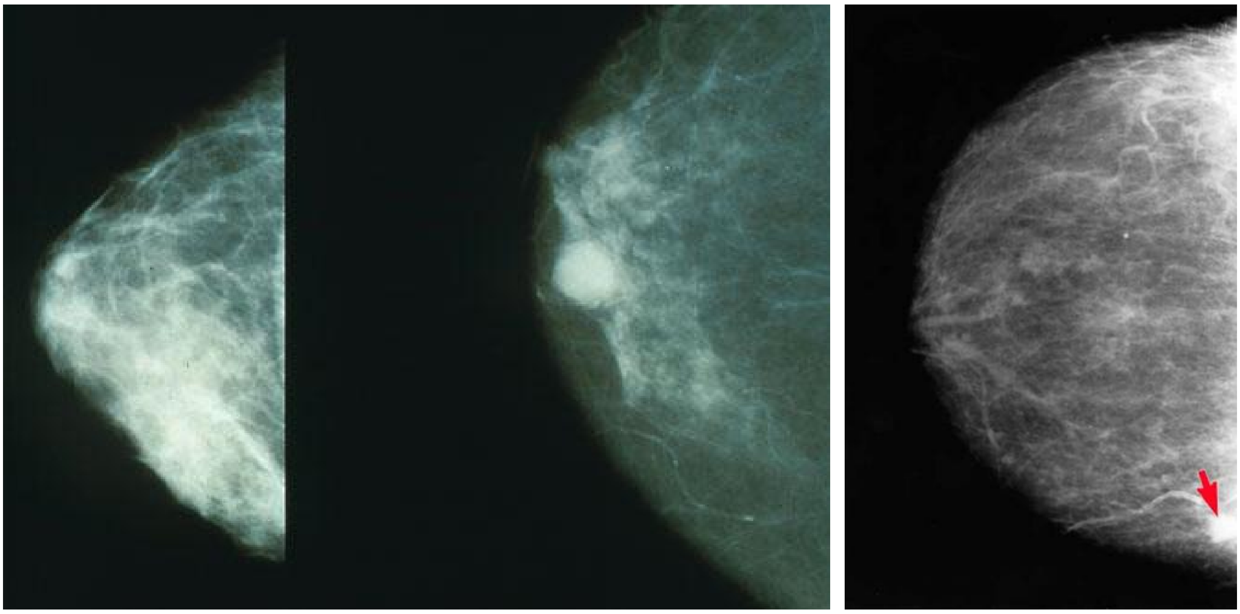
Question *5.3.1* There are special challenges in critically evaluating reports with mathematical, statistical or quantitative claims. Discuss these challenges.

[a]Wikipedia is a great source of general information, if used correctly and carefully. However, it is not a suitable primary source of detailed scientific information

5.4 Huh?

Case Study 5:
Losing patients with mathematics?

www.imagingpathways.health.wa.gov.au/includes/images/mass/mammo.jpg



From left: normal breast (en.wikipedia.org); breast with tumour (en.wikipedia.org); breast with tumour highlighted (breastcancer.about.com).

- Sometimes, particularly in a medical context, understanding and critically evaluating quantitative communications and concepts can be a matter of life and death.

- An important recent research paper[a] covered this.

[a] Gigerenzer *et al.*, *Helping Doctors and Patients Make Sense of Health Statistics*, Psych. Science in the Public Interest **8 (2)** (2007) 53–96.

***Question** 5.4.1* Many SCIE1000 students aim to become doctors, and everyone visits doctors. The Australian Medical Association (AMA) states on its website:

> *"The AMA believes that in order to support and enhance the collaborative nature of the doctor-patient relationship, patients must be able to make informed choices regarding their health care. An informed choice is dependent on receiving reliable, balanced health information, free from the influence of commercial considerations, that is communicated in a manner easily understood by patients."*

Meeting this goal places a range of responsibilities on patients, doctors, researchers, medical companies and the media. Discuss these responsibilities from the perspective of quantitative science.

***Example* 5.4.2** (From *Gigerenzer et al.*) "Many doctors, patients, journalists, and politicians alike do not understand what health statistics mean or draw wrong conclusions without noticing.... We provide evidence that statistical illiteracy:

(a) is common to patients, journalists, and physicians;

(b) is created by nontransparent framing of information that is sometimes an unintentional result of lack of understanding but can also be a result of intentional efforts to manipulate or persuade people; and

(c) can have serious consequences for health.

The causes of statistical illiteracy should not be attributed to cognitive biases alone, but to the emotional nature of the doctor/patient relationship and conflicts of interest in the healthcare system. The classic doctor/patient relation is based on (the physician's) paternalism and (the patient's) trust in authority, which make statistical literacy seem unnecessary; so does the traditional combination of determinism (physicians who seek causes, not chances) and the illusion of certainty (patients who seek certainty when there is none).

We show that information pamphlets, Web sites, leaflets distributed to doctors by the pharmaceutical industry, and even medical journals often report evidence in nontransparent forms that suggest big benefits of featured interventions and small harms. Without understanding the numbers involved, the public is susceptible to political and commercial manipulation of their anxieties and hopes, which undermines the goals of informed consent ...

Statistical literacy is a necessary precondition for an educated citizenship in a technological democracy. Understanding risks and asking critical questions can also shape the emotional climate in a society so that hopes and anxieties are no longer as easily manipulated from outside and citizens can develop a better-informed and more relaxed attitude toward their health."

Example 5.4.3 (From *Gigerenzer et al.*)

"In October 1995, the U.K. Committee on Safety of Medicines issued a warning that third-generation oral contraceptive pills increased the risk of potentially life-threatening blood clots in the legs or lungs ... by 100%. This information was passed on ... to 190,000 general practitioners, pharmacists, and directors of public health and was presented in an emergency announcement to the media. The news caused great anxiety, and distressed women stopped taking the pill, which led to unwanted pregnancies and abortions. ...

How big is 100%? The studies on which the warning was based had shown that of every 7,000 women who took the earlier, second-generation oral contraceptive pills, about 1 had a thrombosis; this number increased to 2 among women who took third-generation pills. That is, the absolute risk increase was only 1 in 7,000, whereas the relative increase was indeed 100%.

Absolute risks are typically small numbers while the corresponding relative changes tend to look big - particularly when the base rate is low. Had the committee and the media reported the absolute risks, few women would have panicked. ...

The pill scare led to an estimated 13,000 additional abortions (!) in the following year ...

For every additional abortion, there was also one extra birth ... with some 800 additional conceptions among girls under 16 ...

Ironically, abortions and pregnancies are associated with an increased risk of thrombosis that exceeds that of the third generation pill.

The pill scare hurt women, hurt the National Health Service, and even hurt the pharmaceutical industry. Among the few to profit were the journalists who got the story on the front page."

Example 5.4.4 (From *Gigerenzer et al.*)

Pharmaceutical leaflets, advertising and doctors

"Researchers from the German Institute for Quality and Efficiency in Health Care searched for the original studies and compared these with the summaries in 175 leaflets [produced for doctors by the pharmaceutical industry] .... The summaries could be verified in only 8% of the cases (!). In the remaining 92% of cases, key results of the original study were often systematically distorted or important details omitted. For instance, one pamphlet from Bayer stated that their potency [male sexual function] drug Levitra (Vardenafil) works up to 5 hours - without mentioning that this statistic was based on studies with numbed hares.

Should doctors have wanted to check the original studies, the cited sources were often either not provided or impossible to find.

In general, leaflets exaggerated baseline risks and risk reduction, enlarged the period through which medication could safely be taken, or did not reveal severe side effects of medication pointed out in the original publications."

Question 5.4.5 (From *Gigerenzer et al.*) "At the beginning of one continuing-education session in 2007, 160 gynaecologists were provided with the following relevant health statistics needed for calculating the chances that a woman with a positive test actually has breast cancer, and then given the following question. *continued...*

Question *5.4.5 (continued)*

'Assume you conduct breast cancer screening using mammography in a certain region. You know the following information about the women in this region:

- The probability that a woman has breast cancer is 1% (prevalence)
- If a woman has breast cancer, the probability that she tests positive is 90% (sensitivity)
- If a woman does not have breast cancer, the probability that she nevertheless tests positive is 9% (false-positive rate)

A woman tests positive. She wants to know whether that means that she has breast cancer for sure, or what the chances are. What is the best answer?

A. The probability that she has breast cancer is about 81%.

B. Out of 10 women with a positive mammogram, about 9 have breast cancer.

C. Out of 10 women with a positive mammogram, about 1 has breast cancer.

D. The probability that she has breast cancer is about 1%.'

The number of physicians who found the best answer, as documented in medical studies, was slightly **less than** chance (21%)."

What is the answer to the above question, and why?

Example 5.4.6 (From *Gigerenzer et al.*)

"A conference on AIDS held in 1987 . . . reported that of 22 blood donors in Florida who had been notified that they had tested positive with the ELISA test [for AIDS], 7 committed suicide.

Indeed, the test (consisting of one or two ELISA tests and a Western Blot test, performed on a single blood sample) has an extremely high sensitivity [proportion of infected individuals who correctly test positive] of about 99.9% and specificity [proportion of non-infected individuals who correctly test negative] of about 99.99%. . . .

To investigate the quality of counseling of heterosexual men with low-risk behaviour, an undercover client visited 20 public health centers in Germany to take 20 HIV tests.

The client was explicit about the fact that he belongs to no risk group, like the majority of people who take HIV tests. In the mandatory pretest counseling session, the client asked: 'Could I possibly test positive if I do not have the virus? And if so, how often does this happen?'

The answers from the medical practitioners were:

No, certainly not	False positives never happen
Absolutely impossible	With absolute certainty, no
With absolute certainty, no	With absolute certainty, no
No, absolutely not	Definitely not ... extremely rare
Never	Absolutely not ... 99.7% specificity
Absolutely impossible	Absolutely not ... 99.9% specificity
Absolutely impossible	More than 99% specificity
With absolute certainty, no	More than 99.9% specificity
The test is absolutely certain	99.9% specificity
No, only in France, not here	Don't worry, trust me"

***Question** 5.4.7* The base rate of infection for heterosexual men with low-risk behaviour is around 1 in 10,000.

(a) What is the (approximate) probability that someone who tests positive on the AIDS test is infected?

(b) Calculate the probability that at least one person who committed suicide after testing positive did not have AIDS.

(c) Comment on the responses of the German doctors, relating your answer to the AMA statement in Question 5.4.1.

***Example** 5.4.8* Consider the following extract from a paper[a].

"This condition [female sexual dysfunction] is claimed by enthusiastic proponents to affect 43% of American women, yet widespread and growing scientific disagreement exists over both its definition and prevalence. In addition, the meaningful benefits of experimental drugs for women's sexual difficulties are questionable, and the financial conflicts of interest of experts who endorse the notion of a highly prevalent medical condition are extensive...

One of the biggest hurdles for drug makers in this area is showing a big enough benefit over placebo to outweigh concerns about short or long term side effects. These concerns are made more acute by recent revelations about hormone replacement therapy, antidepressants, and anti-arthritis drugs...

In anticipation of regulatory approval of its testosterone patch - the first drug assessed for female sexual dysfunction - Proctor and Gamble unleashed a multilayered global marketing campaign... Long before its testosterone patch had even been assessed for approval, the company's global marketing had been strategically targeting health professionals, reporters, and the general public, seeking to shape their perceptions of female sexual problems and how to treat them. Enthusiastic media coverage has often followed these presentations, most notably when a press release carried a headline suggesting the patch caused a *74 per cent increase in frequency of satisfying sexual activity...*"

Preliminary results of 24-week randomised controlled trials of a patch in surgically menopausal women are shown in the following table (there were two trials, with $n \approx 500$ in each case).

continued...

[a]Moynihan, *The marketing of a disease: female sexual dysfunction*, British Medical Journal **330** (2005) 192–194.

Example *5.4.8 (continued)*

Outcome	Placebo	Patch	Placebo	Patch
Sexual activity (episodes/month)	0.98	2.13	0.73	1.56
Sexual desire (100 point scale)	6.9	11.85	6.21	11.38

(Figures for 'sexual activity' represent an increase from a baseline of about 3 satisfying episodes a month. Figures for 'sexual desire' represent an increase from a baseline score of 20−23.)

Question *5.4.9* Discuss the claims and results in Example 121. (For interest, two patches are required per week; in January 2010, packets of 24 patches were selling online for about $USD400.)

- It is easy to think that the above examples "do not apply to me. . . I am different". If you are tempted to believe that, then note the following results from a recent two-year Australian study.

Extension *5.4.10* (From The Australian newspaper, February 01, 2010.)

"**Training fails to prepare new doctors**

Medical students are emerging from the nation's universities feeling inadequately prepared to deal with crucial tasks such as calculating safe drug doses and writing prescriptions.

In a challenge to Kevin Rudd's twin promise to improve university education and doctor shortages, a government study has also revealed that medical supervisors feel the abilities of hospital interns fall short of their expectations.

The study reveals just 36 per cent of junior doctors think they have been adequately or well-prepared to do wound management.

And only 29 per cent of final-year medical students feel they have been adequately prepared to calculate accurate drug doses.

The landmark review of the nation's medical education system was finalised 19 months ago but released only on Friday.

Medical leaders warn that the extra influx of students since the Education Department commissioned the research has made the failings it describes even worse. . .

The report found medical students feared for their skills in a number of key areas, including knowledge of basic sciences, while hospitals increasingly struggled to make time for effective teaching in the face of packed waiting rooms."

End of Case Study 5.

***Question** 5.4.11* Critically evaluate each of the following items quoted from various news sources and websites.

(a) (Courier mail, November 27, 2009)
"HERE is something to get you in the mood tonight: a 10-year Welsh study found that those who enjoyed an active sex life were 50 per cent less likely to have died during that time than those who did not."

(e) (Australian Vaccination Network publications[a])

"According to medical reports, children are now less healthy than they have ever been before. More than 40% of all children now suffer from chronic conditions, something that was unheard of prior to mass vaccination. Vaccines have been associated with such conditions as Asthma, Eczema, Food Allergies, Chronic Ear Infections, Insulin Dependent Diabetes, Arthritis, Juvenile Rheumatoid Arthritis, Autism, Attention Deficit Disorder, Ulcerative Colitis, Irritable Bowel Syndrome, Hyperactivity, Schizophrenia, Multiple Sclerosis, Cancer and a raft of other chronic and auto-immune conditions which are experiencing dramatic rises in incidence."

continued...

[a]The Australian Vaccination Network is opposed to mass vaccinations

Question *5.4.11 (continued)*

(c) (www.naturalnews.com/023032.html, April 16, 2008)
"Odds of intensive care medication errors are over one hundred percent

A report produced by PubMed Central states that 1.7 errors per day are experienced by patients in intensive care units (ICU). At least one life-threatening error occurs at some point during virtually every ICU stay. 78% of the serious medical errors are in medications. 1.7 errors per day times 78% equals the likelihood of experiencing a medication error while in an ICU of well over 100% per day. That means the odds are that you will receive the wrong medication or the wrong amount of a medication at least once every single day of an ICU stay."

(d) (www.news.com.au/heraldsun; December 16, 2008.)
"The institute tracked more than 350 patients receiving treatment for back pain. They were followed over one year and contacted at six weeks, three months and 12 months. Dr Maher said the research showed one-in-four would go on to suffer a recurrence of back pain within a year. 'This explains why around 25 per cent of the Australian population suffers from back pain at any one time', he said."

continued...

Question *5.4.11 (continued)*

(e) (Courier mail, November 27, 2009)
"You fall in love, you get married, you have kids – or so the story goes. Sadly, the statistics prove otherwise: one in eight couples in Australia will have difficulty conceiving, and be classified 'infertile'. And while infertility usually falls into the category of 'secret women's business' and is often perceived as a female problem, it is estimated that in Australia, infertility affects about one in every 20 men. For half of all infertile couples, the problem lies with the male partner, while in 40 per cent of infertile couples using assisted reproduction technologies, the underlying reason is male infertility. "

(f) (www.abc.net.au) "Cliff Arnall, a health psychologist at the University of Cardiff, specialising in confidence-building and stress management, told AFP the prediction was the result of some gruelling mathematics. He says post-Christmas blues, the return to work after the holidays, mounting bills to pay for the parties, the challenge of keeping New Year's resolutions, the slender prospects of fun in the weeks ahead and chilly winter temperatures for those in the northern hemisphere all add up. These factors, which he combined in a complex formula, came out showing the Monday closest to January 24 [2006] would be the most dismal of the year."

continued...

Question 5.4.11 (continued)

(g) (www.mentalhealth.org.uk) "The equation [by Cliff Arnall] calculates that Monday 19 January 2009 is the worst day of the year, when the Christmas glow has faded away, New Year's resolutions have been broken, cold Winter weather has set in and credit card bills will be landing on doormats across the land whilst the January pay-cheque is still some way away. Blue Monday was devised using the following mathematical equation:

$$\frac{(W + (D - d)) \times T^Q}{M \times N_a}.$$

The model was broken down using six immediately identifiable factors; weather (W), debt (d), time since Christmas (T), time since failing our new years resolutions (Q), low motivational levels (M) and the feeling of a need to take action (N_a)."

(h) (www.msnbc.msn.com/id/6847012) "Arnall, who specializes in seasonal disorders at the University of Cardiff, Wales, created a formula that takes into account numerous feelings to devise peoples' lowest point. The model is:

$$\frac{(W + (D - d)) \times TQ}{M \times NA}.$$

The equation is broken down into seven variables: (W) weather, (D) debt, (d) monthly salary, (T) time since Christmas, (Q) time since failed quit attempt, (M) low motivational levels and (NA) the need to take action."

5.5 Space for additional notes

6 Philosophy of science

Immanuel Kant was a real pissant
Who was very rarely stable.
Heidegger, Heidegger was a boozy beggar
Who could think you under the table.
David Hume could out-consume
Wilhelm Freidrich Hegel,
And Wittgenstein was a beery swine
Who was just as schloshed as Schlegel.

Artist: Monty Python

(www.youtube.com/watch?v=m_WRFJwGsbY)

(rude word at time 1:10; song starts at 1:20)

The Philosopher in Meditation (1632), Rembrandt van Rijn (1606 – 1669), Musee du Louvre, Paris. (Image source: en.wikipedia.org/wiki/Image:Rembrandt_-_The_Philosopher_in_Meditation.jpg)

What is knowledge, and how is it different from belief?

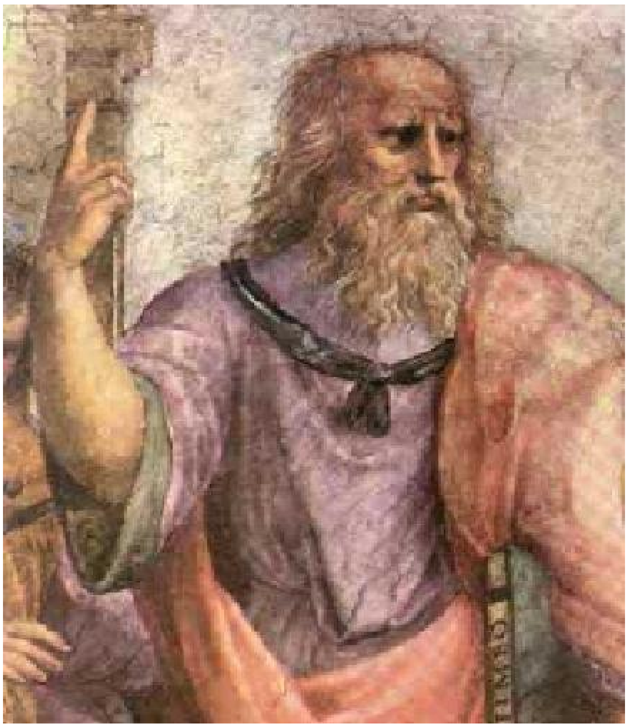
I believe that Liverpool will win the FA Cup, I believe that I was born in Walgett, and I believe that my four year old daughter is a child genius. Do any of these beliefs count as knowledge? What conditions would have to be met for them to do so? And when we do have knowledge, when can it be said to be *scientific*?

Philosophy of Science involves broad conceptual and critical thinking about the general nature and value of science. Sometimes a look at the history of such thinking can provide a helpful perspective. We will do just that in this module, focusing on the concept of knowledge. We will explore three visions of scientific knowledge, each of which remains relevant today.

6.1 Knowledge – the Platonic Vision

Plato (428–348 BC) was a Greek philosopher who had a vision about the difference between belief and knowledge, and for how knowledge should be our rule of life in society, which he set out in his book *The Republic*. The Greek word for belief is *doxa*. Plato believed that 'right belief', *orthodoxy* in Greek, should rule society (for Plato, a city state) in the sense that we should all hold and share the right beliefs about how the city should be developed and governed. This commitment to orthodoxy is in contrast with other Greek thinkers such as Protagoras (490–420 BC) and Hippocrates (460–370 BC), who believed in *heterodoxy*, the flowering of multiple radical or non-orthodox views. But Plato was aware of the dangers of mere consensus. In Nazi Germany it was orthodox to believe that Jews are inferior, but being a consensus view doesn't make it **right** thinking. It was important to which orthodoxy society subscribed: it must be based on true knowledge. The Greek word for knowledge is *episteme*, from which we get the word epistemology, the study of knowledge. The Latin translation of episteme is *scientia*, from which we get the word science, although it had a more general meaning, that is, knowledge.

According to Plato, 'true knowledge' is knowledge of unchanging truths, the ultimate reality that lies behind the buzzing, changing world of our experience. Our senses are not the means to gaining such knowledge, rather, it is gained by conceptualising, 'seeing in our mind's eye'. The true nature of a circle, or of justice, the results of geometry, and the ultimate physical principles that explain our world, are only gained by the act of conceptualising in our minds. Like Pythagoras (569–475 BC) before him, Plato thought true reality is mathematical or mathematics-like.



Plato: "prove it".

Our senses, which reveal the buzzing, changing world, do not provide us with true knowledge. They reveal the world of *appearance*. In his ‘Allegory of the Cave’ (*The Republic* Book VII), Plato describes prisoners chained in a cave, unable to turn their heads, so that all they can see is the wall of the cave. Behind them burns a fire. Between the fire and the prisoners there is a parapet, along which puppeteers can walk. The puppeteers, who are behind the prisoners, hold up puppets that cast shadows on the wall of the cave. The prisoners are unable to see these puppets, the real objects that pass behind them, only shadows and echoes cast by objects Similarly, if all we attend to is the world of our senses, we are like prisoners trapped in a cave. To see beyond appearance we need to conceptualise eternal truths.

To attain such knowledge, those with sufficient aptitude need the right education. Only those who attain this knowledge, episteme, are fit to rule society. Plato called such people *Philosopher Kings*. In ruling, they establish orthodoxy, to which the rest of society should subscribe, since the latter are themselves incapable of much true knowledge.

Two good examples of Plato’s vision of knowledge are Euclid (325–270 BC) and Archimedes (287–212 BC). Euclid proved from “self-evident” geometrical axioms and definitions various theorems such as ‘the angles of a triangle make two right angles’. Archimedes proved from certain axioms concerning levers, that two unequal weights balance at distances from the fulcrum that are inversely proportional to their weights. Both results involved conceptualising definitions, self-evident axioms, and proofs based on those axioms. Philosophers call this type of reasoning *deductive*, by which they mean an argument whose conclusion cannot be false if its premises (axioms) are true. It was not Plato, but Aristotle (384–322 BC) who set out a system of deductive logic, which remained the best of its kind until the late nineteenth century.

The Platonic vision had a powerful influence among some in the sixteenth and seventeenth centuries, a period of time where many of what we know as the traditional areas of science commenced in earnest, such as Newtonian physics, chemistry, anatomy and astronomy. Rene Descartes (1596–1650) held that true knowledge comes from having "clear and distinct ideas", and utilising those to prove deductively results from self-evident truths. Descartes thought that true knowledge could not possibly be doubted. Evidence of our senses, even of most obvious things like 'this is my hand in front of me' could conceivably be doubted. I don't know for certain that I am not dreaming when I see my hand, or that I am not being tricked by an evil demon into thinking I see my hand. Nevertheless, we can have knowledge of the world around us by deductive reasoning. Mathematical physics deals with quantities to which a number can be attached, and mathematical relations between those quantities can be established beyond doubt, on Descartes' view.

Galileo (1564–1642) also held that mathematical physics enabled us to establish true knowledge that takes us beyond the buzzing confusion of the world of our immediate experience. Galileo clearly understood the significance of idealisation when he wrote:[a]

> Just as the Computer who wants his calculations to deal with sugar, silk and wool must discount the boxes, bales, and other packings, so the mathematical scientist when he wants to recognise in the concrete the effects which he has proved in the abstract must deduct the material hindrances, and if he is able to do so, I assure you that things are in no less agreement than arithmetical computations. The errors, then, lie not in the abstractness or concreteness, not in geometry or physics, but in a calculator who does not know how to make a true accounting.

The Platonic Vision was an emphasis, but it didn't mean there was no place at all for experiments. Descartes did a lot of experimental work on human anatomy, and one of Galileo's many contributions was to turn the telescope on the stars to find that there are many more stars than previously thought. But even so, Galileo was a theoretician, and even the experiments for which he is famous were actually thought experiments, such as dropping objects from the leaning tower of Pisa (to show that different objects of different weights fall at the same speed). In theory, the approach of proving theorems from self-evident axioms leaves you with theorems which can be tested in experiment. But if you believe you already have certain knowledge of those theorems, you would not feel any urgency to go and test them.

[a]Galileo, *Dialogue Concerning the Two Chief World Systems*, trans. Stillman Drake, Berkeley: Univ. California Press (1953) 207.

Key point: the Platonic Vision of knowledge is of mathematical and logical conceptualising, and proofs.

Notes:

6.2 Knowledge – the Baconian Vision

Francis Bacon (1561–1626) has traditionally been credited as being the 'father of modern science and technology', who 'has permanent importance as the founder of modern inductive method and pioneer in the attempt at logical systematisation of scientific procedure'. He did not share Galileo's and Descartes' appreciation of the importance of mathematics in science, but is famous rather for his vision for experimentation and application.

As suggested by the title of one of Bacon's works (*The New Organon*, his account of scientific method and logic was developed with the explicit intention of replacing Aristotle's system of deductive logic. There seems to be a fundamental flaw in a purely deductive system, namely, the so-called problem of *premise regress*. A valid argument tells me that if the premises are true, then the conclusion must be true, but how do I know the premises are true? I could have another deductively valid argument with the first premise as the conclusion. But again, how do I know the premises are true? This leads to a regress. How do we ever reach a starting point - premises which are certainly true, on which knowledge can be built via deductive inferences based on those certain truths? Euclid and Descartes were very clear about what their answer to this problem was. The axioms must be self-evident, beyond any possible doubt. But are there really any such truths? One of Euclid's axioms was that parallel lines never meet, but one can derive a different geometry by dropping this assumption, and in fact Einstein's General Theory of Relativity suggests that our own space-time is non-Euclidean in this way.

Bacon: "stick to the facts".

Bacon begins the preface to another work (*The Great Insaturation*) with the manifesto:

> "That the state of knowledge is not prosperous nor greatly advancing, and that a different way must be opened for the human understanding entirely different from any hitherto known."

Bacon claimed that the whole scholastic scheme, with its Aristotelian base, was not producing knowledge at all, as evidenced by the fact that it never produced anything of practical benefit for humanity. He thought of the scholastic university as an 'ivory tower', dominated by obscurantist Aristotelian texts and deductive logic, and characterised by a disregard, possibly derived from a Greek disdain for manual labour, for the hands-on knowledge of things of the humble artisan. In the mechanical arts of, say, the silversmith, Bacon saw genuine practical ability and knowledge of the workings of nature.

So, how to attain this new knowledge? Bacon sets out three requirements. The first is a willingness to discard all personal bias, and a desire to know nature as it is, undistorted by theories and presuppositions. Bacon outlines four 'idols of the mind'; habits and ideas which corrupt our capacity for knowledge. The 'idols of the tribe' are tendencies in human nature to accept what we want to believe and what our raw senses tell us, when it suits us, and to our own purposes. 'Idols of the den' are distortions that arise from our particular perspective, 'idols of the market-place' are errors we pick up from each other, often involving the abuse of words, and 'idols of the theatre' are errors associated with grand theories such as Aristotelianism.

The second requirement is to collect all relevant data. In fact, the *New Organon* was a small part of a scheme to produce one huge encyclopaedia of nature incorporating all the available data of observation and experiment. Towards the end of the *New Organon*, Bacon sets out the general plan for what is to be included in this encyclopaedia. For example, suppose we are studying heat and want to know everything about it, free from bias and presupposition. The method involves formulating what Bacon calls the 'Tables of Investigation'. The first Table of Investigation is the 'Table of Affirmation', where everything that contains heat should be listed, according to the 'Rule of Presence': the sun's rays, blood that circulates around the body, certain chemicals, iron after it has been in fire, chilli peppers, and so on. In the second, the 'Table of Negation', everything that does not contain heat should be listed according to the 'Rule of Absence': the moon's rays, the blood in a dead body, or chemicals which are cold. At this point we can formulate a 'Table of Comparisons', in which the different types of data are compared. The 'Prerogative Instances', are twenty-seven ways in which something might stand out when we are studying a particular case.

For example, the ‘Solitary Instance’ is where two things are similar in many ways, but different in just one way, while the ‘Glaring Instance’ is where there is just one feature of a particular thing that is conspicuous; for example, the weight of quicksilver. In the Preface to the *New Organon*, we find a catalogue of 130 ‘Particular Instances’ by title, including the history of the heavenly bodies, the history of comets, the history of air as a whole, the history of sleep and dreams, the history of smell and smells, the history of wine, the history of cements, the history of working with wood and so on.

Bacon’s third requirement concerns the method for deducing from this collection of facts certain generalisations about nature; that is, scientific laws. For example, in studying heat, we may discover the rule that metals expand when heated. The process will be something like this:

> This piece of iron expands when heated
>
> This piece of iron expands when heated
>
> This piece of copper expands when heated
>
> This piece of copper expands when heated
>
> This piece of bronze expands when heated
>
> and so on.
> Therefore all iron expands when heated
>
> All copper expands when heated
>
> All bronze expands when heated
>
> and so on.
> Therefore all metals expand when heated.

From sufficient observations of iron expanding we draw the conclusion that all iron expands when heated. Then, from the observation that various kinds of metals expand when heated, we conclude that all metals expand when heated.

This method of simple enumeration is one kind of ‘inductive’, as opposed to deductive, inference. The premises, particular observations, do not guarantee the truth of the conclusion in the logical sense, since it is logically possible for the premises to be true and the conclusion to be false. The premises simply render the conclusion probable. The problem of premise regress, however, is overcome, since the entire process is grounded in simple particular observations, which, according to empiricism, are the root of all knowledge. So by following the Baconian inductive method, we arrive at generalisations from observation, that is, the laws of nature.

Bacon believed that true knowledge always leads to practical application, since true knowledge of nature gives us power over nature. (Of course, such practical application may not be immediate.) If I understand metal to the point that I know with certainty that heating a certain piece of copper will cause it to expand, then that knowledge gives me power to control it. If I want it expanded, I can heat it. If I do not, I can prevent it from being heated. For example, suppose part of the deck of a ship is made from metal, and I want to prevent expansion because that tends to warp the wood which can cause leaking. I can prevent that expansion by preventing the heating; for example, shielding the metal from the sun if that is the source of heat. In this way Bacon thought that understanding of nature would automatically lead to control of nature, with practical benefit. Knowledge is power. As Bacon claims in the *New Organon*, in a rather self-satisfied tone:

> "I may hand over to men their fortunes, now their understanding is emancipated and come, as it were, of age; whence there cannot but follow an improvement in man's estate and an enlargement of his power over nature."

In *The New Atlantis*, Bacon describes a utopia in which scientists work hard to apply their knowledge to the improvement of the quality of human life. Bacon cites three inventions as evidence that such a utopic vision would be realised if his understanding of science were followed. The first is the printing press, which aids the dissemination of knowledge, the second is gunpowder, an obvious source of power, and the third is the compass, which greatly improves navigation. For Bacon, these three inventions demonstrated conclusively the capacity of scientific knowledge to give power over nature. They lend support to the idea that if we pour our efforts into true science, we will be rewarded with such technological advances, which in turn improve the quality of life. Bacon's optimistic view of human achievement marks the early stages of a trend which dominated Western thought right through until the early twentieth century.

Unlike Descartes and particularly Galileo, Bacon himself did not make much progress with any actual scientific projects. He is seen rather as a philosopher of the scientific method and its technology, who succeeded in specifying the methodology and research program required for successful science. It was not long, however, before the kind of scientific successes that Bacon had hoped for did, in fact, occur. Eighty years after Bacon's death, his philosophy of science was adopted by the Royal Society in London, which set itself up with the explicit aim of carrying out the work that Bacon had envisioned, adopting him as a kind of patron saint. At their meetings, the Royal Society reported on and discussed those experiments, collected data, and so on. Society members included figures such as Boyle, Hooke, and Harvey; in other words, many of the founders of modern science.

Key point: According to the Baconian Vision true knowledge is derived directly from observations and experiments, and will produce practical benefit.

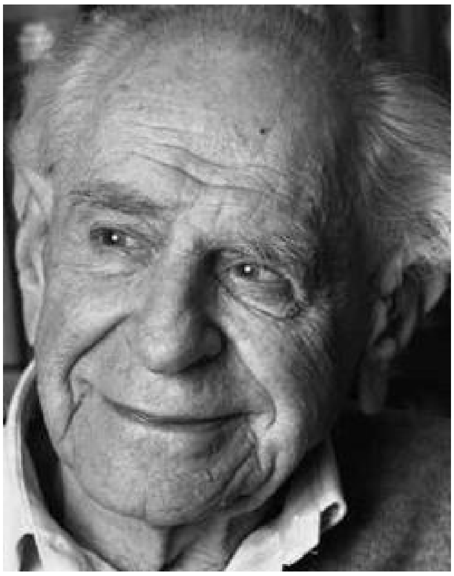
Notes:

6.3 Knowledge – the Popperian Vision

Karl Popper (1902–1994) was an Austrian philosopher who fled Nazi Germany for New Zealand, and later London. He opposed the Baconian vision on a number of points. First, it doesn't match much of scientific practice. Scientists do not in general conduct experiments without preconceptions. Usually they have a good idea of what they are looking for, and are selective in the facts that they collect. No-one records the name of the cleaner or the colour of the paint on the laboratory wall. Generally theories come first, and the experiments which distinguish them from the alternatives come along later. And second, Popper thought the very mechanism of induction is dubious, as it falls short of a proof. Related to this is the Problem of Induction, first pointed out by David Hume (1711–1776). This is the problem that, while you can formulate a 'Rule of Induction' which tells you to make generalisations in the right circumstances, you can never prove this rule. It can't be proved mathematically or logically, since it is always logically possible that the next metal you observe, for example, will not expand when heated even though previously all observations suggested that it would. There is no logical contradiction to suppose it doesn't. And secondly, a Law of Induction cannot be proved by experiment, since that proof would itself be an inductive generalisation. That would be to beg the question. You may as well say 'I know my crystal ball is a good predictor because it tells me it is'. So it seems that the use of induction always has an unproved assumption, that nature will continue working the way it always has, as assumption Hume called the uniformity of nature.

Popper therefore proposed an alternative vision of how we come to scientific knowledge. Science proceeds, he said, by *conjectures* and *refutations*[a]. Conjectures are the starting point. They are hypotheses, educated guesses proposed for the purpose of being tested. In fact, the key thing about a conjecture is that it must be *falsifiable*, able to be proved false. According to Popper this is the mark of true science. Any claim that cannot be falsified in principle is not scientific. For example, open today's newspaper and read your horoscope. It probably makes predictions about how your day will go. Now try and think of a set of circumstances that could happen today which, if they did happen, would refute the horoscope's prediction. Often you find this is very difficult, because the claim is not actually falsifiable. So it's not scientific, according to Popper. Popper was a trenchant critic of Marx and Freud, claiming that their theories were meaningless because they were not falsifiable. A theory is not scientific if it can explain everything, no matter how things turn out.

[a]Popper, *The Logic of Scientific Discovery*, London: Hutchinson (1934).



Popper: “prove me wrong, please”.

Scientific conjectures should be bold, and clearly able to be refuted. They do not need to be unbiased in any sense. Thinking up bold and novel hypotheses can be a very creative process, and can be prompted by all kinds of things, such as in the case of August Kekule (1829–1896), who said he discovered the ring shape of the benzene molecule after having a day-dream of a snake biting its own tail.

Once one has a hypothesis, one can deduce the particular results that it predicts, which are then able to be tested. This is not an inductive step, it is deductive. The hypothesis ‘all metals expand when heated’ entails as a matter of deductive certainty that a particular example of a metal being heated will expand. So there is no problem of induction. Thus Popper’s vision is of what is often called the hypothetico-deductive scientific method.

The second key to Popper’s vision is that if proved wrong the theory should be immediately rejected. This is scientific progress. At least we know that particular hypothesis is not right. The scientific attitude is to be able to throw out a theory if it is proved wrong. But a theory or hypothesis can be accepted if it survives all attempts to refute it.

Like Plato’s and Bacon’s visions, Popper’s vision has its critics. One problem is that scientists in many areas are looking to test whole theories, or in effect groups of hypotheses ‘joined together’. Then, if you refute the group of hypotheses as a whole, the next question would be which part is the part to be rejected. A second problem is that scientists do not always throw out the theory just because there is a problem. If there is no better theory available, it may be held onto, at least for the foreseeable future. Just because a theory has a difficulty with one particular experiment does not mean the theory gets thrown out immediately. And finally, if all we ever have in science is unrejected hypotheses, where is the vision that we ever come to true knowledge in science? On Popper’s account we can know a theory is false, but we can never know it is true.

One prominent critic of Popper is Thomas Kuhn (1922–1996), whose book *Structure of Scientific Revolutions* was the most cited book in the twentieth century. According to Kuhn, science goes through different stages historically. There are periods of *normal science*, where scientists are essentially puzzle solving, and periods of *revolution*, where everything is thrown up in the air and completely new theories come to the fore. Normal science is governed by a *paradigm*, which involves certain big theories such as those of Newton, Einstein, or Darwin, together with methodological assumptions, protocols and conceptual elements. Scientists from all around the world work 'together' in that they subscribe to the paradigm.

To take a not-very intellectual example, unlike in Newton's day, today if one writes a scientific paper reporting the outcomes of experiments or experimental studies, one should set out the method so that it can be repeated. Only when the experimental result is reproduced two or three times by independent groups working in different locations is the result accepted as fact. But before it gets to that stage, the paper has to be published in a reputable scientific journal and to achieve that it must be *peer reviewed*, that is, approved by other (usually two) independent scientists. This means normal science is conservative, tending not to accept ideas and approaches that are too radical or unrecognisable from the perspective of the paradigm. Thus to work in normal science you have to be orthodox in Plato's sense. Kuhn did not make these observations in order to denigrate normal science. On the contrary, its conservative nature enables scientists to get on with solving problems and exploring the technological potential of the paradigm. Another feature of normal science is that it permits anomalies, unresolved difficulties. We mentioned above that scientists do not always throw out the theory just because there is a problem. A paradigm can always tolerate a certain amount of anomaly.

However, if the number and the significance of anomalies become too great, the paradigm can enter into a period of crisis, where the tenets of the paradigm can be questioned. This is the beginning of a scientific revolution. Alternative theories and methodologies emerge, and science takes on a more *heterodoxical* look. Eventually, once one of these wins out and a consensus emerges, we enter into another period of normal science with a new paradigm. The new paradigm may be radically different from the old one, to the point that Kuhn argued that successive paradigms are *incommensurable.*

One advantage of Kuhn's developmental approach to the nature of science is that it draws our attention to the defeasible nature of scientific theories. Even our best theories today may be overthrown down the track and replaced by something we cannot even envisage from our perspective today.

Key Points: According to the Popperian Vision, science proceeds by falsifiable conjecture, and refutation. According to Kuhn, science proceeds by periods of paradigm consensus, punctuated by the occasional radical scientific revolution.

Notes:

***Question** 6.3.1* Create your own glossary by writing down the definitions of the following terms:

(a) Deductive proof

(b) Experiment

(c) Fact

(d) Hypothesis

(e) Hypothetico-deductive method

continued...

Question *6.3.1 (continued)*

(f) Induction

(g) Law

(h) Measurement

(i) Observation

(j) Theory

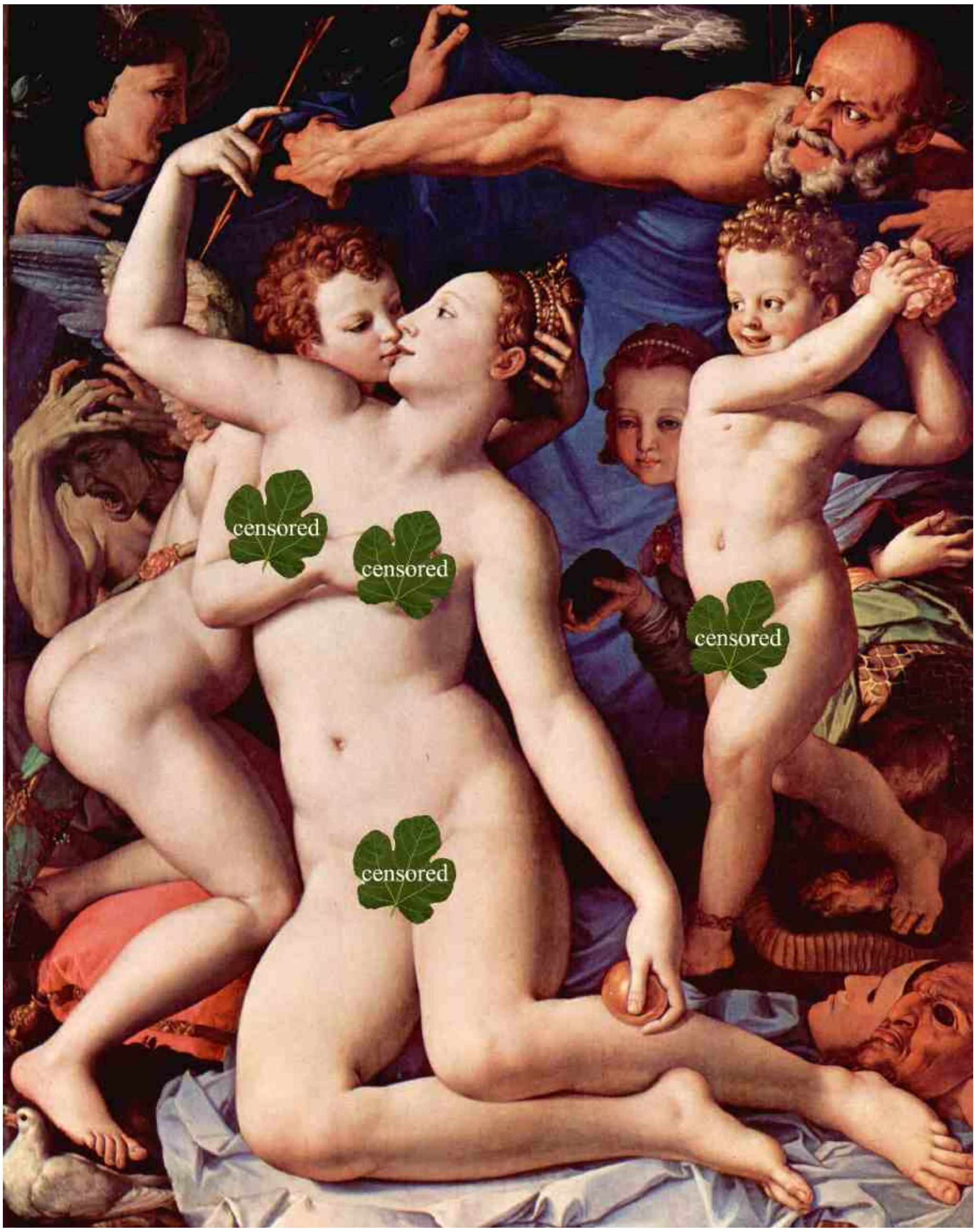
6.4 Space for additional notes

7 Introduction to Python programming

The coiling is fast
This time it's your last
Your soul asphyxiated
Final chance for escape terminated.
Enveloped in python
constriction complete
where dreams become nightmares
of total defeat.

Artist: Torniquet

(www.youtube.com/watch?v=c107Aor329g)



Venus, Cupid, Folly and Time (1540 – 1545), Agnolo di Cosimo (usually known as Il Bronzino) (1503 – 1572), National Gallery, London.

(Image source: en.wikipedia.org/wiki/Image:Angelo_Bronzino_001.jpg)

Introduction

Almost everyone is quite familiar with using computers to perform tasks, like writing documents or looking up internet sites. Every such action requires the computer to run a number of computer programs, each of which was written in one of many computer languages, by one or more programmers.

In science and many other disciplines you will sometimes need to use a computer to solve a problem for which there is no program already written. In such cases you will need to write a new program yourself.

Different computer languages are best suited for different tasks. Python is a language that is becoming widely used in science, and is fairly easy to use. In SCIE1000 we will cover introductory programming in Python. You will learn how to design and write programs, investigate some of the most useful programming concepts and constructs, and apply these in your own programs.

We will cover programming in the context of an unsolved mathematical research problem. You may well find this section to be difficult and confusing at first, but you do not need to understand it all straight away. We will keep returning to the programming concepts throughout semester, and you will practise them extensively during tutorials.

Some of the examples/contexts we will discuss are:

- The *Collatz conjecture*.

Specific techniques and concepts we will cover include:

- Specifying, designing and writing programs.
- Python commands.
- Interpreting programs.
- Errors.

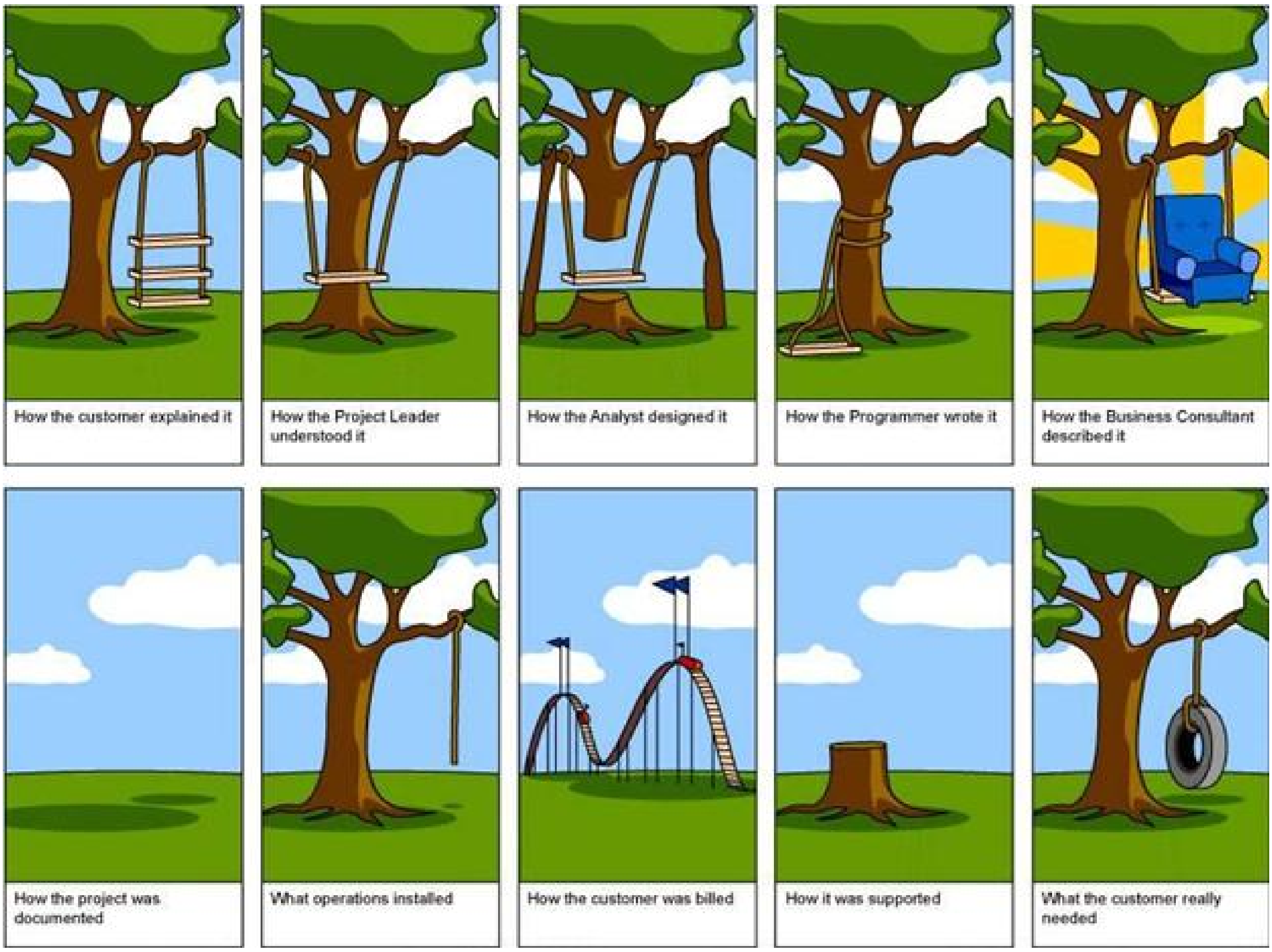
7.1 Designing programs

Software design

"Software is built on abstractions. Pick the right ones, and programming will flow naturally from design, modules will have small and simple interfaces, and new functionality will more than likely fit in without extensive reorganization. Pick the wrong ones, and programming will be a series of nasty surprises: interfaces will become baroque and clumsy as they are forced to accommodate unanticipated interactions, and even the simplest of changes will be hard to make. No amount of refactoring, bar starting again from scratch, can rescue a system built on flawed concepts."

From: Software Abstractions, *by Daniel Jackson.*

- Before starting to write a program, it is **essential** to have clear specifications of what the program needs to do.



softwareindustrialization.com/content/binary/design.jpg

- Once the problem has been specified, there are many approaches to writing the program.
- One common technique is to use *top-down design* .
- This involves subdividing the problem into smaller or simpler steps, and to continue breaking these into even smaller steps, until they can directly be converted into lines of code.
- We will illustrate this with a non-computing task.

***Example** 7.1.1* In Question 9.3.3 we will consider a 2007 research study on the likely impact of climate change on the distribution of the bird species *Catharus bicknelli* (Bicknell's thrush). As part of this study, biologists required a practical way of collecting thrush distribution data, based on temperature zones within habitats.

- Consider a top-down approach to designing the data collection method for Example 7.1.1. First we have the program specifications.

Python Example 7.1.2

```
Estimate distribution of thrush according to temperature zones.
```

- If every line in the previous description is easy to implement in practice, then the top-down design approach would stop.
- However, the total current habitat size for Bicknell's thrush is 140,000 hectares; this is too large for exhaustive measurements, so refinement of the approach is needed.
- The next stage splits the single step into four simpler steps.

Python Example 7.1.3

```
Identify different temperature zones in the habitat.
Select a representative sample of regions in the habitat.
Identify thrush distribution within the sample regions.
Extrapolate to the full habitat.
```

- Again, any lines that are easy to implement do not need further subdivision. In the next stage, Lines 2 and 3 have been split into new Lines 2 to 5.

Python Example 7.1.4

```
1 Identify different temperature zones in the habitat.
2 Divide the habitat into regions 30 m square.
3 Decide how many squares are required to represent the habitat.
4 Choose that many squares at random.
5 Identify which squares contain thrush.
6 Extrapolate to the full habitat.
```

- In the next stage the language has been formalised, and Line 5 has been split into Lines 5 to 8.

Python Example 7.1.5

```
1 Identify different temperature zones in the habitat.
2 Divide the habitat into regions 30 m square.
3 Decide how many squares are needed, say numRegion.
4 Choose numRegion squares at random.
5 for each chosen square in turn:
6   Record temperature in that square.
7   Conduct field trial in that square to search for thrush.
8   Record whether the square contained thrush.
9 Extrapolate to the full habitat.
```

- It is possible that further refinement is unnecessary, as each step may be sufficiently simple. (We will assume that this is the case.)
- If not (for example, Line 6 may be too complicated to be implemented) then further splitting can be undertaken.
- Essentially, the top-down approach is based on starting with a simple description of the problem, then continually refining it into smaller steps until all of the steps are easy to do. In computing, this means they are easy to convert to programming commands.

- As you write programs, you should always be guided by a number of "good programming" principles.

Good programming

There are many features of a "good" computer program. In general, programs should be:

- *correct;*
- *easy to read;*
- *easy to understand;*
- *simple;*
- *efficient; and*
- *thoroughly tested.*

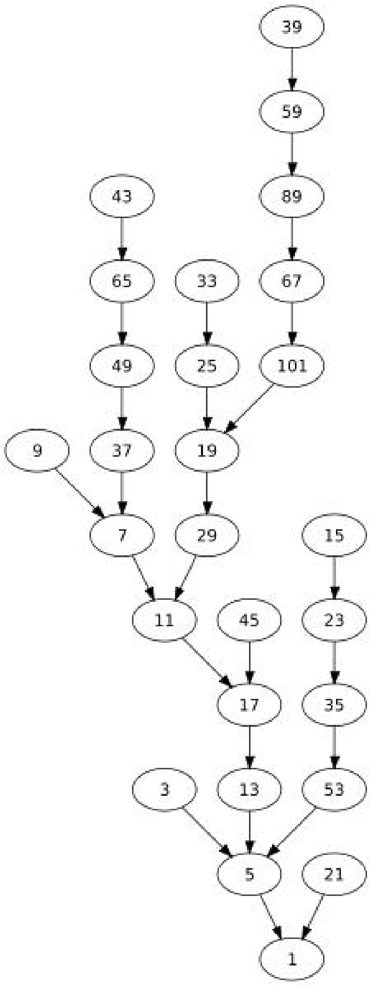
- To assist with achieving these goals, programs should:
  - include blank lines and spacing to assist readability;
  - have extensive comments to explain what is happening; and
  - use *meaningful names* for variables and functions.
- Using top-down design and good programming principles will:
  - make the initial programming job easier;
  - make debugging and maintaining the program easier; and
  - result in a program which is more likely to be correct.

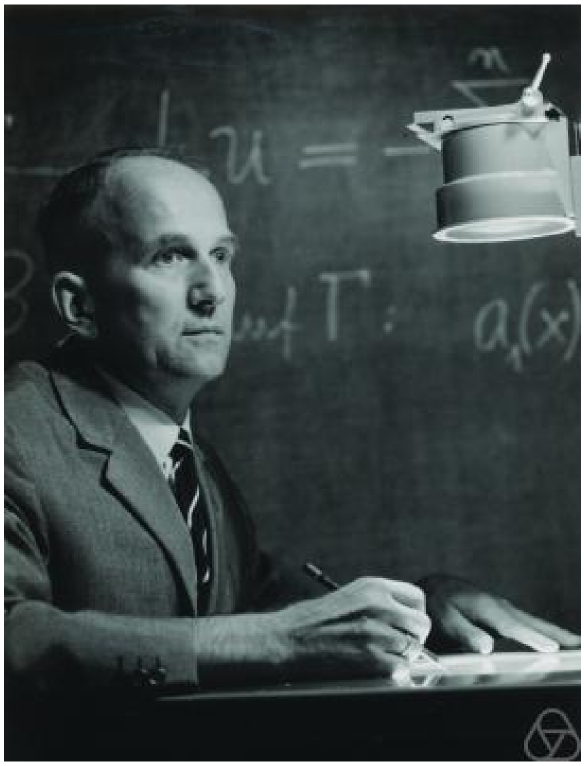
7.2 An unsolved mathematical problem

- We will continue our study of programming and Python in the context of a specific mathematics research problem.

Case Study 6:

Collatz and his vexing conjecture





`3x+1@home is a distributed non-profit project trying to find high 3x+1 conjecture stopping times. The 3x+1 conjecture is also known as Collatz conjecture... You can participate by downloading and running a free program on your computer.` http://www.allprojectstats.com/collatz/

- Many people understand what it means to do research in science: we often see in the media that researchers have invented new vaccines, isolated a previously unknown gene, discovered a new planet or identified a previously undescribed insect.
- However, very few people understand what research in mathematics entails. There is a perception that such research involves "discovering new numbers or making up new equations".

- The *Collatz conjecture* (or "$3x + 1$ problem") is an unsolved research problem in number theory, which is a branch of pure mathematics.
- (In mathematics, a *conjecture* is similar to a hypothesis. However, conjectures are stronger than hypotheses, in that people believe they are "very likely" to be true but cannot yet be proved.)
- Some mathematicians have spent most of their careers (unsuccessfully) trying to solve the Collatz conjecture.
- It is very easy to understand, but is exceedingly difficult (or perhaps even impossible) to prove.
- There is no currently known practical application for the conjecture.
- However, other results obtained using number theory have had no known practical application for a long time, but then proved to be crucial in unexpected ways.
- For example, Euclid's division algorithm was discovered 2500 years ago and thought to just be a mathematical curiosity.
- Its first important use was discovered only 30 years ago, and now it underpins the encryption algorithms used in all secure communication on the internet.
- Maybe an important use of the Collatz conjecture will be discovered in 2500 years?
- We will use the Collatz conjecture as an introduction to Python programming, so make sure you understand it.

Collatz conjecture (informal description)

Choose a positive integer (that is, a whole number greater than 0), and apply the following process:

1. *If the integer equals 1, stop.*

2. *If the integer is even then divide it by two; otherwise (the integer must be odd) multiply it by three and then add one.*

3. *Return to Step 1.*

The Collatz conjecture predicts that: **regardless of which positive integer is chosen initially, this process will always ultimately stop, with the result equal to 1.**

- Of course, there is an unlimited number of possible choices for the initial value.
- The conjecture has not been proved, so no-one knows whether the claim (that the process always results in the number 1) is true or false. However, it is easy to test with some small specific initial values.

***Example** 7.2.1* Is the Collatz conjecture true for $n = 10$?

Answer: The following table shows the values arising during the above process, starting with $n = 10$.

Step	n (before)	n is:	Operation	n (after)
1	10	even	$\div 2$	5
2	5	odd	$\times 3 + 1$	16
3	16	even	$\div 2$	8
4	8	even	$\div 2$	4
5	4	even	$\div 2$	2
6	2	even	$\div 2$	1
7	1	1	stop	

After six operations the process gives the value 1, so the Collatz conjecture is true for the initial value $n = 10$.

Question *7.2.2* With respect to the Collatz conjecture:

(a) Work through the process with an initial value of 6.

(b) How many times do you need to apply the process with an initial value of 7 before you get to 1?

- Although the conjecture is yet to be proven true or false, most mathematicians who have worked on it believe that it is true.
- It has been tested and found to be true for all starting values less than or equal to about 10^{17}. It is also known to be true for infinitely many positive integers (for example, all powers of 2).
- Even though there is an impressive amount of data to *suggest* that the conjecture is true, this data does not *prove* that it is true.
- Proving that a conjecture like this is true requires it to hold in *every* case; to show that the conjecture is false, all that is needed is a *single* case that does not hold (called a *counter example*).
- In the past there have been mathematical conjectures that are true in very many cases, but have been falsified with a particular choice of value.
- With their ability to check many cases rapidly, computers are excellent tools to use in a search for counter examples.

End of Case Study 6.

7.3 Computers and Collatz's Conjecture

- The Collatz conjecture is a genuine example of a research problem in which large computer searches have been used.
- We will work through a Python program which can be used to test the Collatz conjecture on chosen initial values.
- This program is ideal for introducing you to some of the fundamental concepts you will require in order to develop models and write programs applicable to your scientific discipline.
- (Even if you are not especially interested in the Collatz conjecture, understanding exactly what it says and how it works will increase your ability to follow what the program is doing, and hence learn how to write your own programs.)
- First we define the specifications for the program.

***Example** 7.3.1* Write a Python program which:

- Asks the user to enter a positive integer.
- Proceeds through calculations of the Collatz conjecture, starting with the given integer. At each step, the program must print the step number and the current value.
- If the number has not become 1 within 10000 steps, print a message and stop. Otherwise, print the number of steps required for the integer to become equal to 1.

- The following stages illustrate a top-down design process for writing this program.
- The first stage is a very high-level description of what the program will do; it is essentially a repeat of the program specifications.

Python Example 7.3.2

```
1 Input the initial value.
2 Repeatedly
3   Calculate next step until value=1 (or step limit exceeded)
4 Print a final message.
```

- The second stage involves splitting Lines 2 and 3 into new Lines 3 to 7 which are each simpler and more like computer language commands.

Python Example 7.3.3

```
1 Input the initial value, say x.
2 Set a step counter equal to 0.
3 While the iteration has not finished:
4   If x is even then divide x by 2,
5   otherwise multiply x by 3 and add 1.
6   Print some output.
7   Add 1 to the step counter
8 Print a final message.
```

- The third stage involves splitting various lines into steps that are even simpler and closer to the commands in a programming language.

Python Example 7.3.4

```
Input the initial value, say x.
Set numSteps = 0.
While x is > 1 and the maximum number of steps is not exceeded:
  If x is even then
    Set x = x/2
  otherwise
    Set x = 3*x + 1
  Print the step number and new value of x.
  Set numSteps = numSteps + 1
Print a final message.
```

- The above examples should be sufficient to give you an idea of how top-down design proceeds in practise.
- To write the final version of this program, a number of additional subdivision stages were required. We will not step through them all here.
- The final version of the program is:

Python Example 7.3.5

```
from __future__ import division
from pylab import *

# This program investigates the Collatz conjecture, printing the
# sequence starting from a given initial value and stopping at 1.
# A message is printed if the value is not 1 within 10000 steps,
# steps, otherwise the number of steps is printed.

# The following function returns True if the given value is even,
# and returns False otherwise.
#
def isEven(x):
    if x % 2 == 0:
        return True
    else:
        return False

#
# Main Program.

x = input("Enter the initial Collatz value: ")
```

continued...

Python Example 7.3.5 *(continued)*

```
# Initialise values.

maxSteps = 10000
numSteps = 0

# Apply steps until we reach 1 or exceed the step limit.

while x > 1 and numSteps < maxSteps:
    if isEven(x):
        x = x/2
    else:
        x = 3*x + 1
    numSteps = numSteps + 1
    print "After step ",numSteps," the value is ",x

# Print a final message.

if numSteps == maxSteps:
    print "This did not become 1 within the step limit."
else:
    print "The initial value became 1 after ",numSteps," steps."
```

- You will have the opportunity to improve your programming skills in tutorials and assignments.
- We will mostly write relatively short programsm in SCIE1000.
- If you wish to develop additional programming expertise then you might like to study a programming course in Computer Science.

Python Example 7.3.6

The output that arises from executing the program with initial value 10 is:

```
Enter the initial value for the Collatz conjecture: 10
After step  1  the value is  5.0
After step  2  the value is  16.0
After step  3  the value is  8.0
After step  4  the value is  4.0
After step  5  the value is  2.0
After step  6  the value is  1.0
The initial value became 1 after  6  steps.
```

Python Example 7.3.7

The output that arises from executing the program with initial value 22 is:

```
Enter the initial value for the Collatz conjecture: 22
After step  1  the value is  11.0
After step  2  the value is  34.0
After step  3  the value is  17.0
After step  4  the value is  52.0
After step  5  the value is  26.0
After step  6  the value is  13.0
After step  7  the value is  40.0
After step  8  the value is  20.0
After step  9  the value is  10.0
After step  10  the value is  5.0
After step  11  the value is  16.0
After step  12  the value is  8.0
After step  13  the value is  4.0
After step  14  the value is  2.0
After step  15  the value is  1.0
The initial value became 1 after  15  steps.
```

7.4 Dissecting the program

- In the next few pages we will summarise some of the key concepts illustrated by the program.
- The contents of the program may at first be confusing, but in tutorials we will discuss in detail each of the major programming ideas. Also, your Python handbook provides a lot of extra information.

***Example** 7.4.1* If you have never seen a program before, you will immediately notice that:

- The program contains lines of computer commands, some of which also make some sense to a human reader – you can probably work out what some lines will do.
- Some lines look like they are messages or comments.
- Some lines are indented, and others are blank.
- Some lines look fairly mathematical.

Python Example 7.4.2

The top of the program.

```
1 from __future__ import division
2 from pylab import *
```

- When a program runs, the basic rule is that each line of code is executed in turn, from the top and working downwards. (This basic rule is modified by some commands within the program, particularly *functions*, *loops* and *conditionals*.)
- Thus, the Python programs starts by executing Line 1.
- Lines 1 and 2 tell Python to 'load in' libraries of useful commands, used later in the program. The library in Line 1 is called `__future__`, and the library in Line 2 is called `pylab`.

Python Example 7.4.3

Comments.

```
3
4 # This program investigates the Collatz conjecture, printing the
5 # sequence starting from a given initial value and stopping at 1.
6 # A message is printed if the value is not 1 within 10000 steps,
7 # steps, otherwise the number of steps is printed.
```

- Line 3 is blank, simply to make the program more readable.
- Lines 4 to 7 commence with a `#` character, which means that they are comments explaining what the program does to a person who reads the code. Python ignores comments.

Python Example 7.4.4

Functions.

```
12 def isEven(x):
13     if x % 2 == 0:
14         return True
15     else:
16         return False
```

- The `def` command tells Python that Lines 12 to 16 are defining a *function* called `isEven`.
- The lines of code within a function are not executed now, but instead can be *called* later in the program by using the name of the function.
- The function `isEven` takes one input value (called `x`), and gives an output value indicating whether or not `x` is even.
- The % command gives the remainder when x is divided by 2; a number x is even if the remainder equals 0.

Python Example 7.4.5

The `input` command.

```
19 # Main Program.
20
21 x = input("Enter the initial Collatz value: ")
```

- Line 19 is a comment, showing a reader where the main part of the program starts.
- Line 21 prints a message prompting the user for some input, and then waits for a value to be typed at the keyboard. This value is placed into a *variable* called `x`, which can be used later in the program.

Python Example 7.4.6

Initialising variables.

```
24 maxSteps = 10000
25 numSteps = 0
```

- Lines 24 to 25 assign some initial values to variables called `maxSteps` and `numSteps`.
- Assigning the value to a variable makes the program easier tol modify in the future.

Python Example 7.4.7

The `while` command.

```
29 while x > 1 and numSteps < maxSteps:
30     if isEven(x):
31         x = x/2
32     else:
33         x = 3*x + 1
34     numSteps = numSteps + 1
35     print "After step ",numSteps," the value is ",x
```

- Line 29 is the start of a *loop* within the program.
- Python uses indentation to show the *body* of the loop; that is, the lines that form the loop. Line 35 is the last line within the body of the loop.
- In general, the order of executing lines of code within a program is from top to bottom.
- Loops change this basic order. Lines within a loop are executed zero or more times, while some condition is satisfied.
- Line 29 gives a condition that must be satisfied for the loop to execute: you can see that Python allows commands like `and`.
- Line 29 should make sense: lines in the loop body (Lines 30 to 35) will be executed in turn, from top to bottom, while the value of the variable `x` is greater than 1 and also the value of `numSteps` is less than the value of `maxSteps`.

Python Example 7.4.8

The `if` command.

```
30      if isEven(x):
31          x = x/2
32      else:
33          x = 3*x + 1
```

- Lines 30 to 33 contain a *conditional* statement.
- In Line 30, the program *calls* the function named `isEven` which was defined in Lines 12 to 16. This function determines whether or not the value of `x` is even, and returns the value `True` or `False`.
- The `if` command in Line 30 tells Python to execute Line 31 if `x` is even. The `else` command in Line 32 tells Python to execute Line 33 otherwise (that is, if `x` is odd).
- Think about the Collatz conjecture: these lines make sense!

Python Example 7.4.9

Updating the value of a variable.

```
34      numSteps = numSteps + 1
```

- Line 34 is a very common programming construct, which may be confusing.
- The right hand side of the `=` sign is evaluated first. That is, the value of the variable `numSteps` is found, then `1` is added to that value.
- Then the left hand side is used; the new value is assigned to the variable `numSteps`.
- The final result of Line 34 is that the variable `numSteps` will be given a value one more than its previous value.

Python Example 7.4.10

The `print` command.

```
35     print "After step ",numSteps," the value is ",x
```

- Line 35 is a print command, which displays the step number and current value to the screen. All programs should produce sufficient output.

Python Example 7.4.11

The `print` command.

```
37 # Print a final message.
38
39 if numSteps == maxSteps:
40     print "This did not become 1 within the step limit."
41 else:
42     print "The initial value became 1 after ",numSteps," steps."
```

- Lines 39 to 42 display the final output to the screen, depending on whether or not the value became 1.
- Line 39 tests whether the number olf steps equals the maximum number of steps. The Python `if` command tests for equality using two equals signs, `==`.
- If the value did not become 1 then a message is printed in Line 40, otherwise the number of steps is printed in Line 42.

7.5 Errors

- The consequences of software errors can be quite serious.

Example 7.5.1 In Example 4.1.1 we noted that in 1999 the Mars Climate Orbiter crashed into Mars as the result of a software error in relation to the units on some calculated values.

Example 7.5.2 (From: news.bbc.co.uk, Tuesday, 9 February 2010)

Toyota in global recall of Prius

"Toyota has announced the recall of about 436,000 hybrid vehicles worldwide, including its latest Prius model, to fix brake problems…'We have decided to recall as we regard safety for our customers as our foremost priority,' the firm said…The Prius was Japan's top-selling car in 2009 and the world's most popular hybrid model.

Peter De Lorenzo, author of the book The United States of Toyota, told the BBC that the latest recall would be particularly painful for the company. 'The Prius is their shining example of their vision of what we should all be driving and it is everything the new Toyota represents. So for them to have to acknowledge a recall of hundreds of thousands of them is a tremendous blow to their image,' he said.

Credit rating agency Moody's said it had put Toyota's credit rating on review for a possible downgrade…Toyota's president has come under criticism from Japan's transport minister Seiji Maehara for not reacting quickly enough to recall faulty vehicles. 'I wish you had taken measures earlier rather than simply saying it was not a major technical problem,' Mr Maehara told Mr Toyoda in a meeting. Mr Maehara said he would meet US ambassador John Roos on Wednesday to discuss the situation. 'Recalling defective products is important, but each country needs to consider how to prevent this from becoming a diplomatic problem'…

There have been complaints in Japan and the US that the brakes momentarily fail when driven on rough or slippery road surfaces. **Toyota blames a software glitch**…"

- Even the best and most experienced computer programmers will sometimes (even often) make errors (*bugs*) in their programs.
- A key skill in programming is minimising the number of errors, and then identifying and fixing any that occur.
- There are many different types of error, including incomplete problem description, design faults in the software, unanticipated 'special cases', coding errors, logic errors and miscommunications within teams of programmers.

Testing and debugging

Most newly written programs include errors, and it is important to adopt a systematic approach to identifying and fixing them. This process is often called testing *and* debugging.

There are many types of programming error; some will be easy to find (like a missing bracket), some will result in error messages (like trying to divide by zero), but in many other cases the program will produce incorrect output without an error message.

To find such errors, you will need to test your program with different input values, and check the output by hand. Testing is a very important part of the overall programming process!

Avoiding errors

When writing programs, make sure that you:

- *understand the specifications* **before** *starting;*
- *think about the best and most logical way to solve the problem;*
- *consider planning your program on paper first;*
- *put comments in your program so you (and others) know what you are trying to do;*
- *test your programs on a range of data;*
- *check some output carefully to make sure it is correct; and*
- *pay attention to any error messages!*

Error messages are your friends!

If Python gives you error messages, make sure you use them in the correct ways:

- *do not ignore them: they give useful advice about what is going wrong;*
- *do not be scared of them;*
- *think about what they are saying;*
- *make full use of all of the information they give; and*
- *think about how you fixed similar errors in the past.*

Python Example 7.5.3

Here is an example of a Python program with an error:

```
from __future__ import division
from pylab import *

a = input('Tell me a number: ')
b = input('Tell me another number: ')

c = a + b
d = a * bb

print a, '+', b, '=', c
print a, 'x', b, '=', d
```

Here is the output from running the program:

```
>>>
Tell me a number: 8
Tell me another number: 7

Traceback (most recent call last):
  File "example.py", line 8, in <module>
    d = a * bb
NameError: name 'bb' is not defined
```

- The error message gives the following information:
  1. The last line of the error message (Line 8 above) identifies *what* the type of error is, in this case:

     `NameError: name 'bb' is not defined`

  2. The second line of the error message (Line 6 above) shows *where* the error was detected.

     `File "example.py", line 8, in <module>`

     This indicates the file and line in which the error occurred. Examine the identified line of the program and look carefully for a mistake. In this case, in Line 8 of the program the programmer has accidentally typed '`bb`' instead of '`b`'.

- If a program contains multiple errors, Python will display the message for the first one it encounters.
- After fixing that error, a different error message may appear. *This is usually a good sign*: it means that the first error is fixed, and you can move on.

Common errors

Here are some common error messages and possible causes.

- `SyntaxError` *The command is not understood by Python. Perhaps:*
  - *your brackets are incorrect (such as* `( )` *instead of* `[ ]`*);*
  - *you have forgotten a bracket; or*
  - *your indentation is incorrect.*
- `NameError` *There is no variable with the given name. Perhaps:*
  - *you have mistyped the name of a variable; or*
  - *you have forgotten to set a starting value for a variable.*
- `ImportError` *A module to be imported does not exist. Perhaps you mistyped the name of the module to import.*
- `OverflowError` *The answer is too large or too small to calculate.*
- `ValueError` *One of the arguments you have given is not valid for this function.*

7.6 Space for additional notes

8 Progress Report 1

- As we work through SCIE1000, it is useful to take the time to consider the course as a whole.
- Students sometimes feel that the course content "jumps around", however we are aiming to build an overall cognitive framework for learning and doing science.

Where are we up to?

- So far we have:
  - presented a broad overview of the nature of science, and the various activities which comprise science;
  - explained how SCIE1000 and your other courses fit into this framework;
  - identified the importance of modelling, and the five common ways of presenting models;
  - introduced some basic science knowledge;
  - discussed the importance of quantitative communication;
  - analysed the philosophical nature of science and scientific thought, including hypotheses; and
  - described how computer programs and Python can be used to model phenomena.
- By now, you should have a reasonably solid understanding of the basis of scientific activities and thought processes, and the role that modelling plays in science.
- In the first lecture we outlined six classes of activity crucial to the scientific process, and we estimated how much of each activity is represented in SCIE1000 (and in some other courses).
- The following table outlines this information, and what we have covered so far in SCIE1000.

Skill/Activity	Overall	Done so far
Scientific discipline knowledge	5%	3%
Scientific thinking and logic	15%	12%
Communication and collaboration	15%	10%
Curiosity, creativity, persistence	15%	5%
Observation and data collection	0%	0%
Modelling and analysis	50%	5%

How does it link together:

- In Chapter 2 we built an overall picture of different skills, approaches and thought processes required to do science.
- In Chapter 6 we refined this, considering the nature of logical, scientific thought.
- In Chapter 4 we covered some basic scientific knowledge, setting the scene for future in-depth study of phenomena.
- In Chapter 5 we discussed the importance of precision, accuracy, honesty and scepticism when communicating quantitative scientific information, and when collecting, analysing and using data.
- In Chapter 3 we considered the role of modelling in simplifying reality whilst also maintaining relevance and sufficient accuracy.
- In Chapter 7 we demonstrated how writing computer programs allows more sophisticated models to be developed, because of their ability to perform calculations rapidly.

What we will do next:

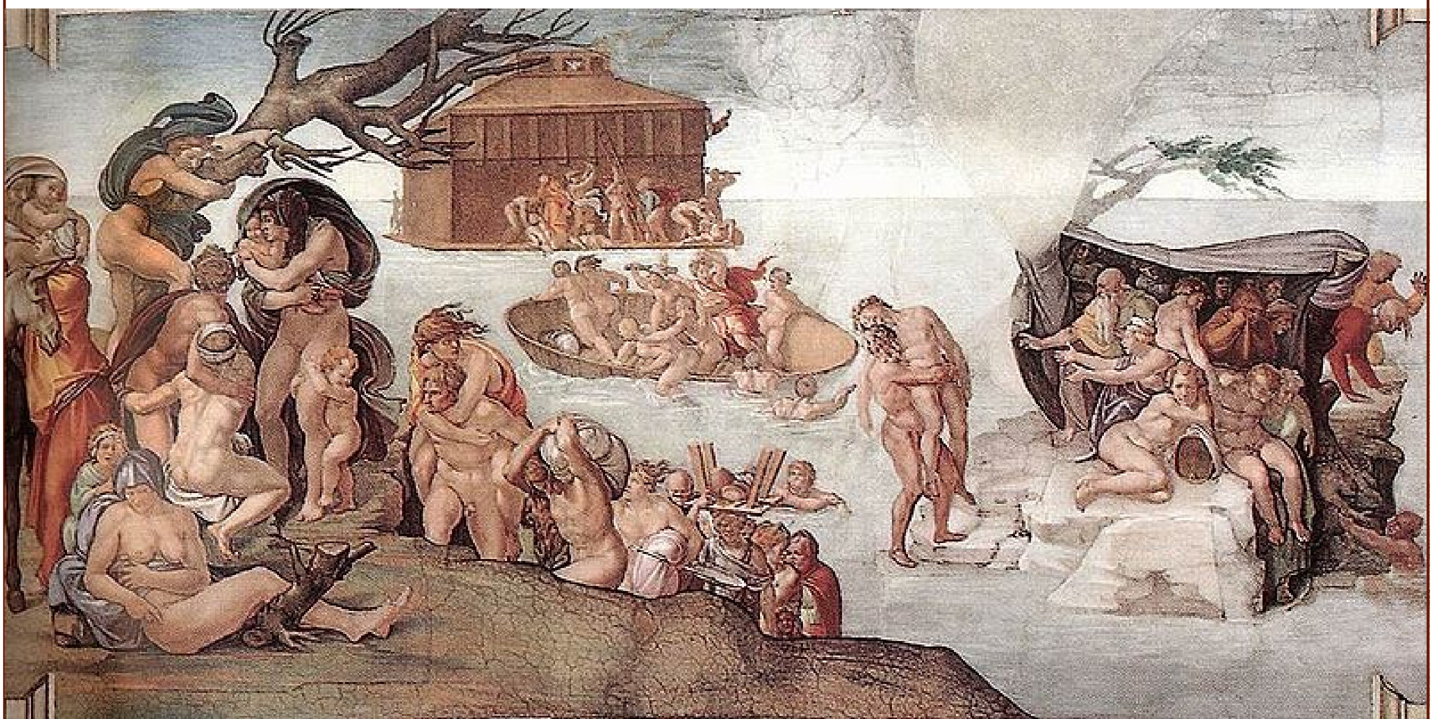
- For most of the rest of semester we will focus on modelling and analysis. In the next three chapters we will:
  - remind you of mathematical functions and their uses;
  - encounter functions which are: linear, quadratic, power, periodic, exponential and logarithmic;
  - see that these functions can be used to model phenomena in a diverse range of scientific areas;
- We will study all of these topics through authentic and important scientific contexts.
- Do not attempt to memorise details of particular contexts or mathematical approaches.
- Instead, understand *when* and *how* each technique can be applied, and how to decide which is the most appropriate to use.
- We will also see examples of how Python programs can assist with the modelling process.

9 Climate, species and functions

We are a rock revolving around a golden sun
We are a billion children rolled into one
So when I hear about the hole in the sky
Saltwater wells in my eyes.
We climb the highest mountain, we'll make the desert bloom
We're so ingenious we can walk on the moon
But when I hear of how the forests have died
Saltwater wells in my eyes.

Artist: Julian Lennon

(www.youtube.com/watch?v=GzvjuMkAEEU)



The Deluge (1508 – 1512), Michelangelo (1475 – 1564), Sistine Chapel ceiling, Apostolic Palace, Vatican.

(Image source:
commons.wikimedia.org/wiki/Image:The_Deluge_after_restoration.jpg)

Introduction

As we saw earlier, scientific models allow us to simplify reality while still making useful inferences and predictions about events and processes. We also noted that in modern science, many models are fundamentally quantitative because they are based on identified frequencies, patterns and relationships between various values. Models are commonly presented in five ways: words, values, pictures, equations and computer programs. In the next few chapters we will consider in detail how equations can be used to represent models.

The mathematical concept that allows patterns to be quantified is the *function*. Essentially, a function is a rule that takes some input (such as a collection of factors that impact on the phenomenon being modelled), applies the rule to the input, and gives a corresponding output. This output is typically compared with reality, testing the accuracy of the model.

You will need to be familiar with a variety of functions, know how to manipulate and apply them, and decide which are likely to be most appropriate in differing situations.

Some of the examples/contexts we will discuss are:

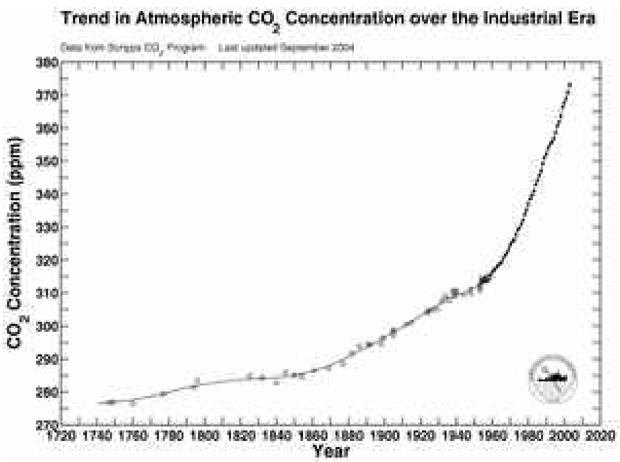
- The Keeling curve and CO_2 concentrations in the atmosphere.
- Temperature and measurement scales.
- Bicknell's thrush and climate change.
- Species-area curves and biodiversity.
- Wind chill.

Specific techniques and concepts we will cover include:

- Definition of a function.
- Linear functions.
- Quadratics and power functions.

9.1 Introduction to functions

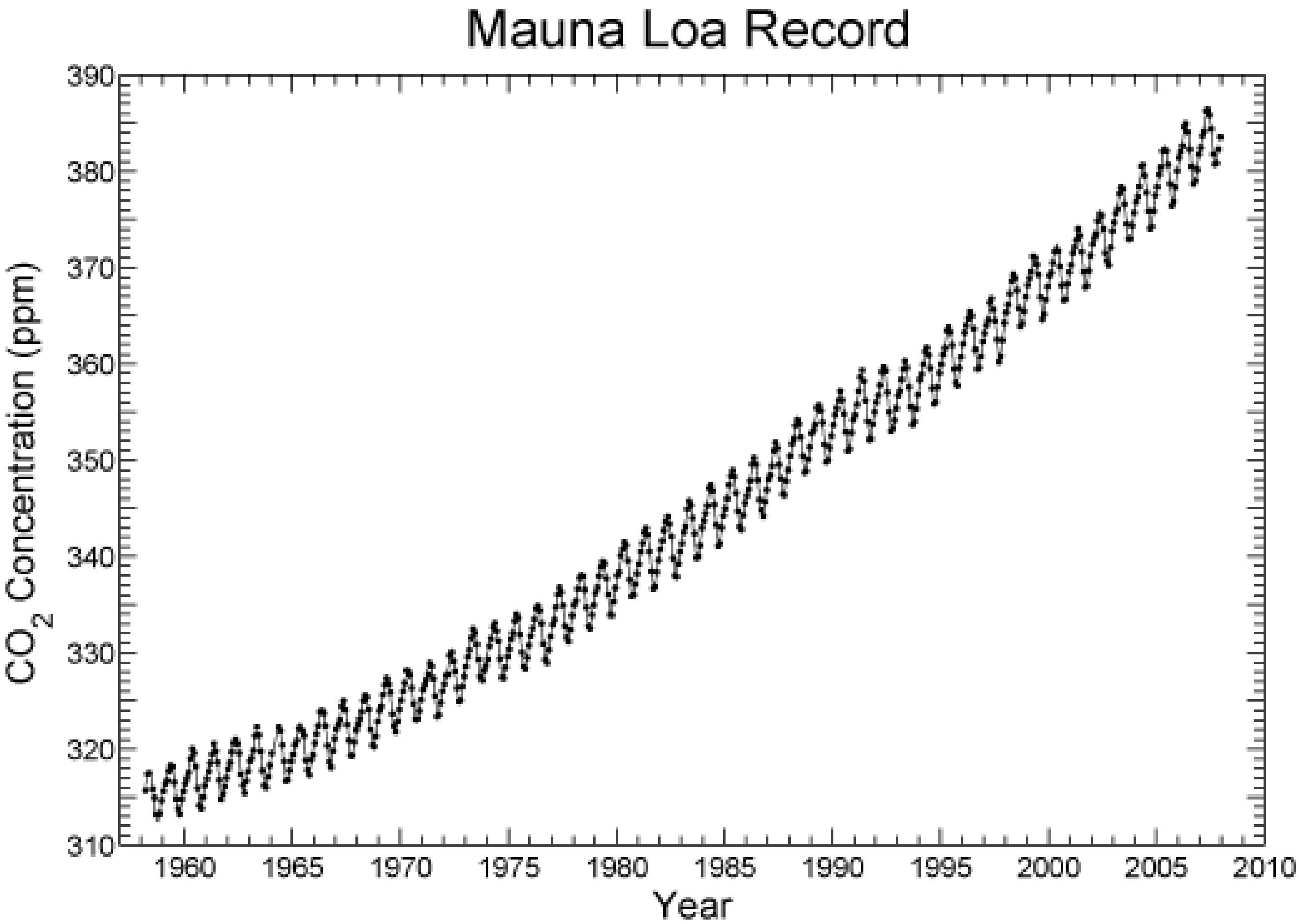
Case Study 7: Atmospheric CO_2 and the Keeling curve



- Scientifically, it is widely accepted that:
  - Earth is undergoing a period of rapid climate change;
  - global temperatures are likely to rise rapidly over coming years;
  - this warming is related to increasing concentrations of carbon dioxide in the atmosphere; and
  - the increase in atmospheric CO_2 concentration is a result of human activity.
- There is a famous, long-running study measuring the change in atmospheric CO_2 concentrations over time.

Example *9.1.1* The Scripps Institution of Oceanography is based in San Diego, USA. Their website includes the following:

> "Charles David Keeling directed a program to measure the concentrations of CO_2 in the atmosphere that continued without interruption from the late 1950s through the present. This program, operated out of Scripps Institution of Oceanography, is responsible for the Mauna Loa record, which is almost certainly the best-known icon illustrating the impact of humanity on the planet as a whole...."



This graph is called the **Keeling** curve.

continued...

***Example** 9.1.1 (continued)*

- This study has continuously measured atmospheric concentrations of CO_2 at the Mauna Loa observatory in Hawaii for around 50 years.
- Gases in the atmosphere mix fairly well, so this measurement is considered as representative of the atmospheric CO_2 concentration world-wide.
- The current level is around 380 parts per million by volume (ppm or ppmv).
- Other data from ice-core samples shows that long-term CO_2 levels for thousands of years have remained relatively constant at 280 ppm, but started increasing in the 19th century.

***Question** 9.1.2* With reference to the Keeling curve shown in Example 9.1.1:

(a) Describe the main features of the graph.

(b) What physical factor(s) could cause those features?

End of Case Study 7.

- Mathematics is the language commonly used to describe quantitative relationships and patterns.

Functions

In mathematics, a function *is a rule which converts input value(s) to output values. If f is the name of a function, then* $f(x)$ *denotes the output that arises from applying the function f to the input x.*

- A key skill in modelling is recognising which type of function is likely to best represent the observed data.
- In the next few sections we will study some phenomena and see how a range of useful mathematical functions allow us to represent and study these phenomena.
- It is not important that you memorise specific details about the particular case studies (such as the scientific name of Bicknell's thrush or the formula for wind chill).
- Instead, understand the concepts **behind** the examples, including which functions should be used to model which type of phenomena, and how to interpret mathematics in a scientific context.
- One point we will continually stress is the diversity of phenomena which can be modelled by the same (or very similar) functions.

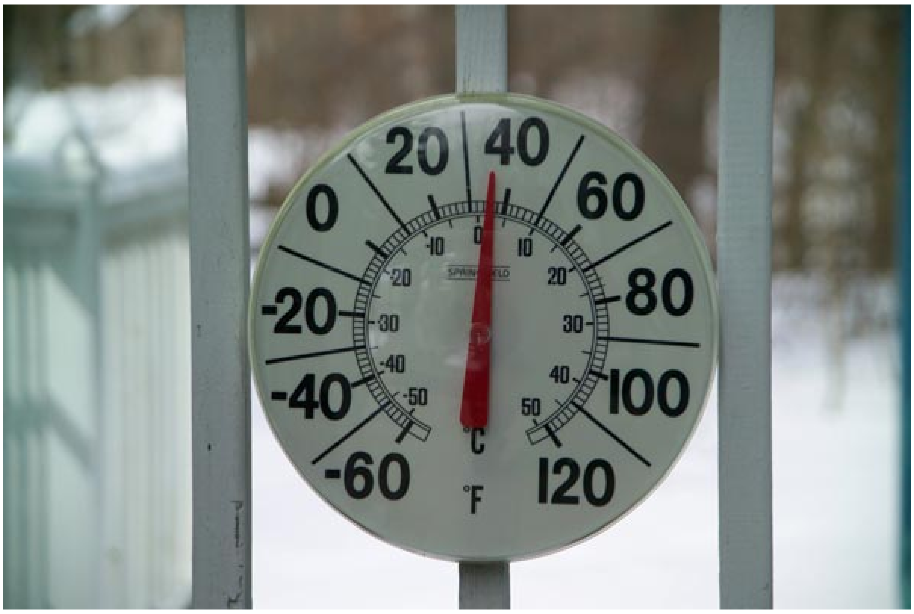
9.2 Linear functions

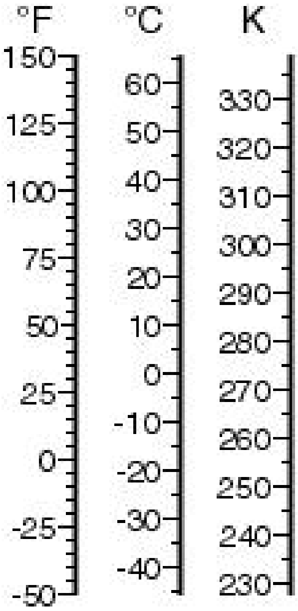
Linear function

Linear *functions have equations* $y(x) = mx + c$ *, where m and c are constants. Graphs of linear equations are straight lines.*

Linear functions are useful for modelling phenomena in which the y value changes by the same amount for each given change in x value, irrespective of the x value.

Case Study 8:
Temperature

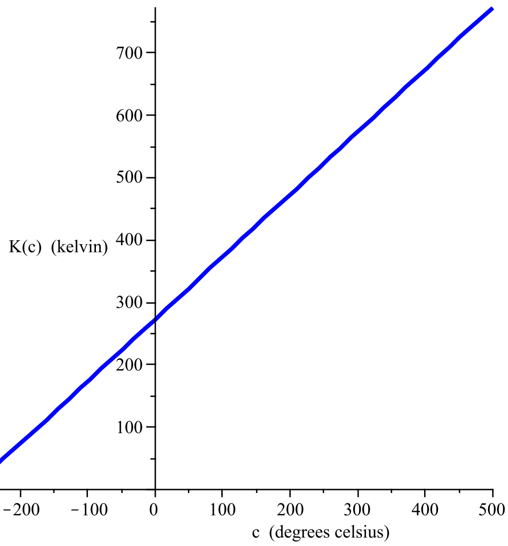




Question *9.2.1* A temperature of c degrees Celsius can be converted to an equivalent temperature on the kelvin scale by the function

$$K(c) = c + 273.15.$$

A graph of this function is:



continued...

Question *9.2.1 (continued)*

(a) The United States is one of the few countries in the world to use the *Fahrenheit* scale as their standard. A temperature c in degrees Celsius can be converted to Fahrenheit by the function

$$F(c) = \frac{9c}{5} + 32.$$

Derive a function that converts a temperature f in **Fahrenheit** to an equivalent temperature k in **kelvin**.

(b) The highest temperature ever recorded on Earth was 160 degrees Fahrenheit, in Libya in 1922. Convert this to degrees Celsius and also to kelvin.

continued...

***Question** 9.2.1 (continued)* Recall that

$$K(c) = c + 273.15 \quad \text{and} \quad F(c) = \frac{9c}{5} + 32.$$

(c) Find the temperature(s) at which the Fahrenheit and Celsius scales give the same reading.

(d) Find the temperature(s) at which the Fahrenheit and kelvin scales give the same reading.

(e) Find the temperature(s) at which the Celsius and kelvin scales give the same reading.

Then we can develop a computer model.

Program specifications: Write a program which allows the user to convert a temperature from Celsius to Fahrenheit, or Fahrenheit to Celsius.

Temperature *(continued)*

Python Example 9.2.2

```
# A program to convert between Celsius and Fahrenheit
from __future__ import division
from pylab import *
origTemp = input("What is the original temperature? ")
choice = input("Type 1 to convert C -> F, or 2 for F -> C: ")

if choice == 1:
# C-> F
    newT = origT * 9 /5 + 32
    newT = round(newT,1)
    print origT," Celsius is approximately",newT,"Fahrenheit."
else:
# F-> C
    newT = (origT - 32) * 5 / 9
    newT = round(newT,1)
    print origT," Fahrenheit is approximately",newT,"Celsius."
```

Python Example 9.2.3

Here is the output from running the above program three times:

```
What is the original temperature? 0
Type 1 to convert C -> F, or 2 for F -> C: 1
0  Celsius is approximately 32.0 Fahrenheit.

What is the original temperature? -40
Type 1 to convert C -> F, or 2 for F -> C: 2
-40  Fahrenheit is approximately -40.0 Celsius.

What is the original temperature? 160
Type 1 to convert C -> F, or 2 for F -> C: 2
160  Fahrenheit is approximately 71.1 Celsius.
```

End of Case Study 8.

9.3 Functions with other powers

- As we just saw, the relationships between equivalent temperatures in Celsius, kelvin and Fahrenheit are all linear, so the highest power of any variable in the equation is 1.
- Many quantities in science are related linearly, but other quantities relate in different ways. One such relationship is to have powers that are not equal to 1.
- We will first study an example in which the power is 2 and then some examples in which the power is between 0 and 1.

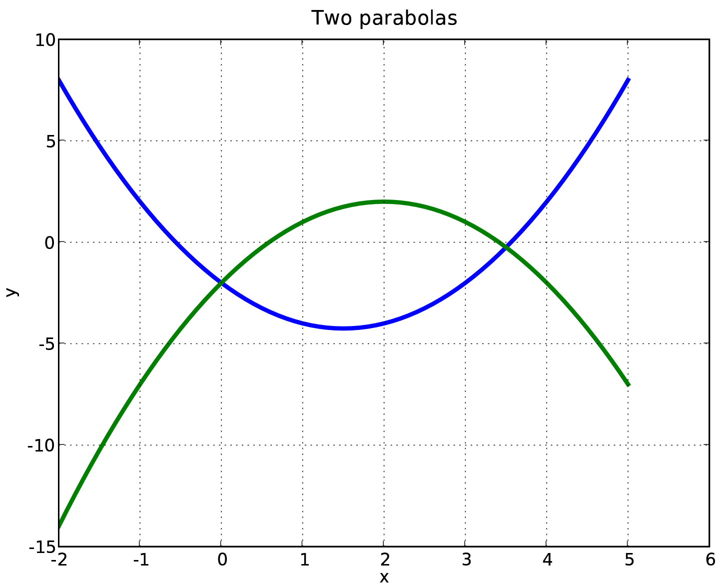
Quadratic function

Quadratic functions have equations

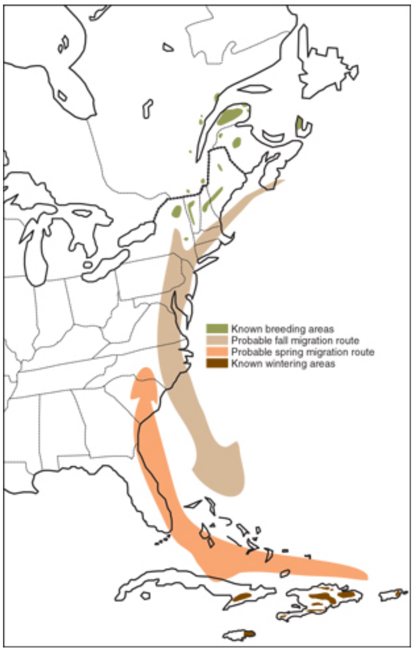
$$y(x) = ax^2 + bx + c,$$

where a, b and c are constants and $a \neq 0$. The graph of a quadratic is a parabola.

***Example** 9.3.1* Here are the graphs of two quadratic equations for x between -2 and 5.:



Case Study 9:
Climate change and Bicknell's thrush



Example *9.3.2* A paper[a] gives a model of the distribution of birds at various altitudes and temperatures in locations in North East USA, and then uses their models to predict the likely impact of rising temperatures on these distributions. Part of their study focused on Bicknell's Thrush, *Catharus bicknelli*.

- Collecting data for this study involved the following process (which we saw earlier in Example 7.1.1):
  - Subdividing the region being studied into rectangular cells each 30 m square;
  - Classifying each cell according to the mean July (summer) daily maximum temperature in that cell (this temperature in general was proportional to the altitude of the cell);
  - Conducting fieldwork on a representative sample of cells to determine which cells were thrush-positive (that is, contained at least one resident thrush).

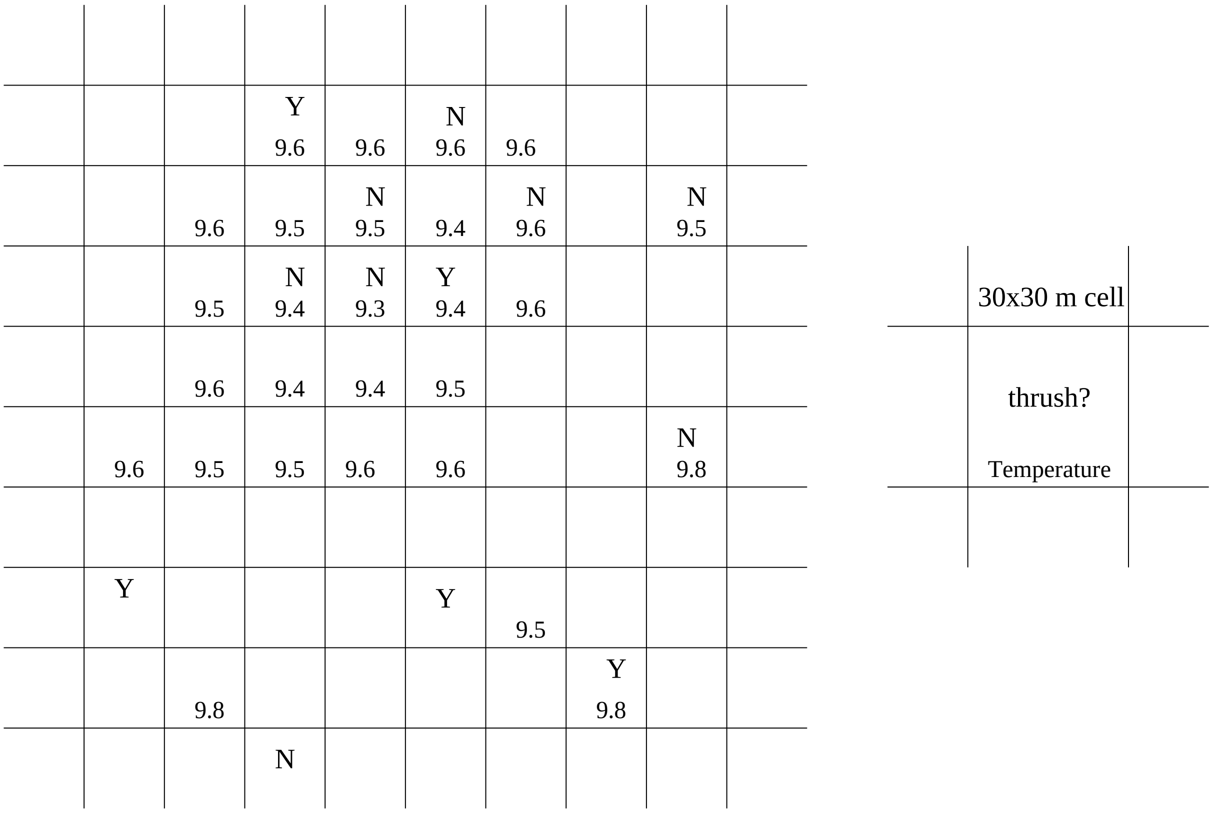
continued...

[a]Rodenhouse et al., *Potential effects of climate change on birds of the north-east*, Mitigation and Adaptation Strategies for Global Change, **13** (2008) 487–516

***Example** 9.3.2 (continued)*

- Data was used to estimate the proportion of cells with each maximum temperature which are thrush-positive.
- This process resulted in a model of thrush distribution across their habitat based on temperatures within that habitat.

The following diagram shows an example of a partial data set that **could** have been collected:



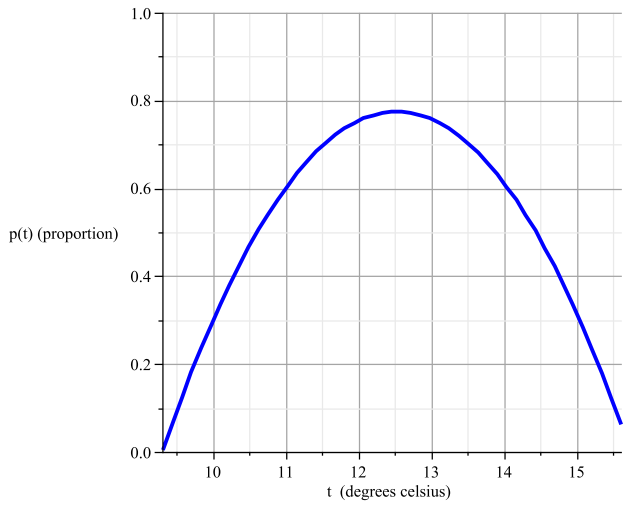
The study found that no significant thrush habitats possess July temperatures outside the range 9.3 °C to 15.6 °C.

After conducting statistical analysis on their data, the researchers showed that the proportion $p(t)$ of thrush-positive cells is closely modelled by the quadratic function

$$p(t) = -0.0747t^2 + 1.8693t - 10.918$$

where t is a temperature in °C, between 9.3 °C and 15.6 °C.

***Question** 9.3.3* The graph of $p(t) = -0.0747t^2 + 1.8693t - 10.918$ is:



(a) What is the probability that a thrush will be found in a sample area in which $t = 11$ °C?

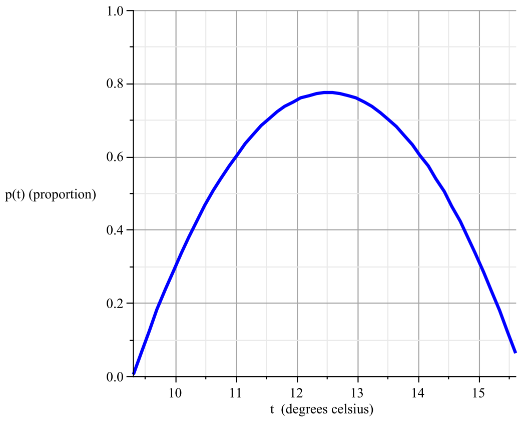
(b) From the graph, at what (approximate) value of t are these thrush most densely distributed, and what is the (approximate) value of $p(t)$?

(c) There is no value of t for which $p(t) = 1$. Explain (in words) what this means in terms of the thrush, and give a reason why it would happen.

continued...

***Question** 9.3.3 (continued)* Average temperature rises in this region over the next century are predicted to range from 2.8 °C under a low greenhouse gas emission scenario, to 5.9 °C under a high emission scenario.

Recall that the graph of $p(t) = -0.0747t^2 + 1.8693t - 10.918$ is:



(d) How would **this graph** change if the average temperature rose by 2.8 °C? What if it rose by 5.9 °C? Explain your answers.

(e) What key factor relevant to the thrush **would** change if there were a substantial rise in average temperatures?

continued...

Question *9.3.3 (continued)* Consider the following measured areas of existing thrush habitat, and the predicted areas remaining after possible temperature rises over time.

Scenario	habitat (hectares)
(current) +0°C	140000
+1°C	32000
+2°C	10000
+3°C	1000
+4°C	200
+5°C	75
+6°C	0

(f) Draw a rough graph of the habitat size as a function of change in temperature.

(g) Give some physical reasons why your graph has this shape.

continued...

Question *9.3.3 (continued)*

(h) What is the likely impact on the thrush population of a temperature rise of 2.8 °C?

(i) What is the likely impact on the thrush population of a temperature rise of 5.9 °C?

(j) What survival strategies are there for the thrush if there is an increase in temperature at the higher end of predictions?

There are many other examples of species at risk from climate change.

Example *9.3.4*

Antarctic beech (*Nothofagus moorei*) is a temperate rainforest tree species found in isolated locations in South East Queensland (Lamington and Springbrook National Parks), and northern New South Wales. They can live for several thousand years.

This species tends to occur only at the highest points of mountains, particularly at the northern extremes of its distribution. Rapid climate change will probably result in local extinction.

Question *9.3.5* Scientists often need to estimate the abundance of something that is difficult to measure. One approach is to extrapolate from a sample; the *tag and release method* is an example.

Melanie the marine biologist wants to estimate the number of fish N living on an isolated reef. She captures a sample of S_1 fish, tags them and releases them. One week later, she collects another sample of size S_2 and finds S_3 tagged fish amongst them. Assuming the population size has not changed, develop a formula to estimate N.

End of Case Study 9.

Case Study 10:
Species-area curves and biodiversity

- The previous case study discussed the abundance and distribution of *individual* species. Ecologists often study the *overall number of species* found in a region (sometimes called the region's *biodiversity* or *species diversity*).
- Species diversity is often modelled using mathematical functions with powers other than 1 (linear) and 2 (quadratic).

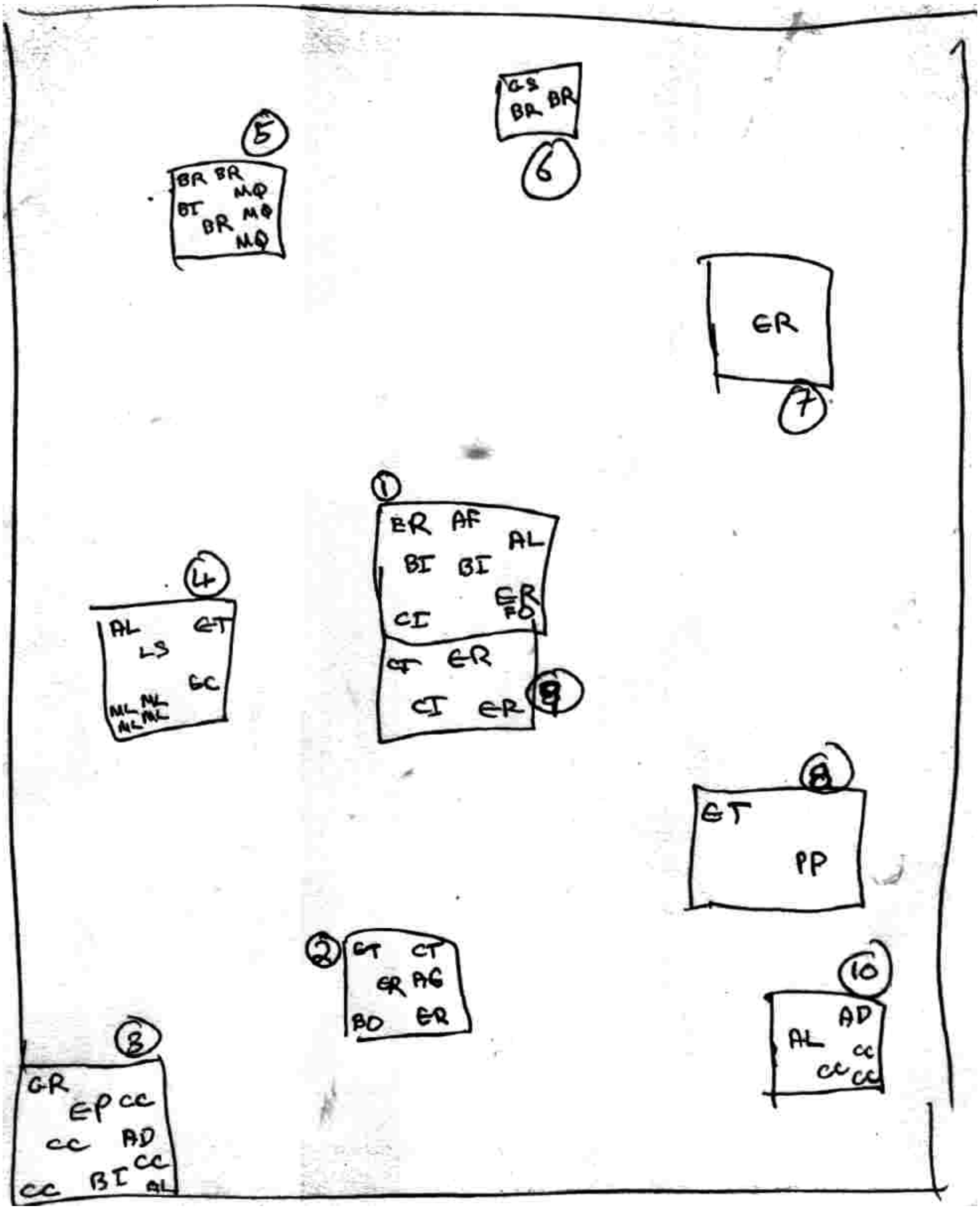




- Rather than undertaking a full species count over the entire region, data from a sample can be extrapolated to cover the entire region.
- This can be used to estimate the abundance of **all** species, or of species satisfying a particular property, or even of the number of individuals showing certain characteristics.

***Example** 9.3.6* Peter lives on 4 hectares in eastern Brisbane. He wishes to estimate the number of distinct, naturally occurring, native plant species with individuals more than 2 m in height which occur on his land.

He divides his land into cells of 10 m square, randomly selects ten cells, and records the locations of individual plants within those cells. The following diagram shows his data sheets (species are shown on the next page.)



continued...

Example *9.3.6 (continued)* The following table collates the species data collected in Example 9.3.6.

The table shows:

- the cell number, from 1 to 10;
- the number of additional species identified in that cell;
- the names of the additional species identified in that cell; and
- the cumulative total C of species identified in this and previous cells.

Note that each species is recorded (and counted) only once.

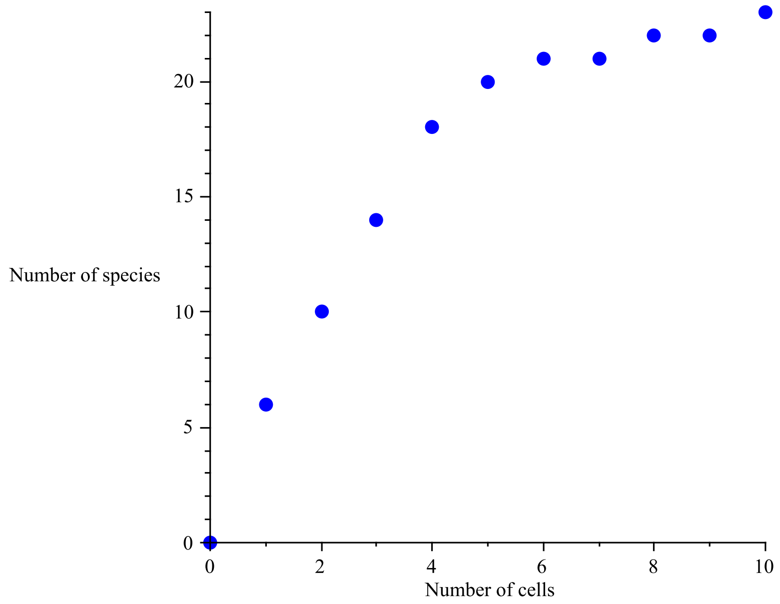
Cell	Num. new sp.	New species	C
1	6	*Eucalyptus racemosa*, *Acacia fimbriata*, *Banksia integrifolia*, *Corymbia intermedia*, *Allocasuarina littoralis*, *Ficus obliqua*	6
2	4	*Eucalyptus tereticornis*, *Alphitonia excelsa*, *Corymbia trachyphloia*, *Breynia oblongifolia*	10
3	4	*Acacia disparrima*, *Eucalyptus propinqua*, *Casuarina cunninghamiana*, *Grevillea robusta*	14
4	4	*Acacia leiocalyx*, *Lophostemon suaveolens*, *Melaleuca linariifolia*, *Eucalyptus crebra*	18
5	2	*Banksia robur*, *Melaleuca quinquinerva*	20
6	1	*Glochidion sumatranum*	21
7	0	–	21
8	1	*Petalostigma pubescens*	22
9	0	–	22
10	1	*Angophora leiocarpa*	23

- Using the above information, it is possible to draw a graph of the number of distinct species recorded versus the number of cells surveyed.

Species-area curves

In ecology, a species-area curve *is a graph showing* *the number of distinct species observed in a particular environment, as a function of the size of the area surveyed.*

Example *9.3.7* The following graph is a species-area curve showing the data in Example 9.3.6:



- The graph has a shape that is typical of many species-area curves: the number of distinct species initially rises rapidly as the area increases, but then rises less rapidly as the area becomes larger.
- In this case, Peter collected additional data (not shown in the graph) to investigate what happened as he surveyed a larger area.
  - after 20 cells were surveyed, the total number of species identified was 25 (so the total only increased by two compared to his survey of 10 cells).
  - After 50 cells were surveyed, the total number of species identified was 28 (so a further increase of only three).
- Mathematically, species-area curves (and similar phenomena) are often modelled using *power functions* .

Power functions

Power functions have equations

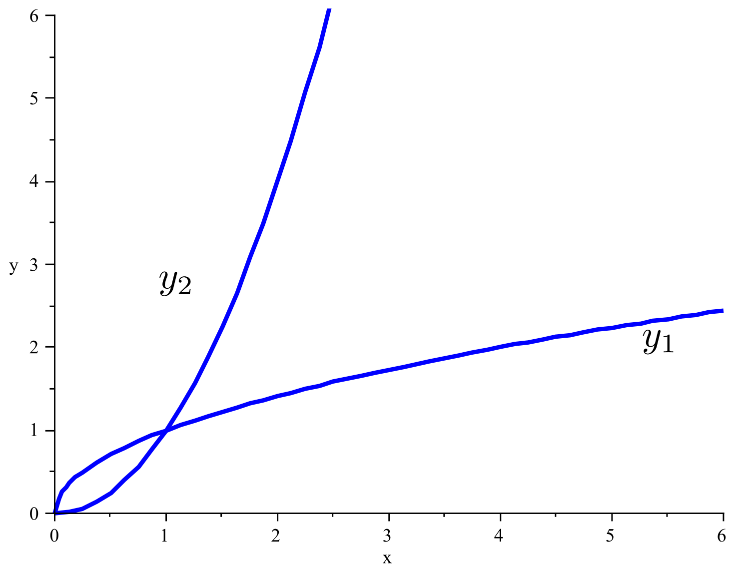
$$y(x) = ax^p$$

where a and p are constants. (Note that the power p does not need to be an integer.)

Changing the value of the power leads to graphs with different shapes. If the power is:

- *0, then the graph is a horizontal line;*
- *between 0 and 1 then the graph increases less rapidly as x gets larger;*
- *1, then the graph is a straight line ; and*
- *greater than 1 then the graph increases more rapidly as x gets larger.*

***Example** 9.3.8* The graphs of $y_1 = x^{0.5}$ and $y_2 = x^2$ are shown in the figure below. The differences in their shapes mean that they are suitable for modelling different phenomena.



Equations for species-area curves

Species-area curves are most often represented using power functions, with power p between 0 and 1.

Their general form is $S(a) = Ca^p$, *where S is the number of species occurring as a function of the area a, and C and p are constants depending on the geographical location, resource availability and biological diversity of that environment.*

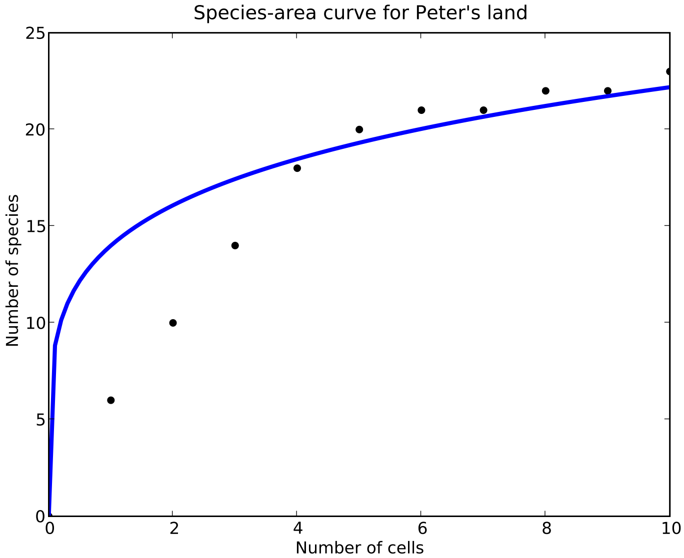
Question *9.3.9* With respect to a species-area curve $S = Ca^p$:

(a) Why do species-area curves have that general shape?

(b) Describe some physical features that would make the values of C and p smaller or larger.

(c) What ramifications does the shape of species-area curves have for sampling techniques?

Example *9.3.10* The graph of $f(x) = 14x^{0.2}$ is shown in the following figure, along with the species data from Example 9.3.7. If x is the number of 10 m square cells in Peter's land then $f(x)$ gives a *reasonable* (continuous) model of the data. (Note that the model is inaccurate for small numbers of cells, but in practise it would only be applied for large numbers of cells.)



(When you study STAT1201, you'll see how to use statistical analysis to judge more precisely whether a model gives a "good fit".)

Question *9.3.11* Assume that Peter's land is ecologically representative of his local area. All parts of this question refer to species of native, naturally occurring plants more than 2 m high.

(a) Estimate the total species diversity on Peter's 4 hectare property.

(b) Peter's street block measures about 1.5 km by 600 m. Estimate the total species diversity of his street block.

continued...

Question *9.3.11 (continued)*

(c) The land on which Peter lives is four times the size of the land on which his neighbour lives. Predict the relative species diversity of these parcels of land.

- The next example shows a Python program which models the species diversity in a given area, assuming Peter's property is ecologically representative of that area.

Python Example 9.3.12

```
# A program to predict species diversity in Peter's neighbourhood

from __future__ import division
from pylab import *

area = input("What is the total area in m^2? ")
numSquare = area/100
numSpecies = 14 * numSquare**0.2

print "Predicted number of species: ",round(numSpecies,0)
```

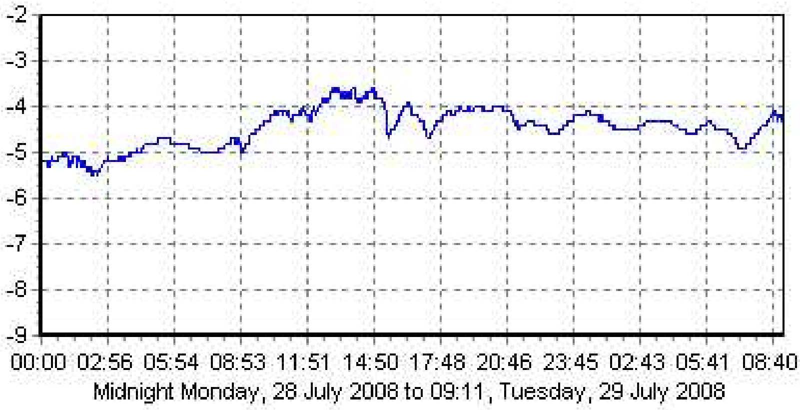
Here is some output from running the program twice; the output checks the answers to Question 9.3.11.

```
What is the total area in m^2? 40000
Predicted number of species:  46.0

What is the total area in m^2? 900000
Predicted number of species:  86.0
```

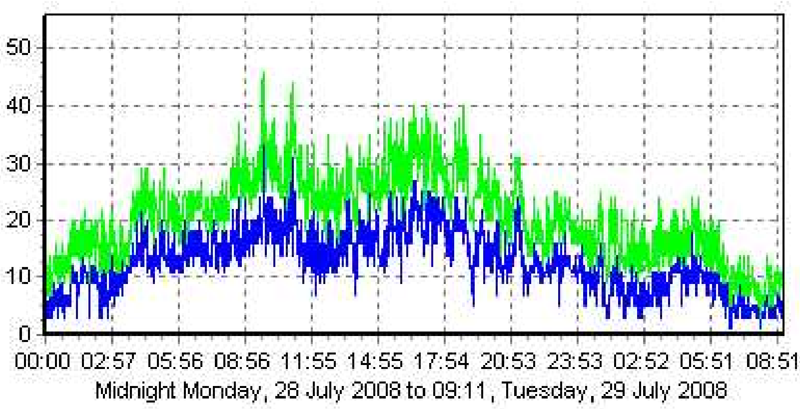
End of Case Study 10.

- In previous examples we have seen how some simple mathematical functions are used to model various phenomena, and how to interpret these models.
- Next we build on the functions we have studied, by combining multiple physical factors in the model.
- Rather than a single independent variable (like time t or area a), the next example considers how the ambient temperature **and** the wind velocity combine to change the apparent temperature that we perceive.

Case Study 11:
Wind chill



(temperatures at Thredbo ski resort)



(Wind velocities at Thredbo ski resort)

Dusting of snow, extra blankets everywhere

Brian Williams
ENVIRONMENT REPORTER

IT snowed in Queensland yesterday but it will pay to rug up because even colder weather is expected tomorrow.

Snow, sleet, wind and rain ripped through the Granite Belt and southern Darling Downs, bringing freezing conditions.

The cold snap was felt virtually all over the eastern seaboard and the ski fields at Perisher in the NSW Snowy Mountains enjoyed a 15cm dump of snow.

In Queensland, overnight temperatures were below average for much of the state. Brisbane is tipped to experience temperatures down to 6C early tomorrow and Thursday.

At Dalby wind dragged the temperature down to -0.2C at 2pm.

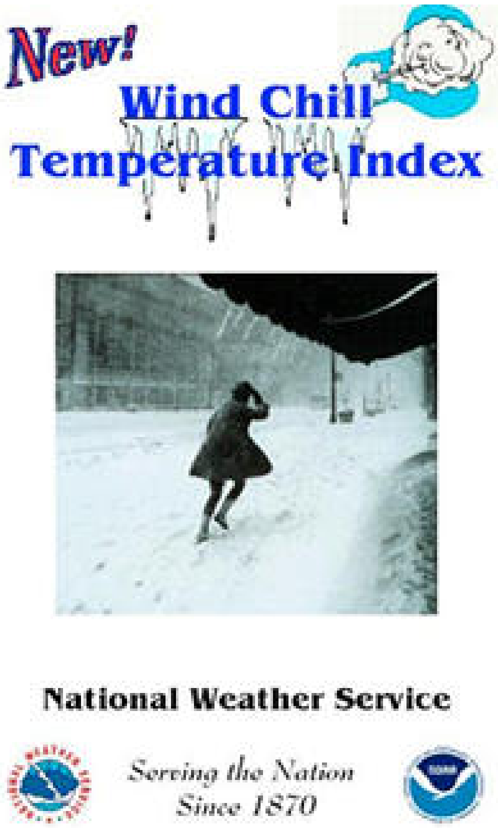
At the same time, the wind chill factor meant Warwick dropped to 1.2C, Applethorpe in the Granite Belt 0.4C and Brisbane City 9.9C.

Granite Belt Wine Country marketing director Michele Cozzi

(Courier mail, 28/7/08)

- We all know that windy days can feel much colder than calm days, even if ambient air temperatures are the same on both days.
- Particularly on cold days, the *apparent* temperature to the human body drops as the wind velocity increases.
- This effect is commonly called *wind chill*.

Question *9.3.13* Derive an equation that models wind chill calculations. (Hint: start by deciding which factors are important, whether they increase or decrease the apparent temperature, whether their effect is linear, and how they interact.)



Wind chill *(continued)*

- It is important to measure, model and predict wind chill. It can cause significant discomfort, and in cold areas it can lead to serious injuries (such as frostbite) and death.
- Wind chill has been measured in a number of ways.
- The most widely accepted current model was developed by the US National Weather Service early in 2001.
- Volunteers were exposed to varying low temperatures and high wind velocities in a wind tunnel.
- Measurements were taken of the physiological impact on the aces of the volunteers, and also their perceptions of the temperatures.
- An equation was formulated which modelled the perceived wind chill temperature as a function of the ambient air temperature and the wind velocity (for velocities of at least 5 km/h).

***Question** 9.3.14* Let t be the ambient air temperature in °C and v be the wind velocity in km/h. Then the wind chill temperature W perceived by the human body in °C is given by the equation:

***Example** 9.3.15* On a cold Brisbane bike ride, the ambient temperature is 2 °C and the effective wind velocity is 30 km/h. Then

$$W \approx 13.12 + 1.24 - 11.37 \times 1.723 + 0.79 \times 1.723 \approx -3.85$$

so the perceived temperature is about -3.85 °C.

Question *9.3.16* Recall that $W = 13.12 + 0.6215t - 11.37v^{0.16} + 0.3965tv^{0.16}$. Discuss the impact/meaning of each term in the equation.

Question *9.3.17* In 2007, Peter rode a snowmobile at 100 km/h in Yellowstone National Park, when the air temperature was -16 °C. What was the perceived temperature?

Question *9.3.18* Recall that $W = 13.12 + 0.6215t - 11.37v^{0.16} + 0.3965tv^{0.16}$. Discuss in detail how this equation will behave under various conditions involving v and t, including:

(a) Days with the same wind velocity but varying temperatures.

(b) Days with the same temperature but varying wind velocities.

(c) The impact on perceived temperature if the wind velocity increases from 5 km/h to 20 km/h, compared to the impact on perceived temperature if it increases from 50 km/h to 100 km/h.

Question *9.3.19* Recall that the five common ways of presenting quantitative models are: words, values, pictures, equations and computer programs. Making wind chill information widely accessible and comprehensible can be a matter of life and death. Briefly discuss the suitability of each of the five ways for making information about wind chill available.

Extension *9.3.20* (From www.ontarioweather.com/winter/safety/...)
Here is how a Canadian website presents wind chill information.

	Air Temperature (°C)										
Wind Speed (Km/h)		0	-5	-10	-15	-20	-25	-30	-35	-40	-45
	10	-3	-9	-15	-21	-27	-33	-39	-45	-51	-57
	20	-5	-12	-18	-24	-31	-37	-43	-49	-56	-62
	30	-7	-13	-20	-26	-33	-39	-46	-52	-59	-65
	40	-7	-14	-21	-27	-34	-41	-48	-54	-61	-68
	50	-8	-15	-22	-29	-35	-42	-49	-56	-63	-70
	60	-9	-16	-23	-30	-37	-43	-50	-57	-64	-71

Color coding to match windchill factors issued by Environment Canada

Windchill (C)	Qualifier	Comfort and/or precautions description
0 to -10	Low	Conditions are slightly uncomfortable for outdoor activity. Dress Warmly. Winter clothing is recommended, including hat, gloves and dry insulating under clothing.
-10 to -25	Moderate	Cold on exposed skin. Conditions can be comfortable for outdoor activity on sunny days. Hat, gloves and layered dry insulating clothing is a necessity. Risk of hypothermia over prolonged periods.
-25 to -45	Cold	Important to keep active. Cover all skin. Take frequent warm up breaks. Frostbite is possible on exposed skin over short periods of time so check frequently. Risk of hypothermia over prolonged periods.
-45 to -59 Warning Level*	Extreme	Very uncomfortable. Outdoor activity should be limited to short periods. Cover all exposed skin. Dress in layers. Limit outdoor activities to short periods. Exposed skin freezes in minutes. Serious risk of hypothermia over prolonged periods.
-60 and colder	Very Extreme	Outdoor conditions are hazardous. Exposed skin will freeze in 2 minutes. Stay indoors.

* In Ontario/Atlantic provinces, the warning level is -35 C. In most areas of Canada, the warning level is -45 C. In northern Quebec, Manitoba, Labrador and the Arctic, the warning level is -50 C. In the high Arctic, the warning level is -55 C. This is due to human adaptability to cold over time.

As usual, we can develop a computer model.

Program specifications: Write a program which allows the user to input the wind speed in km/h and air temperature in °C, and calculates the apparent wind chill temperature.

Wind chill *(continued)*

Python Example 9.3.21

```
# A program to calculate apparent wind-chill temperatures
# given the wind speed and air temperature.

from __future__ import division
from pylab import *

airT = input("What is the air temperature in degrees Celsius? ")
windS = input("What is the wind speed in km/h? ")

x = pow(windS,0.16)
windC = 13.112 + 0.6215 * airT - 11.37 * x + 0.3965 * airT * x

print "An air temperature of ",airT," Celsius and wind speed of"
print windS,"km/h has a wind chill of",round(windC,1)," Celsius."
```

Python Example 9.3.22

Here is the output from running the above program three times:

```
What is the air temperature in degrees Celsius? -16
What is the wind speed in km/h? 100
An air temperature of  -16  Celsius and wind speed of
100 km/h has a wind chill of -33.8  Celsius.

What is the air temperature in degrees Celsius? 2
What is the wind speed in km/h? 30
An air temperature of  2  Celsius and wind speed of
30 km/h has a wind chill of -3.9  Celsius.

What is the air temperature in degrees Celsius? -45
What is the wind speed in km/h? 60
An air temperature of  -45  Celsius and wind speed of
60 km/h has a wind chill of -71.1  Celsius.
```

End of Case Study 11.

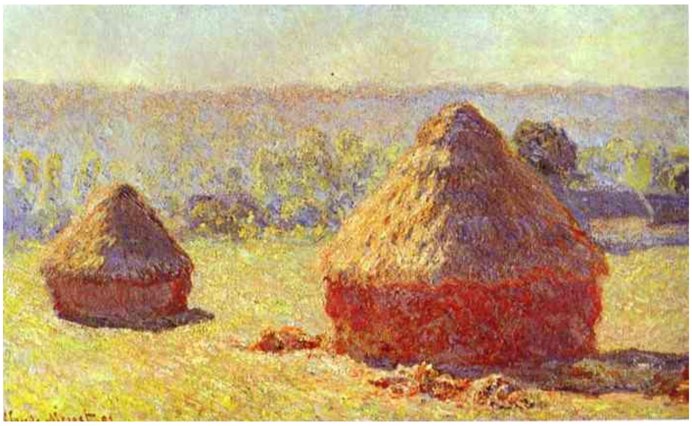
9.4 Space for additional notes

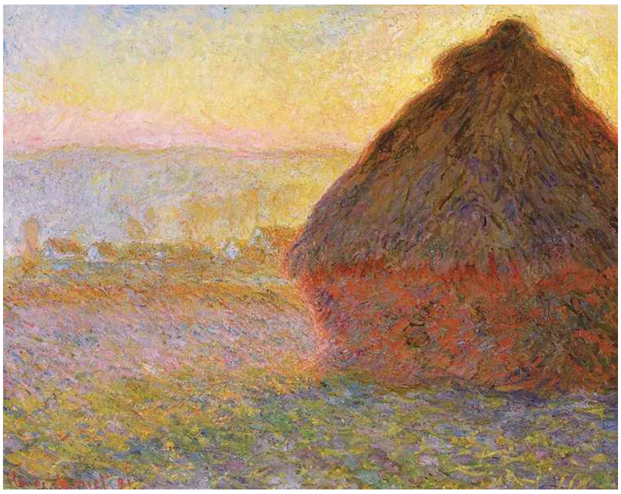
10 Waves, cycles and seasons

I cannot lie
From you I cannot hide
I'm losing the will to try
Can't hide it (can't hide it),
can't fight it (can't fight it)
So go on, go on,
come on, leave me breathless

Artist: The Corrs

(www.youtube.com/watch?v=2eBkXXSbwlE)





From the series *Haystacks* (1890 – 1891), Claude Monet (1840 – 1926), various museums. (Image source: see en.wikipedia.org/wiki/Haystacks_(Monet))

Introduction

The previous section showed how some simple mathematical functions (linear, quadratic and power functions) can be used to model a range of scientific phenomena.

In this section we will encounter examples of phenomena which regularly *cycle* over time; this is quite common in science and nature. Modelling such phenomena requires a new type of function, called a *periodic* function. The graphs of periodic functions are waves.

Some of the examples/contexts we will discuss are:

- Periodic functions and breathing.
- Seasons and daytimes.

Specific techniques and concepts we will cover include:

- Periodic functions.
- Varying frequency and amplitude.

10.1 Waves, cycles and periodic functions

- Science and nature include many phenomena which *repeat* or *cycle*. The graph of such processes is called a *wave*.

Waves

Key features of the graph of a wave include the:

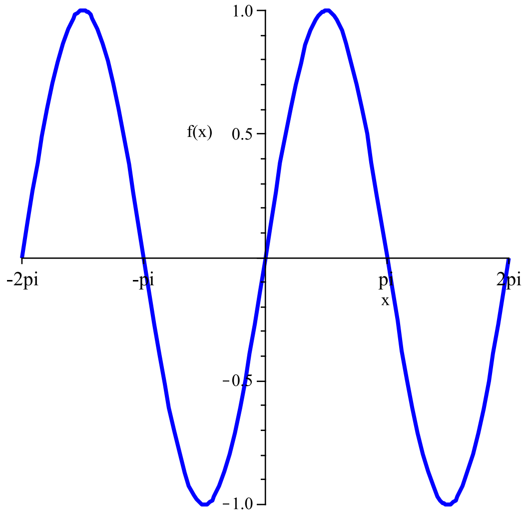
- **peaks and troughs**, *which are, respectively, the highest and lowest points on the wave;*
- **equilibrium value** *or* central value, *which is the function value around which the wave is centred.*
- **wavelength**, *which is the distance of one* **cycle**, *or the distance from one peak to the next;*
- **amplitude**, *which is the maximum variation from the equilibrium value during one cycle;*
- **phase shift**, *which is a partial horizontal shift of the wave;*
- **period**, *which is the time for one complete cycle; and*
- **frequency**, *which is the rate at which the peaks pass a given point. The frequency equals the reciprocal of the period, and is measured in cycles per second, with SI base unit* **hertz** *or* **hz**.

- To represent waves accurately we require functions which cycle between certain values and repeat at regular intervals.
- The most common choices for cyclic functions are the standard *trigonometric functions* sin and cos .
- (You will have seen these functions before, in the context of angles. However, in many scientific models they are used not for angles but instead because they cycle periodically.)
- In SCIE1000 we will always use sin (we could have used cos).

The periodic function sin

The function $f(x) = \sin x$ *is a smoothly repeating function with a period of* 2π *and an amplitude of 1, with an equilibrium value of 0.*

A graph of $\sin x$ *is shown for* x *between* -2π *and* 2π*; this graph shows two cycles of a* **sine wave***.*



- In practice, modelling different phenomena usually requires functions with: periods other than 2π; and/or amplitudes other than 1; and/or an equilibrium value other than 0; and/or a phase shift.

Question *10.1.1* Suggest some scientific phenomena that cycle, along with appropriate periods, amplitudes and equilibrium values (where possible).

- The equilibrium value, period, amplitude and phase of a wave can be changed by using different constants in sin functions.

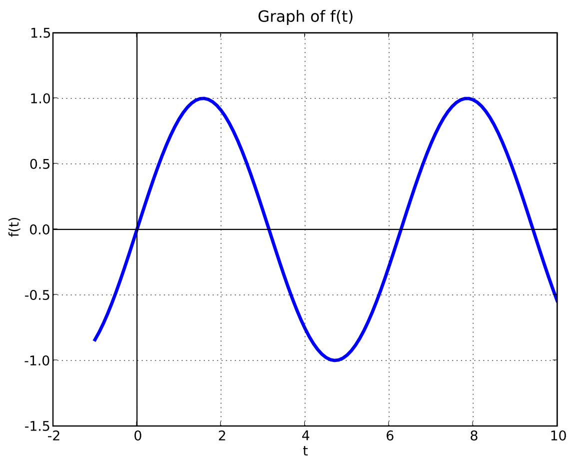
***Question** 10.1.2* Four copies of the graph of $f(t) = \sin t$ are shown below. In each case, write the equation for a sin function with the given property, then sketch the graph of that function.

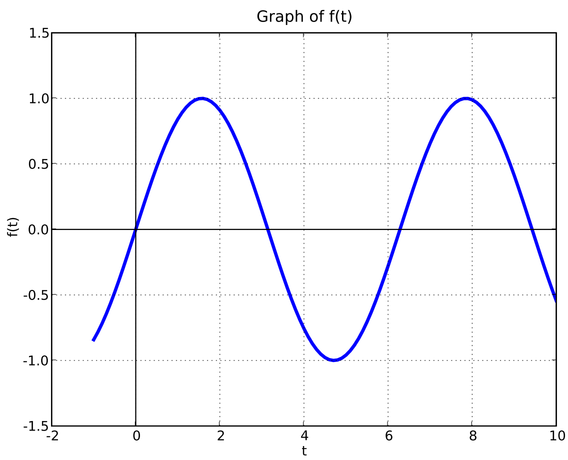
(a) Centred around $y = 0.5$.

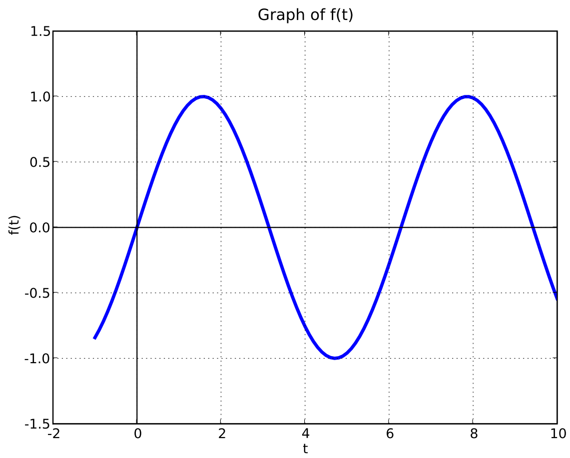
(b) Amplitude of 0.5.

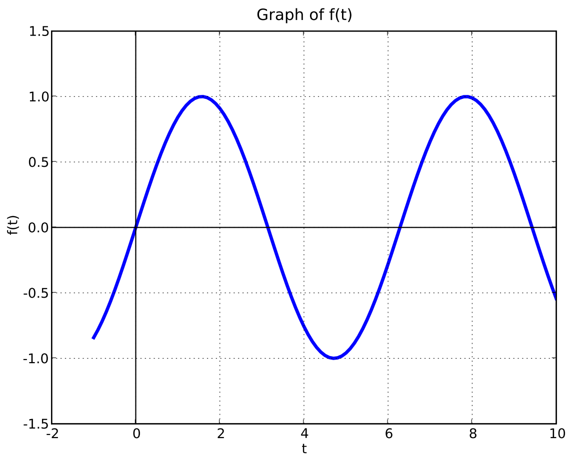
(c) A period of 5.

(d) A phase shift of one half of a cycle.









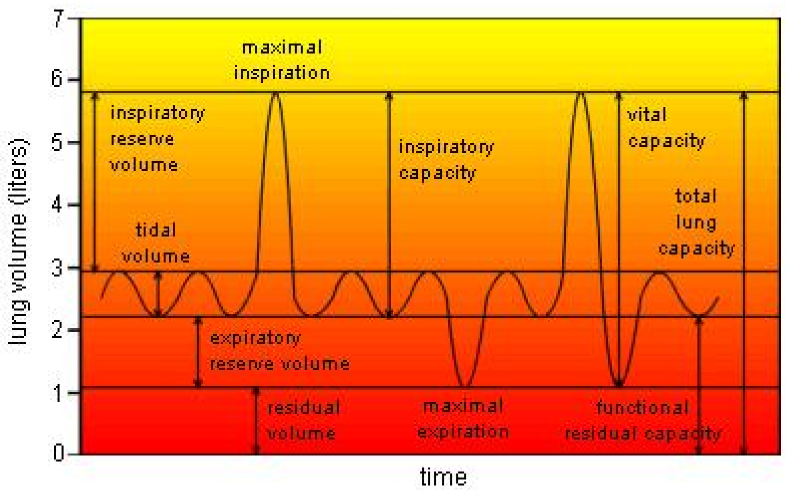
Case Study 12:
Periodic functions and breathing

Spirometer

healthy lung

lung with emphysema

- The human lung (indeed, any lung) has a certain maximum capacity, which depends on factors such as the size, gender and level of physical activity of the individual. In an adult human male, a reasonable estimate of the total lung capacity is 6 L.
- Normal breathing involves rhythmic inhalation and exhalation. After each (normal) exhalation the lung contains a volume of air, called the **functional residual capacity**.
- The volume of air breathed in and out is called the **tidal volume**.
- Tidal volumes can be measured using a *spirometer*, and recorded in a *spirogram*. (One common type of spirometer uses the Hagen-Poiseuille equation to measure flow rates of air out of the lungs.)



***Question** 10.1.3* The breathing of an individual at rest was monitored. Each cycle took 5 s, the functional residual capacity was 2.2 L, and the tidal volume was 0.5 L.

(a) Sketch a rough graph of lung capacity (that is, the volume of air in the lung) over time. Assume that at time $t = 0$ s the person is inhaling and has inhaled exactly one half of the tidal volume.

(b) Write a function using sin to model the lung capacity in (a).

continued...

***Question** 10.1.3 (continued)* Recall that a breathing cycle takes 5 s, functional residual capacity is 2.2 L, and tidal volume is 0.5 L.

(c) How would you expect the function to change after a period of intense physical activity?

(d) Hyperventilation is characterised by rapid, deep inhalations and exhalations. How would your function change during hyperventilation compared to normal breathing?

(e) Emphysema is a type of Chronic Obstructive Pulmonary Disease in which lung tissue is destroyed. The resulting impairment decreases the ability to interchange carbon dioxide and oxygen during breathing due to a decrease in lung surface area. Emphysema is often caused by smoking. How would your function change for an individual with emphysema?

End of Case Study 12.

10.2 Daytimes, seasons and periodic functions

- An important property of any location on the surface of Earth is the amount of sunlight available on a given day.
- We will approximate this with the *daytime*, which we will define as the time between sunrise and sunset. This definition is independent of clouds and other weather events that might obscure the sun.
- Daytimes, seasons and climate are all very closely linked.
- At large distances from the equator, summer daytimes are very long; on some occasions there is no sunrise or sunset for a period greater than one day. For simplicity, in such cases we say that the daytime is 24 hours.
- At each location on the surface of Earth, the length of the daytime varies from day to day throughout the year. However, from year to year the daytimes on a given date are very similar, so we can assume they form a repeating, yearly pattern.
- Hence the sin function, with appropriate periods and amplitudes, can be used to model daytimes at different places on the surface of Earth, depending on the day of the year.
- (In reality there are slight variations from these functions as days are discrete time steps whereas the Sun and Earth move continuously. If you look at a calendar you will see very small changes in daytimes on a given date from year to year.)
- Some features of daytimes throughout the year include:
  - The **summer solstice** and **winter solstice**, which are the days with the longest and shortest daytimes (respectively).
  - The **vernal equinox** and **autumnal equinox**, which are the days in spring and autumn (respectively) in which the daytimes are exactly 12 hours.

***Question** 10.2.1* Describe the daytime lengths in midsummer and midwinter in each of:

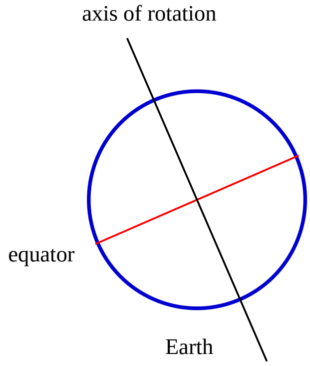
(a) Brisbane;

(b) Kuala Lumpur (which is very close to the equator); and

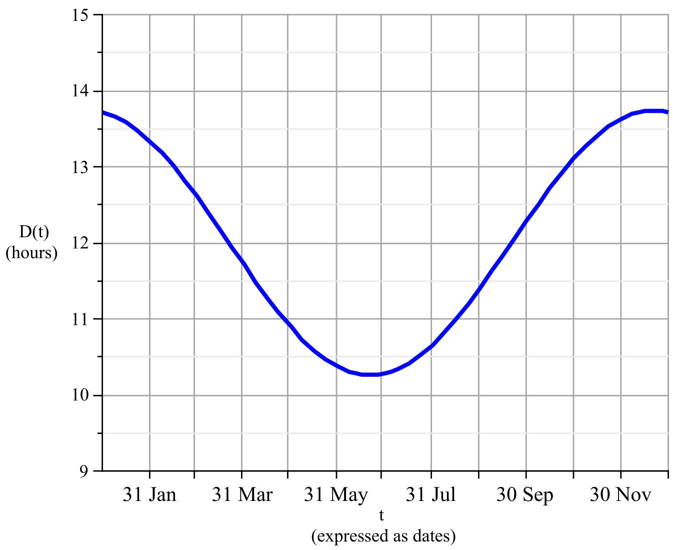
(c) the Santa Claus village, near Rovaniemi in Finland, slightly north of the Arctic Circle.



***Question** 10.2.2* Explain why daytimes vary between locations, and from day to day. (This is closely related to the reason seasons occur.) Your explanation should include solstices and equinoxes. (Hint: Earth has a tilt of 23.45 degrees on its axis of rotation.)



***Question** 10.2.3* The daytimes for Brisbane are:



(Note that this should be graphed as discrete points but because the points are so close it is instead drawn as a smooth curve.)

Use the graph to answer the following questions.

(a) Approximately when are the solstices in Brisbane, and how long are the daytimes?

(b) When are the equinoxes in Brisbane?

Case Study 13:
Equations for daytimes

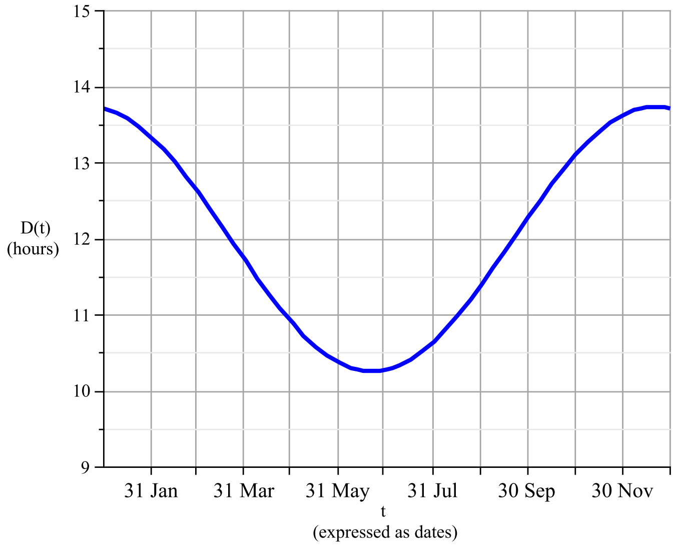


- Any point on the surface of Earth has a *latitude*, which is a measure in degrees of how far it is north or south of the equator.
- For example, the latitude of Brisbane is about 27 degrees, 29 minutes south. (Note that a *minute* is 1/60 of a degree.)
- On any given day, at **every point with the same latitude the daytime has the same length**. For example, New York (USA) and Madrid (Spain) have very similar latitudes, so will have very similar daytimes on every day of the year.
- Thus the daytime function for a given latitude can be written as a function of the number of the day in the year (starting from $t = 0$ on January 1st).
- The daytime function at any location cycles with an (approximate) period of 365 days, so the function we use will need to be periodic, with a period of 365 days.

***Question** 10.2.4* If t is the day number in the year (starting from $t = 0$ on January 1st) then the length of the daytime in hours at any point in the southern hemisphere is given by

$$D(t) = 12 + K \times \sin\left(\frac{2\pi}{365}(t - 264)\right)$$

where K is a constant determined by the latitude of the point; at the equator $K \approx 0$, and its value increases for more southerly locations. For Brisbane $K \approx 1.74$; the graph with this value of K is plotted.



Discuss the physical and mathematical significance of each term in $D(t)$.

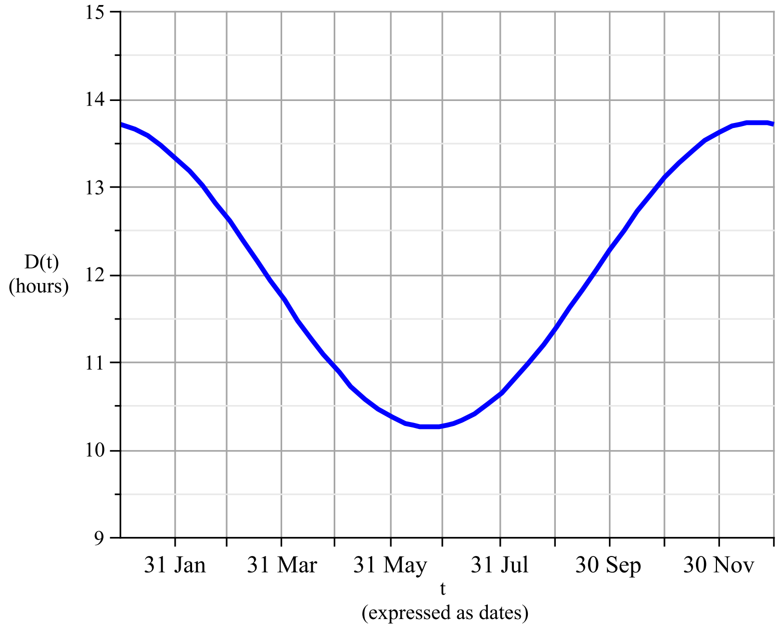
***Question** 10.2.5* In Brisbane, $D(t) = 12 + 1.74\sin\left(\frac{2\pi}{365}(t-264)\right)$. Answer each of the following. (This is very similar to Question 10.2.3, but use the function rather than the graph to answer the questions.)

(a) Approximately when are the solstices in Brisbane, and how long are the daytimes?

(b) When will the solstices occur in Townsville (north of Brisbane) and in Hobart (south of Brisbane)? Why?

(c) The equinoxes have daytimes of length 12 hours everywhere in the world. When are the equinoxes?

Question 10.2.6 In $D(t)$, $K \approx 1$ for Townsville, $K \approx 1.74$ for Brisbane, and $K \approx 3.3$ for Hobart. The graph for Brisbane is:



(a) Roughly sketch the graphs of $D(t)$ for Townsville and Hobart on the above graph.

(b) By how much is the daytime on the **summer** solstice in Hobart **longer** than in Townsville? What is the difference on the **winter** solstice?

(c) What does this suggest for the total amount of daytime in a year at any location on Earth? Is this true, and what does it mean?

continued...

Question *10.2.6 (continued)* Recall in the **southern** hemisphere, $D(t) = 12 + K \times \sin\left(\frac{2\pi}{365}(t - 264)\right)$. In the **northern** hemisphere the corresponding equation is $ND(t) = 12 + K \times \sin\left(\frac{2\pi}{365}(t - 81)\right)$.

For Hobart, $K \approx 3.3$, and at the Arctic Circle, $K \approx 12$.

The Sanderling, *Calidris alba*, is a migratory wading bird which typically inhabits areas of coastal Australia from September until April, when it migrates to the northern hemisphere for its breeding season.

(d) An individual Sanderling leaves a latitude equivalent to Hobart in April and arrives in the Arctic Circle on June 15th. Calculate how much longer daytime it has on June 15th in the Arctic Circle compared to Hobart on June 15th.

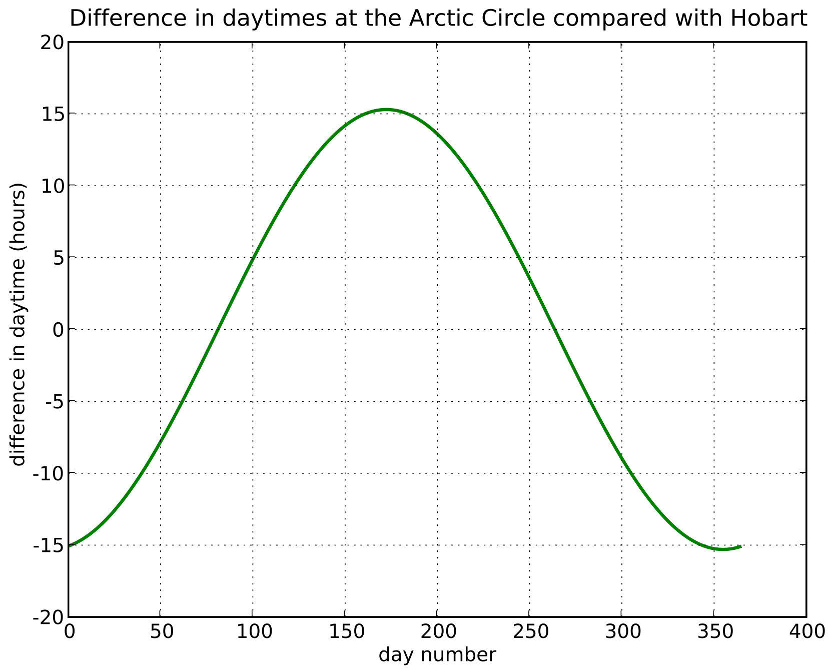
As usual, we can develop a computer model to investigate this.

Program specifications: Write a program which graphs the difference in daytime on each day between the Arctic Circle and Hobart.

Python Example 10.2.7

```
# A program to calculate the difference in daytime at
# the Arctic Circle versus Hobart on each day of the year.
from __future__ import division
from pylab import *

# Calculate the daytime for each day at each place.
days = arange(0,365)
dayTHob = 12 + 3.3 * sin(2 * pi/365 * (days - 264))
dayTArc = 12 + 12 * sin(2 * pi/365 * (days - 81))

# Plot the difference, and draw the labels and title.
plot(days, dayTArc - dayTHob, "g-", linewidth=2)
xlabel("day number")
ylabel("difference in daytime (hours)")
title("Difference in daytimes at the Arctic Circle compared
                                  with Hobart")
grid(True)
show()
```

Here is the output from running the above program:



End of Case Study 13.

10.3 Space for additional notes

11 Exponentials and logarithms

dum dum, diddle dum dum,
diddle dum dum, diddle dum dum.
There was a turtle by the name of Bert
And Bert the Turtle was very alert
When danger threatened him he never got hurt
He knew just what to do. (bang)
He'd duck (quack) and cover, duck (quack) and cover.
He did what we all must learn to do
You and you and you and you. (bang)
Duck (quack) and cover!

Artist: US Federal Government Civil Defense.

(www.youtube.com/watch?v=C0K_LZDXp0I)

(Take the time to watch this and think about it.)

Stonehenge (1835), John Constable (1776 – 1837), Victoria and Albert Museum, London.

(Image source: en.wikipedia.org/wiki/File:John_Constable_Stonehenge.jpg)

Introduction

A graph of global human population over the last two thousand years starts off fairly flat, but then "takes off" in recent years. This is an example of *exponential growth*. Similar behaviour is shown by populations of many organisms, at least over some range of times.

Other quantities show *exponential decay*, where the quantity initially falls very rapidly, but then "flattens out" over time. Two common examples of exponential decay are the decrease in size of a population when a disease is introduced, and decay of radioactive isotopes.

Many quantities in nature, and also many man-made phenomena, change exponentially. This includes phenomena in: physics (such as the electrical discharge of a capacitor); psychology (the rate at which an individual learns new knowledge); marketing (the rate at which the impact of an advertising campaign drops off); business (the balance of a bank account earning interest); and chemistry (the rates at which some chemical reactions occur).

Other functions closely related to exponentials are *logarithms*. They can simplify calculations on exponential functions, and also are the foundation of numerous physical measurement scales, including the Richter scale and the pH scale.

Some of the examples/contexts we will discuss are:

- Algal blooms.
- Radioactive decay.
- Carbon dating.
- The pH scale.

Specific techniques and concepts we will cover include:

- Exponentials.
- Logarithms.

11.1 Growth, decay, exponentials and logarithms

- In nature, the size, number or amount of most phenomena change over time. Often, the rate of change at any time is proportional to the amount that is currently there.
- This is typical of many populations. For example, each year the size of the global human population is increasing by around 1.5% of its current size.
- Any phenomenon which has a rate of change proportional to the current amount follows an *exponential* function. (We will see why this is when we study differential equations later.)
- When we studied power functions (such as $y = x^{0.25}$) the *power* was always constant, with the variable x in the *base*.
- With exponential functions the *variable* occurs in the *power* and the *base* is *constant*.

Exponential functions

Exponential functions have equations

$$f(x) = Ca^{kx},$$

where C, a and k are constants. The constant a is called the **base***. The two most common values used for the base a are*

- *the number 10; and*
- Euler's number, *denoted e, where $e \approx 2.71828\ldots$.*

Note that when x=0 the function value equals C. The constant k is the **growth rate** *or* **decay rate** .

- Phenomena that change exponentially can be classified as follows:
  - If they *increase* as x gets larger, they are said to display exponential *growth*.
  - If they *decrease* as x gets larger, they are said to display exponential *decay*.
- For exponential functions, knowledge about how long it takes the function value to double (for growth functions) or halve (decay) allows us to study the behaviour of the phenomenon over time.

Doubling time/Half-life

The **doubling time** *for an exponentially growing quantity is the time taken for it to increase to twice its original size.*

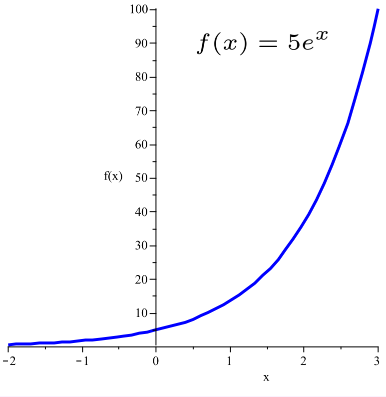
The **halving time** *or* **half-life** *for an exponentially decreasing quantity is the time taken for it to decrease to half its original size.*

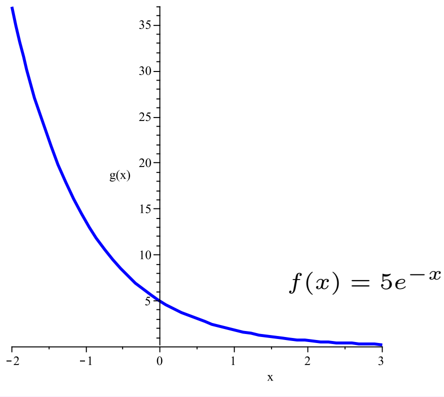
- Many exponential phenomena in science have relatively constant doubling times/half lives over extended time periods.
- It is easy to tell from an exponential function whether it gives growth or decay.

***Example** 11.1.1* Let $f(x) = Ce^{kx}$ where $C > 0$. Then:

- If k is positive then the function displays *exponential growth.*
- If k is negative then the function displays *exponential decay.*

The following graphs show an example of exponential growth (left, with $k = 1$) and exponential decay (right, with $k = -1$).





***Example** 11.1.2* Exponential functions occur very frequently in nature and society. For example, they occur in:

- Unconstrained and constrained population growth.
- Radioactive decay and carbon dating.
- Modelling the concentration of a drug in the bloodstream.
- Modelling *habituation* to a stimulus (in psychology).

- *Logarithms* are very closely related to exponential functions.
- Many people find logarithms confusing. However there is nothing mysterious about them.

Logarithmic functions

Logarithmic functions are of the form $f(x) = \log_a x$. *This is pronounced "f of x equals the* **logarithm** *of x to the* **base** *a".*

In the special case that the base a is Euler's number e then the logarithm function is often written as $f(x) = \ln x$. This is pronounced "f of x equals the **natural logarithm** *of x".*

Logarithms and exponentials

The relationship between exponentials and logarithms is:

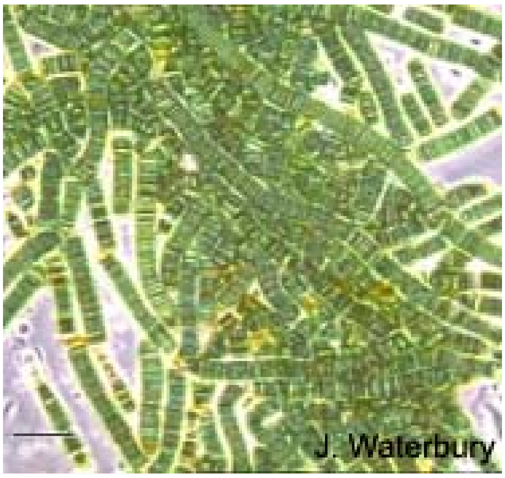
- *If $y = 10^x$ then $x = \log_{10} y$ (and vice-versa).*
- *If $y = e^x$ then $x = \ln y$ (and vice-versa).*

***Example** 11.1.3* Here are some examples of the relationships between exponentials and logarithms.

- $1000 = 10^3$, so $\log_{10} 1000 = 3$.
- $0.01 = 10^{-2}$, so $\log_{10} 0.01 = -2$.
- If $y = e^{0.02x}$ then $\ln y = 0.02x$.
- $\ln 1 = 0$ because $e^0 = 1$.

11.2 Exponentials in action

Case Study 14: Algal blooms


***Example** 11.2.1* Most microscopic algae reproduce asexually, with the *mother* cell splitting to form two *daughter* cells.

Under normal conditions, factors such as predation and limited resources keep algae populations under control. However, sometimes uncontrolled reproduction occurs, leading to an **algal bloom**. In algal blooms, the population of algae can reach 10^6 individuals per mL of water. Some blooms are harmful to humans, producing dangerous biotoxins that can be passed on in food sources. Many algal blooms result directly or indirectly from human activities. It is believed that their frequency and severity will increase as a result of further environmental degradation.

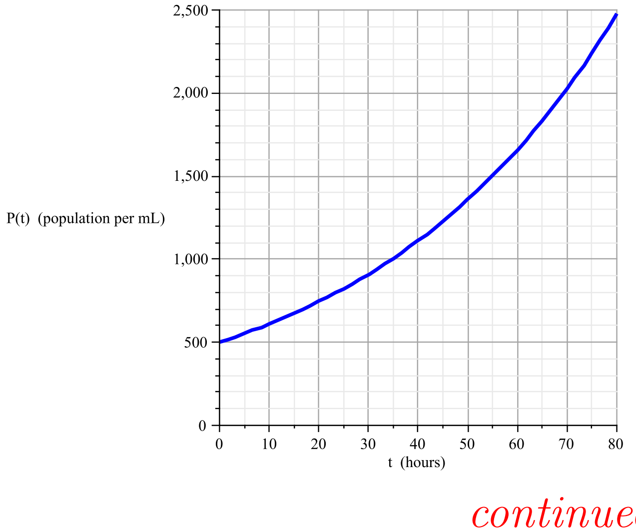
Because the rate at which algae reproduce is proportional to the current population, populations must follow exponential functions.

Question *11.2.2* A certain species of algae grows exponentially over a given time period. The initial population at time $t = 0$ is 500 individuals per mL of water, with a growth rate of 2% per hour. Then the population size $P(t)$ at any time t in hours is (approximately)

$$P(t) = 500e^{0.02t}.$$

(a) Find the population after 2 hours.

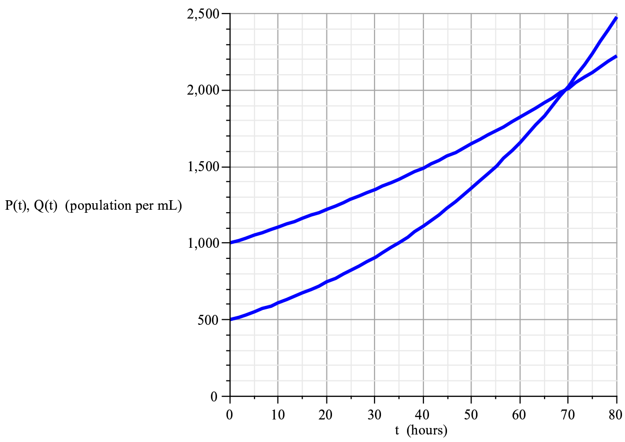
(b) Use logarithms to calculate the doubling time of this population. That is, find the time at which the population size reaches 1000. (Hint: $\ln 2 \approx 0.693$.)



continued...

***Question** 11.2.2 (continued)* Recall that the population size $P(t)$ per mL for the algae after t hours is given by $P(t) = 500e^{0.02t}$.

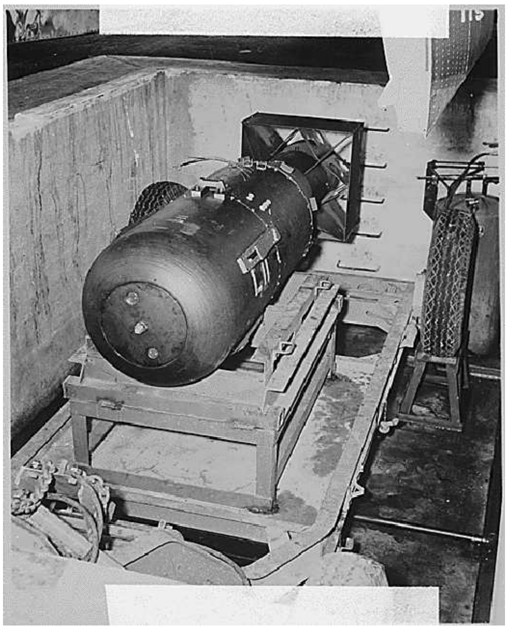
(c) A second species of algae also grows exponentially. There are 1000 individuals per mL at time $t = 0$ with a growth rate of 1% per hour, so the population $Q(t)$ per mL is $Q(t) = 1000e^{0.01t}$. At what time are the populations P and Q the same size?

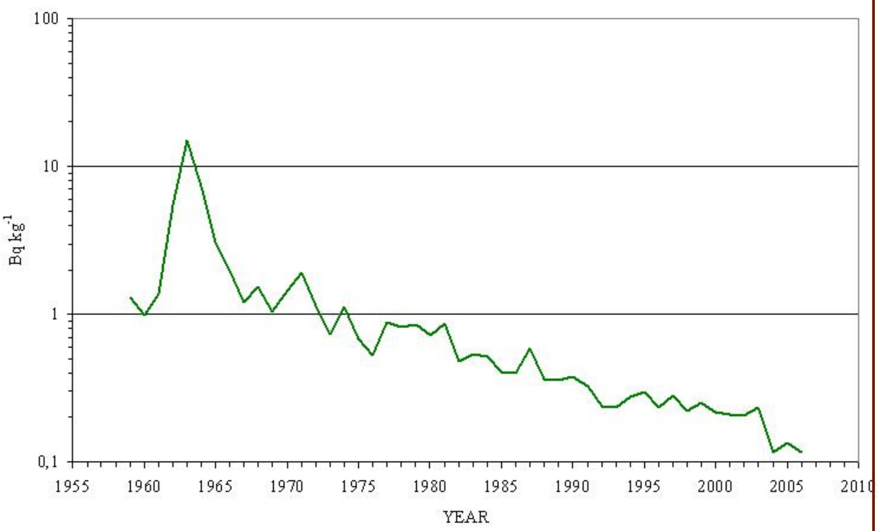


End of Case Study 14.

- In Example 11.2.2 the population *increased* exponentially. Other phenomena *decrease* exponentially, showing exponential *decay*.

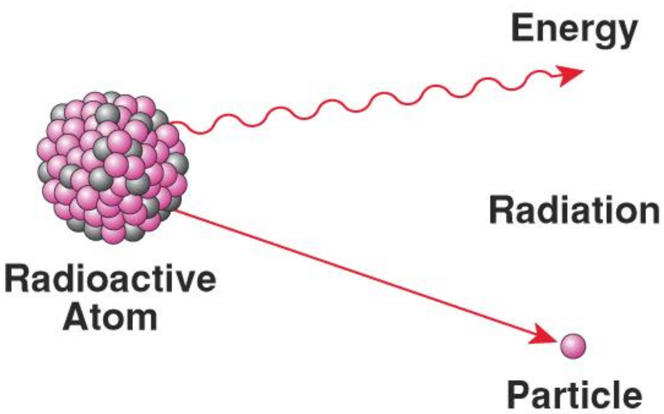
Case Study 15:
Radioactive decay and exponentials





Strontium-90 in barley collected in 1959-2006.

http://www.risoe.dk/



- Not all atoms remain the same over time; some undergo a process known as *radioactive decay*.
- Radioactive decay involves a change in the arrangement of the nucleus of an atom, sometimes changing into a different element.
- Substances that undergo this type of decay are called *radioactive*.
- When an element undergoes radioactive decay but remains the same element (so maintains the original number of protons), the new atom is called an *isotope*.

- Isotopes can be denoted in several ways. One standard way is to write the name or chemical symbol of the element, hyphenated with its atomic mass. For example, Deuterium (an isotope of Hydrogen and the main ingredient in "Heavy water") is written as Hydrogen-2 or H-2.
- Another style writes the atomic mass as a superscript before the chemical symbol, so Deuterium would be written ^{2}H.
- Radioactive isotopes are important in a range of scientific and industrial fields, including chemistry, biology, medicine, physics and engineering.
- Radioactive decay is spontaneous, so there is no way of knowing *when* a *specific* individual atom is going to undergo decay.
- However, it *is* known that in any given time period a certain *proportion* of the total quantity in a sample will have decayed.
- Thus, radioactive material undergoes continuous decay at a rate **proportional** to the **quantity** of material (which is similar to the algae population in Example 11.2.2 which was growing at a rate proportional to the current value).
- Hence radioactive decay is an exponential process.

Decay constant

For a radioactive element, the **decay constant** k *is a constant that reflects the rate of decay of the element, and is a property of the chemical element.*
The half-life can be calculated from the value of k*, and vice-versa.*

Example 11.2.3 Decay constants and half-lives vary greatly between radioactive elements. For example:

- Polonium-212 has a half-life of about 3×10^{-7} s.
- Uranium-236 has a half-life of about 4.5×10^{9} years.

Example 11.2.4 Strontium-90 is a radioactive isotope of Strontium (atomic symbol Sr, atomic number 38) frequently used in radiotherapy. Strontium-90 has a half-life of about 28.9 years.

Sr-90 is found in nuclear fallout after atomic blasts and nuclear accidents (for example, the Chernobyl nuclear accident in 1986 caused extensive Sr-90 contamination). During nuclear fallout Sr-90 falls onto grass, which is eaten by cows and incorporated into their milk, and then passed to humans when the milk is consumed.

One of the health risks posed by Sr-90 is that it is chemically similar to calcium. Hence the body absorbs Sr-90 and incorporates it into bones and teeth, potentially leading to bone cancer.

Extension 11.2.5 (From Gould *et al.*, *Strontium-90 in baby teeth as a factor in early childhood cancer*, International Journal of Health Services **30:3** (2000) 515 – 539.)

> "Strontium-90 concentrations in baby teeth of 515 children born mainly after the end of worldwide atmospheric nuclear bomb tests in 1980 are found to equal the level in children born during atmospheric tests in the late 1950s. Recent concentrations in the New York-New Jersey-Long Island Metropolitan area have exceeded the expected downward trend seen in both baby teeth and adult bone after the 1963 ban on atmospheric testing... In Suffolk County, Long Island, Strontium-90 concentrations in baby teeth were significantly correlated with cancer incidence for children 0 to 4 years of age. A similar correlation of childhood malignancies with the rise and decline of Strontium-90 in deciduous teeth occurred during the peak years of fallout. . . ."

Question *11.2.6* Strontium-90 has a half-life of approximately 28.9 years.

(a) Find its decay constant.

(b) It is about 65 years since the first nuclear bomb used in war ("Little Boy") was dropped on Hiroshima. Estimate the proportion of Sr-90 released in that explosion which has not yet decayed.

***Example** 11.2.7* Carbon-14 (C-14, also known as *radiocarbon*) is used extensively throughout science to determine the age of organic-based artifacts (of age up to around 60,000 years).

C-14 is produced in the upper atmosphere by cosmic rays striking nitrogen. It then reacts chemically with oxygen to form radioactive carbon dioxide which permeates living creatures in a fixed proportion, either directly (by absorption from the atmosphere), or indirectly (via food chains).

When an organism dies, the C-14 it contains is no longer continually replenished, so undergoes net decay over time. Measuring the remaining level of C-14 allows an organic artifact to be dated; this process is called *carbon dating*.

The half-life of C-14 is about 5730 years.

***Question** 11.2.8*

(a) Stonehenge is a well-known prehistoric site located on the Salisbury Plain in the UK. Less well-known is nearby *Woodhenge*, which was a similar site constructed (mostly) of wood, somewhat earlier than Stonehenge. In the 1970s, Archaeologists discovered the body of a child at Woodhenge, with an injury suggesting human sacrifice. It is believed that Woodhenge was constructed around 2200 BC. If so, what is the expected proportion of non-decayed C-14 in organic artifacts discovered at Woodhenge compared to the initial level?

continued...

Question *11.2.8 (continued)*

(b) Consider the following information from a paper[a].

> "The Shroud of Turin, which many people believe was used to wrap Christ's body, bears detailed front and back images of a man who appears to have suffered whipping and crucifixion. It was first displayed at Lirey in France in the 1350s …Very small samples from the Shroud of Turin have been dated by accelerator mass spectrometry in laboratories at Arizona, Oxford and Zurich. As Controls, three samples whose ages had been determined independently were also dated. The results provide conclusive evidence that the linen of the Shroud of Turin is mediaeval…"

Researchers discovered that around 91.9% of the 'expected original' amount of C-14 was present in a sample they analysed. Hence deduce the (approximate) age of the Shroud.

[a] Damon *et al.*, *Radiocarbon Dating of the Shroud of Turin*, Nature **337: 6208** (1989) 611–615.

End of Case Study 15.

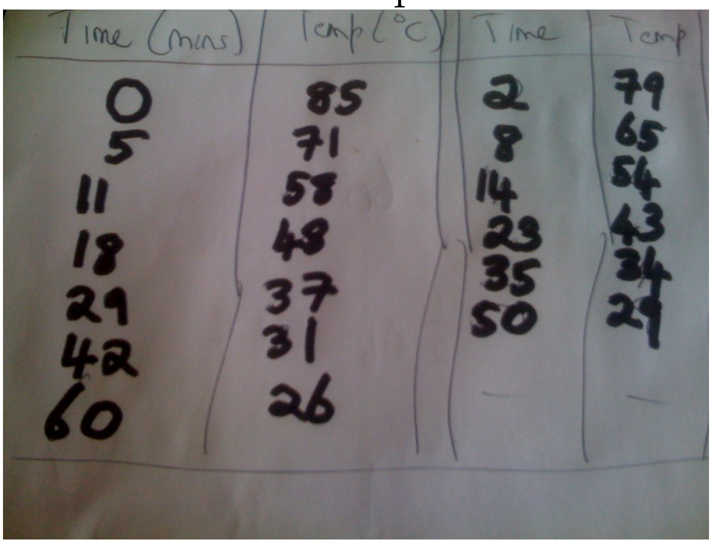
Case Study 16:
Hot stuff


www.readersdigest.com.au

- When an object with one temperature is moved to a location with a different (but constant) temperature, the temperature of the object will gradually change to match that of the location.

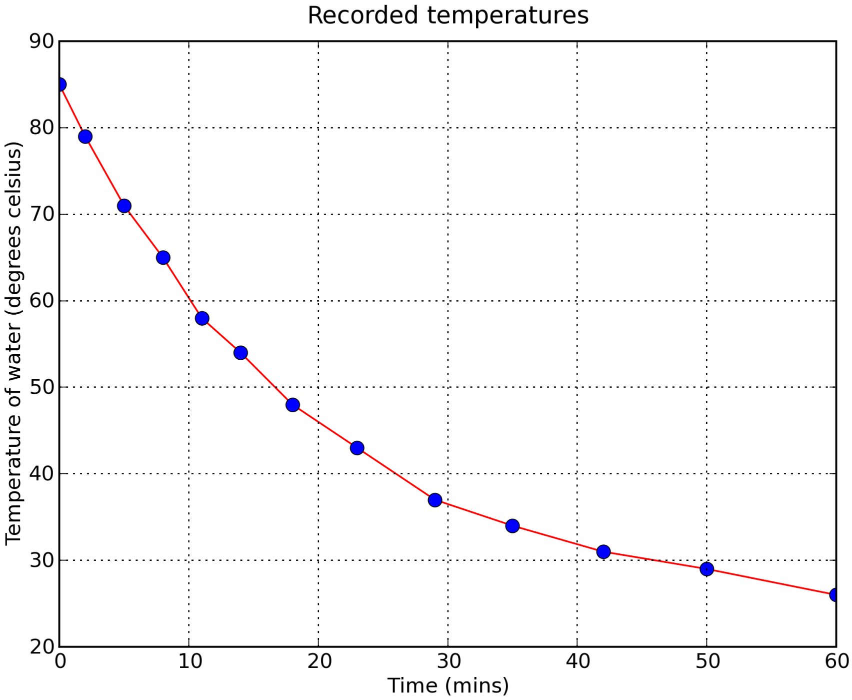
Question *11.2.9* Explain why a graph of the temperature of the object over time is exponential.

Example *11.2.10* Peter conducted an experiment in which he recorded the temperature of hot water in a container over one hour; the room temperature was 25 °C. The following pictures show his experimental apparatus and the recorded temperatures.

Time (mins)	Temp (°C)	Time	Temp
0	85	2	79
5	71	8	65
11	58	14	54
18	48	23	43
29	37	35	34
42	31	50	29
60	26	—	—

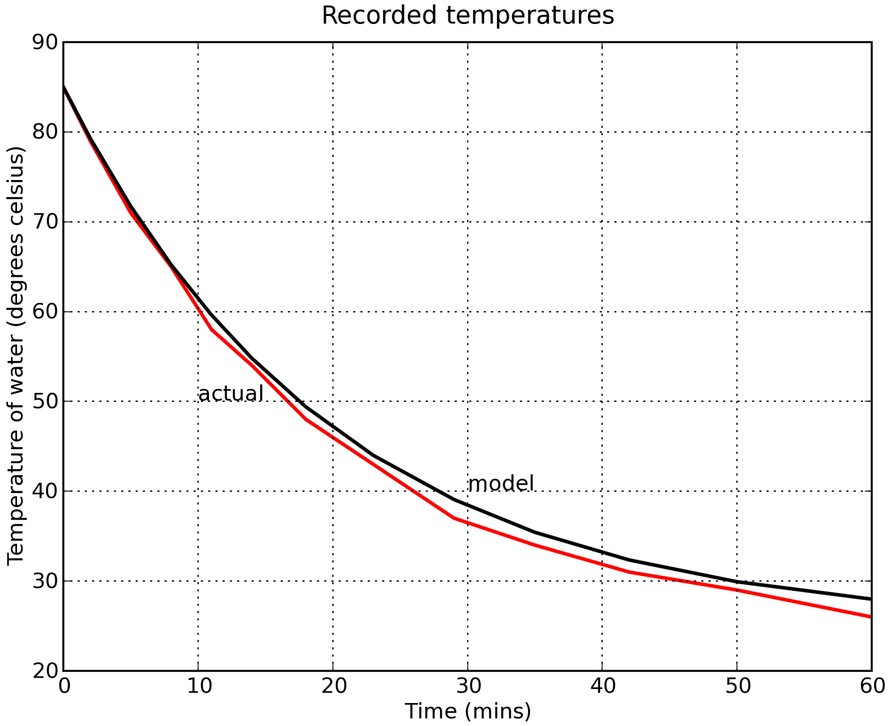
***Question** 11.2.11* Here is a graph of the measured temperatures.



Derive an equation for the water temperature at any time in minutes. (Hint: note that it approaches room temperature of 25 °C, not 0 °C.)

Python Example 11.2.12

```
# Program to plot measured and modelled temperatures.
from __future__ import division
from pylab import *

# Initialise variables
times = array([0, 2, 5, 8, 11, 14, 18, 23, 29, 35, 42, 50, 60])
temps = array([85, 79, 71, 65, 58, 54, 48, 43, 37, 34,31,29,26])
model = 60 * exp(-0.05 * times) + 25

# Draw graphs
plot(times, temps, 'r-', linewidth=2)
plot(times, model, 'k-', linewidth=2)
xlabel("Time (mins)")
ylabel("Temperature of water (degrees celsius)")
title("Recorded temperatures")
grid(True)
text(30,40,"model")
text(10,50,"actual")
show()
```



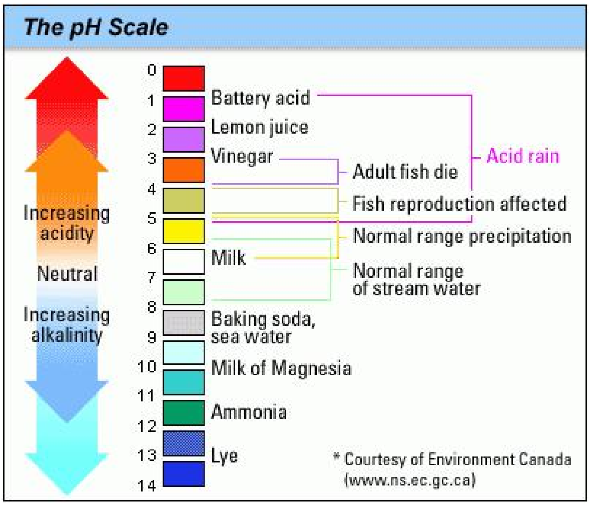
End of Case Study 16.

11.3 Logarithms in action

Example 11.3.1 As well as helping to solve calculations involving exponential functions, there are some very well-known scientific measurement scales that measure log to base 10 of particular quantities. These include:

- *the Decibel scale*, which measures the 'loudness' of sounds (which is directly related to the amplitudes of sine waves);
- the *Richter scale*, which measures earthquake intensity; and
- the *pH scale* (discussed below).

Case Study 17:
Logarithms and the pH scale



- An important application of logarithms in Chemistry is the pH scale, which is a measure of the *acidity* or *alkalinity* of solutions.

***Question** 11.3.2* A pH of 7.00 represents a neutral solution, and **decreasing** pH values correspond to an **increase** in acidity. Most substances have pH values between 0.00 (very acidic) and 14.00 (very alkaline).

The pH of a solution reflects its relative concentration of positive hydrogen ions $[H^+]$, in mol/L. The pH is defined as the *negative of the logarithm to base* 10 *of this concentration*, so

$$pH = -\log_{10}[H^+].$$

(a) Find the pH of gastric digestive juice in which

$$[H^+] \approx 10^{-2} \text{ mol/L}.$$

(b) Pure water has a pH of 7.00 and coffee has a pH of about 5.00. What is the relative concentration of hydrogen ions in coffee compared with pure water?

continued...

Question *11.3.2 (continued)* The rising level of CO_2 in the atmosphere due to greenhouse gas emissions poses a significant risk to the survival of coral reefs. Atmospheric CO_2 dissolves into the ocean and reacts with water to produce carbonic acid (H_2CO_3), leading to ocean acidification with a major impact on coral skeletons.

Ice core samples suggest that the long-term average pH of sea water was about 8.25. Recent studies have predicted that this could drop to 7.65 by the year 2100.

(c) If this prediction is correct, what will be the relative concentration of hydrogen ions in sea water in the year 2100 compared to the long-term historical average?

continued...

Question *11.3.2 (continued)*

(d) Discuss some ways in which acidification of sea water affects coral.

Extension *11.3.3* (From Hoegh-Guldberg *et al.*, *Coral Reefs Under Rapid Climate Change and Ocean Acidification*, Science **318:5857** (2007) 1737 – 1742.)

> "Increases in atmospheric $CO_2 > 500$ ppm will push carbonate-ion concentrations well below 200 μmol kg^{-1} ... and sea temperatures above +2 °C relative to today's values. These changes will reduce coral reef ecosystems to crumbling frameworks with few calcareous corals... Under these conditions, reefs will become rapidly eroding rubble banks such as those seen in some inshore regions of the Great Barrier Reef, where dense populations of corals have vanished over the past 50 to 100 years."

End of Case Study 17.

11.4 Space for additional notes

12 Progress Report 2

Where are we up to?

- So far we have:
  - presented a broad overview of the nature of science, and the activities and attributes involved with science;
  - explained how SCIE1000 and other courses fit into this framework;
  - identified the importance of modelling, and the five common ways of presenting models;
  - introduced some basic science knowledge;
  - discussed the importance of quantitative communication;
  - analysed the philosophical nature of science and scientific thought, including hypotheses;
  - described how computer programs and Python can be used to model phenomena;
  - introduced some mathematical techniques which allow quantitative models to be developed; and
  - demonstrated how linear, quadratic, power, periodic, exponential and logarithmic functions can model a range of phenomena.
- By now, you should have a solid understanding of the basis of scientific activities and thought processes, and some of the roles that modelling and mathematics play in science.
- In the first lecture we outlined six classes of activity crucial to the scientific process, and we estimated how much of each activity is represented in SCIE1000 (and in some other courses).
- The following table outlines this information, and what we have covered so far in SCIE1000.

Skill/Activity	Overall	Done so far
Scientific discipline knowledge	5%	4%
Scientific thinking and logic	15%	13%
Communication and collaboration	15%	13%
Curiosity, creativity, persistence	15%	10%
Observation and data collection	0%	0%
Modelling and analysis	50%	30%

How does it link together:

- In Chapter 2 we built an overall picture of different skills, approaches and thought processes required to do science.
- In Chapter 6 we refined this, considering the nature of logical, scientific thought.
- In Chapter 4 we covered some basic scientific knowledge, setting the scene for future in-depth study of phenomena.
- In Chapter 5 we discussed the importance of precision, accuracy, honesty and scepticism when communicating quantitative scientific information, and when collecting, analysing and using data.
- In Chapter 3 we considered the role of modelling in simplifying reality whilst also maintaining relevance and sufficient accuracy.
- In Chapter 7 we demonstrated how writing computer programs allows more sophisticated models to be developed, because of their ability to perform calculations rapidly.
- In Chapter 9 we saw how some simple mathematical functions, including linear, quadratic and power functions, can model a range of phenomena.
- In Chapter 10, we modelled "cycling" phenomena using periodic functions.
- In Chapter 11, we modelled a range of phenomena using exponential and logarithmic functions.

What we will do next:

- For most of the rest of semester we will focus on modelling and analysis. We will:
  - stress the importance of studying change;
  - remind you about derivatives and rates of change, and use these concepts to solve some important problems;
  - develop a numerical algorithm to solve equations approximately.
  - describe how integrals relate to the area under a curve, and why this is useful;
  - introduce the concept of a differential equation, and practice formulating DEs to represent phenomena; and
  - develop numerical algorithms to solve DEs approximately.
- We will study all of these topics through authentic and important scientific contexts.
- Do not attempt to memorise details of particular contexts or mathematical approaches.
- Instead, understand *when* and *how* each technique can be applied, and how to decide which is the most appropriate to use.
- We will also see examples of how Python programs can assist with the modelling process.

13 Sex and drugs and rates of change

I met with a gal and we went on a spree
She taught me to smoke and to drink whuskey.
Cigareets and whuskey and wild wild women
They'll drive you crazy, they'll drive you insane.
And now I'm feeble and broken with age
The lines on my face make a well written page.
I'm leavin' this story how sad but how true
On women and whuskey and what they will do.

Artist: Jim Croce

(www.youtube.com/watch?v=yVw96wzmZC8)

The Garden of Earthly Delights (1503 – 1504), Hieronymus Bosch (c. 1450 – 1516), Museo del Prado, Madrid.

(Image source: en.wikipedia.org/wiki/Image:GardenED_edit1.jpg)

Introduction

Change is an important part of life. Whether it is a change in the length of days, the behaviour of rats in a maze, the level of CO_2 in the atmosphere or the species diversity of an island, change is universal.

Indeed, all modelling and prediction revolves around change: if something does not change then the future value of that quantity is certain and there is no need to model or make predictions.

Since change is such a fundamental part of the world in which we live, it makes sense that finding the *rate* at which things change is an important activity for scientists. You will need to know how to: find rates of change; apply these techniques to a variety of problems; and interpret your answers.

Some of the examples/contexts we will discuss are:

- Pharmacology.
- Antidepressants.
- Nicotine.
- Pharmacokinetics and drug concentrations.
- Alcohol.
- Caffeine.
- Mathematics and contraception.
- Forensic science.

Specific techniques and concepts we will cover include:

- Interpreting rates of change from graphs.
- Finding average rates of change.
- Instantaneous rates of change and derivatives.
- Finding derivatives.
- Newton's method for numerically solving equations.

13.1 Pharmacokinetics and rates of change

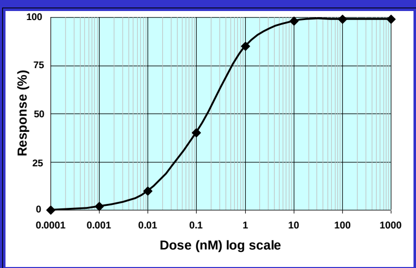
Pharmacology

Pharmocodynamics (PD)
study of what drug does to body
- mimic/inhibit normal processes
- inhibit pathological processes
- stimulants, depressants, toxins

Pharmacokinetics (PK)
study of what body does to drug
- Absorption
- Distribution
- Metablism
- Excretion

Pharmacodynamics (PD)

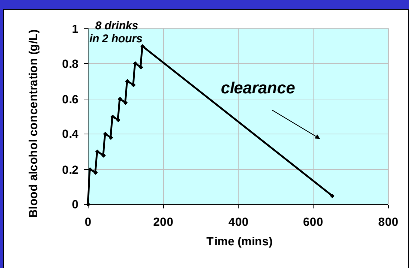
DOSE – RESPONSE CURVE



Sigmoidal (S-shaped) curve
reminiscent of logistic growth curve

Pharmacokinetics (PK)

CONCENTRATION-TIME CURVE



Linear functions
Surge functions

Some drug-related terminology

Broadly speaking, a **drug** *is any chemical substance that affects the function of an organism, usually introduced from outside the organism. Drugs are commonly used to enhance physical or mental well-being, and include both medicinal and so-called recreational drugs.*

Pharmacology *is the study of how drugs interact with living organisms and the mechanisms by which they result in a change in function.*

Pharmacokinetics *is the study of what happens to a drug inside the body (particularly the extent and rate of* **absorption**, **distribution**, **metabolism** *and* **excretion** *of drugs).*

Pharmacodynamics *is the study of what effects a drug has on the body. (We will not cover this in any detail in SCIE1000; there are many other courses in which you can study this important area.)*

Drug concentrations

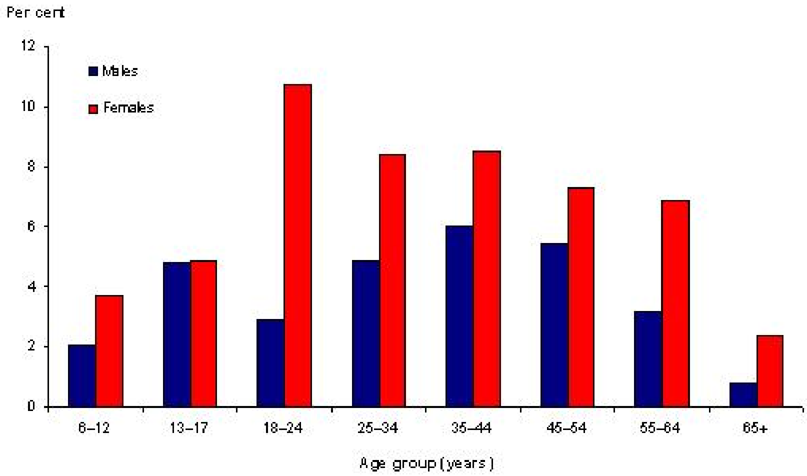
After a drug is administered, a key determinant of the impact of a drug is its **concentration** *in the bloodstream, which is commonly measured as mass per volume (such as mg/L).*

Typically, concentrations are measured (or predicted) over some time period after the drug is administered, and can be shown graphically using a drug concentration curve.

- Mathematics and functions are particularly important when modelling the change in drug concentrations over time.

Case Study 18:
Zoloft

Source: upload.wikimedia.org



Age-specific prevalence of depression, Australia, 1997.
Source: www.aihw.gov.au

- *Zoloft* (and a number of generically-branded equivalents) is the brand name of the drug sertraline hydrochloride. It is an antidepressant of the SSRI class (Selective Serotonin Reuptake Inhibitor).
- The Consumer Medicine Information fact sheet states that SSRIs "...are thought to work by blocking the uptake of a chemical called serotonin into nerve cells in the brain. Serotonin and other chemicals called amines are involved in controlling mood."
- Zoloft is the most commonly prescribed antidepressant in Australia, and one of the most prescribed drugs overall on the Australian Pharmaceutical Benefits Scheme.
- Zoloft is taken orally as a pill. The usual dosage ranges from 25 mg per day to 200 mg per day.
- Zoloft has a number of comparatively mild side effects (including insomnia, loss of appetite, and some sexual impairment), and is generally believed to be both effective and well tolerated.
- There has, however, been media controversy over some years about possible adverse impacts in a small number of people.

Example 13.1.1 When recommending a dosage of a therapeutic drug, pharmacologists need to consider a range of physiological factors, including:

- how rapidly the drug is absorbed;
- whether it should be taken with food;
- how often should a dose be administered;
- what proportion of administered drug is absorbed;
- how quickly the drug is distributed in the body;
- how the drug is metabolised;
- what concentration of the drug is required to have the desired effect, and for how long; and
- how rapidly the drug is excreted.

In terms of concentration graphs, pharmacologists will observe and measure:

(a) the peak concentration;

(b) the time at which peak concentration occurs;

(c) the *half-life* of the drug, which is the time taken for the concentration to fall to half of its previous value;

(d) the minimum effective concentration, below which the drug does not have the desired therapeutic effect;

(e) the maximum rate of drug absorption and when this occurs;

(f) the maximum rate of drug removal and when this occurs;

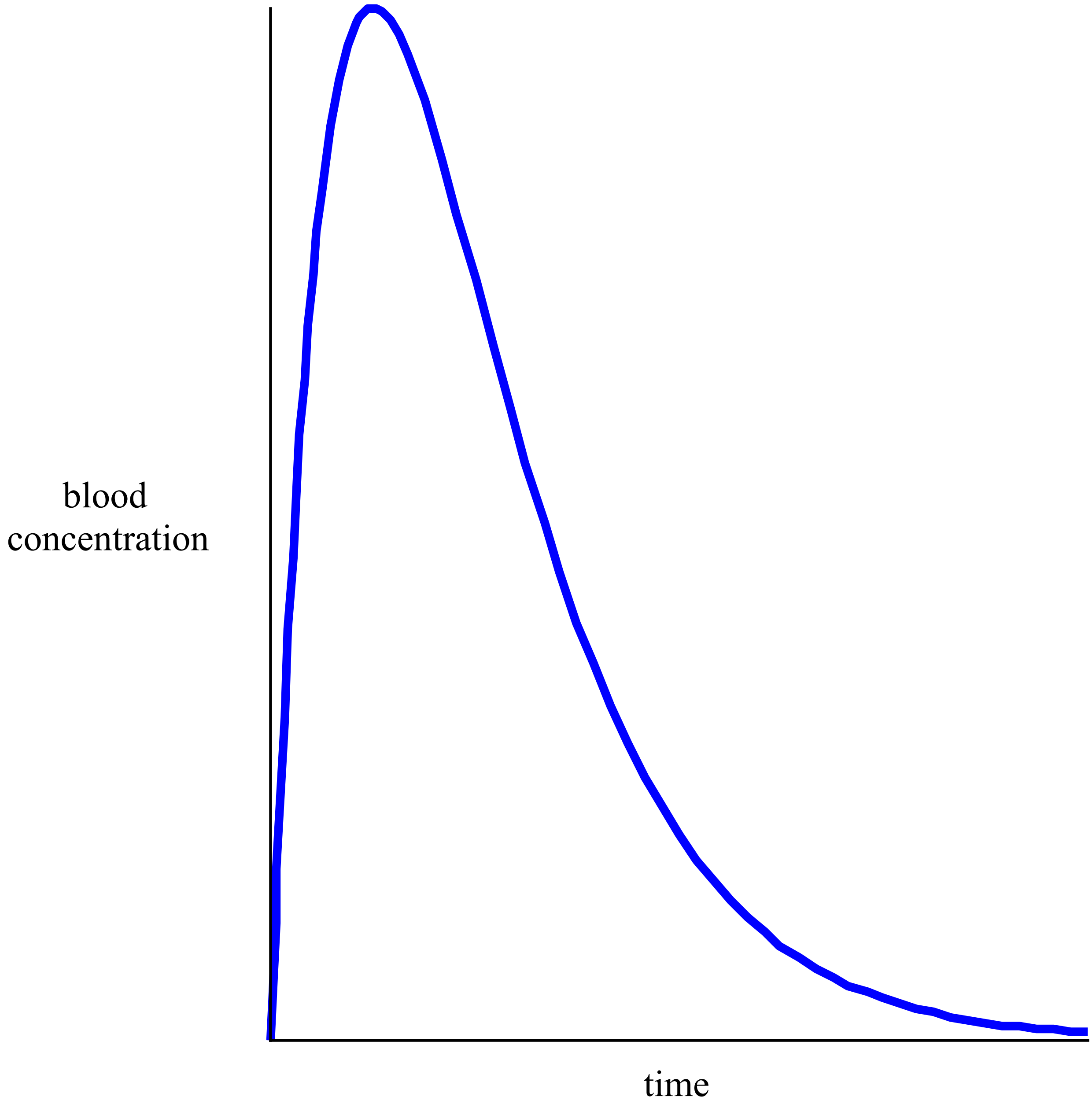
(g) a possible "danger level" of drug concentration, above which the person may require monitoring; and

(h) the "total exposure" of the body to the drug.

Understanding rates of change plays an important role in analysing most of these factors.

Zoloft *(continued)*

***Question** 13.1.2* An idealised drug concentration graph is shown. Mark on the graph the values (or possible values) of each of (a) to (h) described in Example 13.1.1.



- Compare the information on Zoloft in the following example with some of the features/observations in Example 13.1.1.

Example 13.1.3 (From the sertraline fact sheet at *www.pbs.gov.au.*)

"**Pharmacokinetics:**

In humans, following oral once-daily dosing over the range of 50 to 200 mg for 14 days, mean peak plasma concentrations (C_{max}) of sertraline occurred between 4.5 to 8.4 hours post dosing. The average terminal elimination half-life of plasma sertraline is about 26 hours. Based on this pharmacokinetic parameter, steady-state sertraline plasma levels should be achieved after approximately one week of once-daily dosing. Linear dose-proportional pharmacokinetics were demonstrated in a single dose study in which the C_{max} and area under the plasma concentration time curve (AUC) of sertraline were proportional to dose over a range of 50 to 200 mg.

Dosage: Adults (18 years and older)

The usual therapeutic dose for depression is 50 mg/day. ...patients not responding to a 50 mg/day dose may benefit from dose increases up to a maximum of 200 mg/day. Given the 24 hour elimination half-life of sertraline, dose changes should not occur at intervals of less than 1 week. The onset of therapeutic effect may be seen within 7 days; however for full activity 2 to 4 weeks are usually necessary ....

Use in Children and Adolescents aged less than 18 years:

Sertraline should not be used in children and adolescents below the age of 18 years for the treatment of major depressive disorder. The efficacy and safety of sertraline has not been satisfactorily established for the treatment of major depressive disorder in this age group.

Overdosage:

On the evidence available, sertraline has a wide margin of safety in overdose. Overdoses of sertraline alone of up to 13.5 g have been reported. Deaths have been reported involving overdoses of sertraline, primarily in combination with other drugs ...."

Extension 13.1.4 (From the Australian newspaper online, 1/11/2008)

"Probe into antidepressants being conducted 'in secret'

The Therapeutic Goods Administration is investigating the adverse effects of SSRI antidepressants, a widely prescribed group of drugs that includes the well-known brands Prozac and Zoloft.

The TGA confirmed in a statement to [the newspaper] that it had established a special expert panel of psychiatrists and epidemiologists to review a number of cases involving patients who had had adverse reactions to these drugs. It is believed hundreds of cases will be reviewed.

"Although there has not been a jump in adverse events from SSRIs, there has been community concern about potential overuse", the TGA said. Medicare figures show that, since 1990, when Prozac first appeared on pharmacy shelves, there have been almost 10,000 reports of suspected adverse reactions to SSRIs received by the TGA's Australian Adverse Drug Reactions Advisory Committee.

More than 12 million SSRI antidepressant scripts were subsidised by the Pharmaceutical Benefits Scheme last year ....

The TGA has also asked all drug companies that market SSRI antidepressants in Australia to update the wording of their suicide warnings concerning children and young people under 24 years in the information provided to patients....

The move comes after an investigation by The Weekend Australian revealed several hundred thousand scripts for antidepressants such as Zoloft and Prozac were last year prescribed to children and subsidised through the Pharmaceutical Benefits Scheme, despite the TGA and Pfizer, the company that markets Zoloft in Australia, recommending they not be prescribed to anyone under the age of 24 for the treatment of depression. Significant discrepancies in the information given to parents about the potential dangers of the drugs to children were also uncovered..."

End of Case Study 18.

- Pharmacokinetics is particularly concerned with the *rate* at which the drug concentration *changes*.
- The concept of one quantity changing as another quantity changes, and the rate at which this change occurs, is crucial to many applications in science, engineering, social sciences and economics.

***Example** 13.1.5* In addition to answering questions about drug concentrations, rates of change are important in solving problems such as:

- landing a space capsule on the moon with minimum fuel usage;
- predicting the spread of ash from a volcanic eruption;
- modelling earthquakes and tsunamis, allowing predictions to be made about which areas will be affected, and when;
- predicting future populations of two interacting species;
- estimating the impact of a vaccination program on the spread of a disease;
- predicting the impact on blood flow due to constriction of an artery;
- minimising risk in a share portfolio;
- determining the time to equilibrium for a chemical reaction; and
- predicting the time at which a student will attain a certain threshold level of knowledge about a topic.

- We will cover two similar ways of studying rates of change:
  - *average* rates of change; and
  - *instantaneous* rates of change.

13.2 Average rates of change

- The *average rate of change* measures the average rate at which some phenomenon changes between two observations.
- In science, average rates of change are usually specified as occurring in some time period (such as 60 m s^{-1}).
- To find the average rate of change of a quantity between two observations over time:

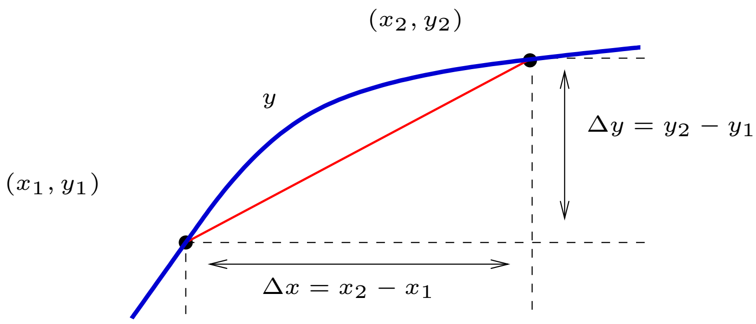
  divide the **total change in the quantity** by the **total change in time**.

Average rate of change

Let (x_1, y_1) *and* (x_2, y_2) *be two points. Then the* **average rate of change of** y **with respect to** x *between those points is defined to be the change in* y *values divided by the change in* x *values, so:*

$$\frac{\text{change in } y}{\text{change in } x} = \frac{\Delta y}{\Delta x} = \frac{y_2 - y_1}{x_2 - x_1}.$$

(Note that Δ *is the Greek capital letter "Delta", and usually means "the change in the value of".)*



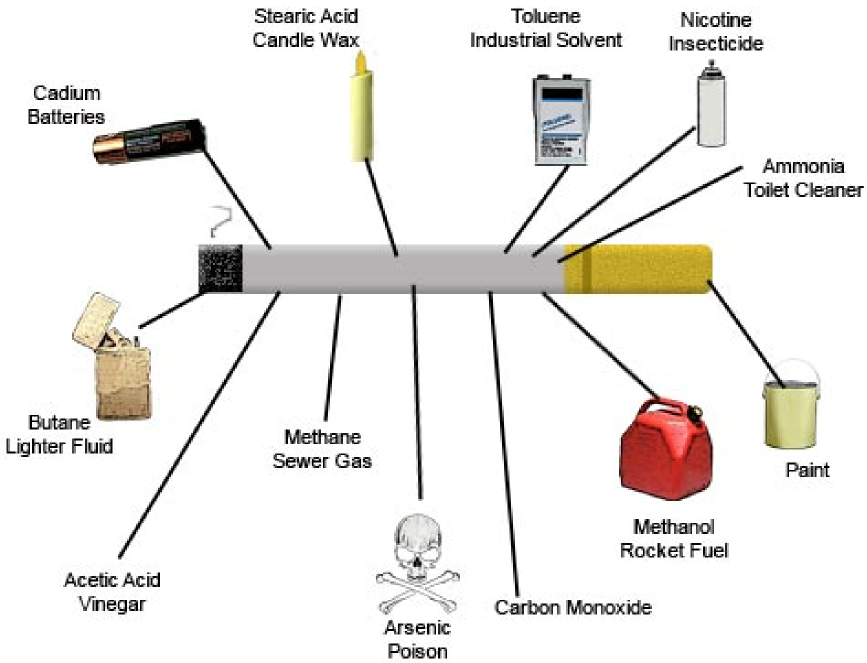
***Example** 13.2.1* The concentration of atmospheric CO_2 has risen by about 70 ppm over the last 50 years. Hence the average rate of change over this time is $\dfrac{70}{50} = 1.4$ ppm/year.

Case Study 19: Cigarettes





- Nicotine is an addictive, poisonous alkaloid found in a number of plants, including tobacco. Tobacco products also contain a large number of other compounds, many of which are damaging to health.



(source: quit-smoking-aid.net)

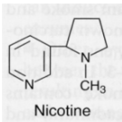
Cigarettes *(continued)*

Tobacco

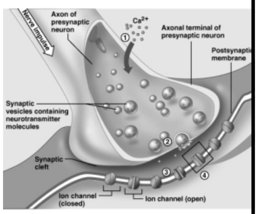
- cigarettes, cigars, pipes, snuff
- widely used stimulants (inhaled, chewed)
- mainstream cigarette smoke
  - 1-3 billion particles/mL
  - 4,000 substances (43 carcinogens)
  - metals (arsenic, cadmium...), promoters (phenols...)
  - irritants (formaldehyde...), toxins (cyanide)
  - carbon monoxide (200x affinity for Hb than O_2)
- causative agents for many diseases, incl.
  - lung cancer
  - chronic respiratory diseases
  - cardiovascular diseases

Why smoke? nicotine addiction

Nicotine



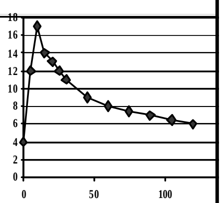
– alkaloid substance (insecticide)
– readily crosses blood-brain barrier
– stimulates receptors in neural synapses
(nicotinic acetyl choline)



Three main effects
– enhanced dopamine release
(reward circuit, ↑ pleasure)
– addictive behaviours
(physical dependence)
(psychologic dependence)
– enhanced neurotransmission
(↑ cardiovascular responses, ↑HR, ↑BP, ↑CO)
(hypertension, arteriosclerosis, MI, stroke)
(COPD – chronic obstructive pulmonary disease)

Nicotine

Pharmacokinetics (PK):
~ 1mg/cigarette, LD_{50} ~ 1 mg/Kg



Absorption
- through lungs, within seconds

Distribution
- throughout body via circulation
- effect on brain within 7 seconds

Metabolism ($t_{1/2}$ ~ 2 hours)
- oxidation in liver
(cytochrome P450 system, CYP2A6, CYP2B6)
(FMO system, flavin-containing monooxygenase)

Excretion
- must be metabolized

Extension 13.2.2 (From a NSW Government Health Dept. fact sheet)

"What is nicotine?

Nicotine is a chemical substance found in tobacco leaves. Addiction to nicotine is what keeps you smoking. Nicotine is as addictive as heroin or cocaine.

How does nicotine work?

From the moment that you inhale tobacco smoke, it takes four seconds for the nicotine to reach your blood stream and about ten seconds to reach the brain. Once the nicotine has attached itself to special sites in the brain, many relaxing chemicals are released. But this effect only lasts for a short time and then the addicted smoker needs to 'top up' their nicotine...

Why is nicotine a problem for health?

The worst problem for health caused by nicotine is that it is so addictive.... Smoking tobacco accounts for the largest proportion of preventable illness and death in Australia. Immediate effects of nicotine on the body include increased heart rate and blood pressure and constriction of blood vessels. Over time, ingestion of nicotine from smoking combines with carbon monoxide to damage the lining of blood vessels and make blood platelets stickier. In combination these effects contribute to the development of heart disease.

Although nicotine is among the most toxic and fast acting of all poisons, the dose from smoking is too low to cause acute poisoning (smoking poisons you slowly)....

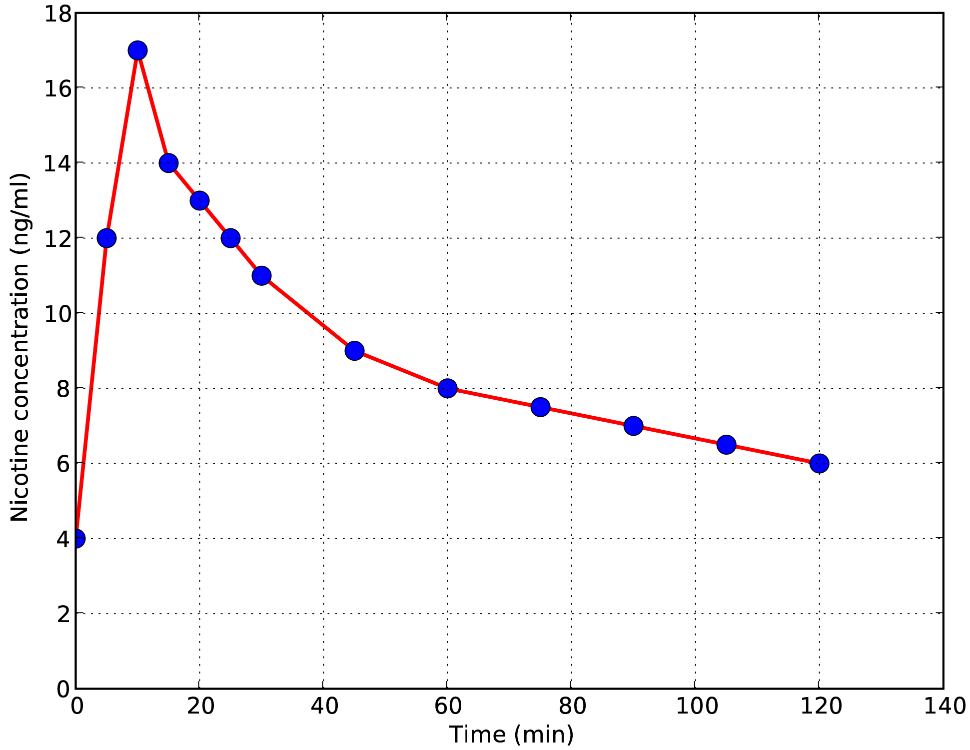
How does your body get rid of nicotine?

Most of the nicotine (80 per cent) is broken down in the liver. Nicotine is also filtered from the blood by the kidneys and removed in urine."

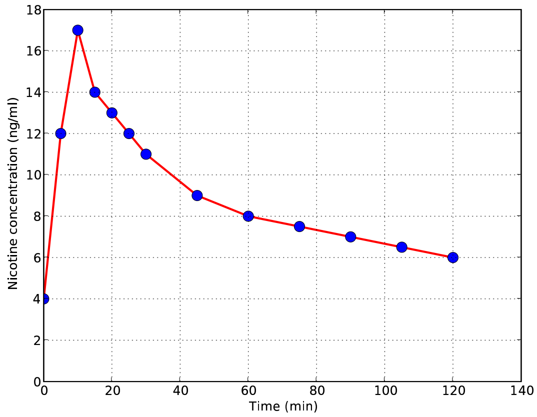
***Example** 13.2.3* When a cigarette is smoked, nicotine is rapidly absorbed into the bloodstream through the lungs. The following table shows measurements of the blood-concentration of nicotine of a person at various time intervals after smoking a cigarette.

t (min.)	0	5	10	15	20	25	30
$C(t)$ (ng/mL)	4	12	17	14	13	12	11
t (min.)	45	60	75	90	105	120	
$C(t)$ (ng/mL)	9	8	7.5	7	6.5	6	

This data is plotted on the following graph.
(Note that the measurements were taken at discrete time intervals. Hence the data points should not be joined on the graph; the connecting lines are there only to make the graph easier to read.)



***Question** 13.2.4* The graph from Example 13.2.3 is:



(a) Explain the main features of the shape of the graph (which is typical of many drugs).

(b) The person commences smoking again at $t = 200$ mins. Roughly estimate their blood-nicotine concentration at that time.

(c) Find the **total** change in blood-concentration of nicotine from $t = 0$ to $t = 120$ min?

(d) Find the **average** rate of change in concentration from:

(i) $t = 0$ to $t = 120$ min; and

(ii) $t = 0$ to $t = 10$ min.

End of Case Study 19.

13.3 Instantaneous rates of change and derivatives

- Average rates of change are often useful.
- However, if a rate of change varies substantially then average rates of change become less useful.
- In many situations it is more useful to measure the *instantaneous* or *exact* rate of change.
- If we know the exact rate of change, we can identify a number of important features. For example, at any *peak* or *trough* the rate of change is 0. (On a drug concentration curve, a peak corresponds to the *peak concentration level.*)
- Hence we require a new approach which finds the *instantaneous* rate of change of a function at a point. The mathematical concept which does this is called the *derivative.*

Derivatives

Let $f(x)$ be a function. Then the **derivative** *of f is a new function denoted $f'(x)$ that gives the instantaneous slope or rate of change of the function f at any point x.*

Another way of writing the derivative is $\dfrac{df}{dx}$.

The process of finding a derivative is called **differentiation**. *In this course we will assume that the derivative always exists when we need it to. (There are situations where derivatives do not exist.)*

The derivative of the derivative *is often called the* second derivative, *denoted f''.*

- You will need to know how to interpret and use derivatives. Make sure you understand what a derivative is, and what information it gives.

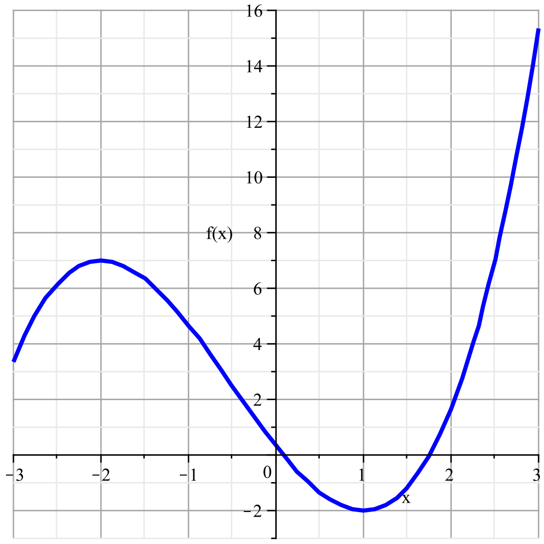
Interpreting derivatives

If $y = f(x)$ is a function then the derivative y' gives the rate at which y is changing with respect to x.

The **value** *of the* **derivative** *at any point describes the behaviour of the* **function** *at that point. At any point:*

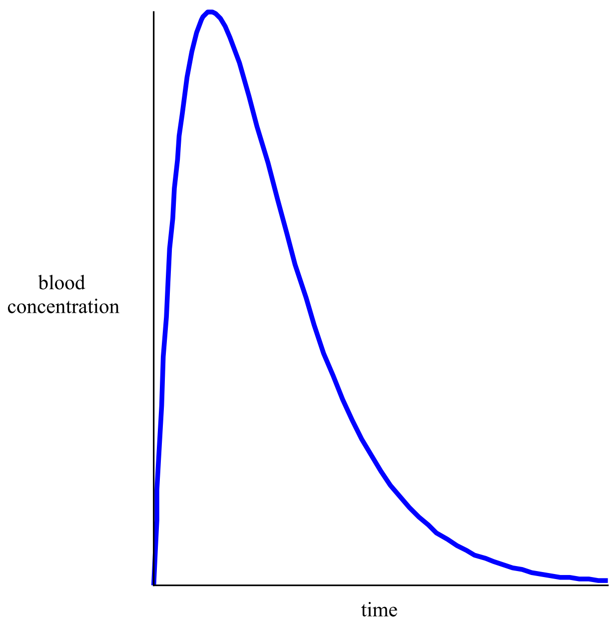
- *if y' is* **positive** *then the function y is* **increasing***;*
- *if y' is* **negative** *then the function y is* **decreasing***; and*
- *if y'* **equals zero** *then the function y has one of:*
  - *a* **local maximum** *or peak at that point; or*
  - *a* **local minimum** *or trough at that point; or*
  - *a* **point of inflection** *at that point (which we will not cover in this course).*

***Example** 13.3.1* Let $f(x)$ be the following function.



- $f' = 0$ at $x = -2$, which is a local maximum.
- $f' = 0$ at $x = 1$, which is a local minimum.
- f' is positive between $x = -3$ and $x = -2$, and also between $x = 1$ and $x = 3$.
- f' is negative between $x = -2$ and $x = 1$.

Question *13.3.2* Consider the concentration function $C(t)$:



(a) What is the physical meaning of C'?

(b) On the graph:

- **(i)** mark with a cross any points at which $C' = 0$;
- **(ii)** label any local maxima with the word 'max';
- **(iii)** label any local minima with the word 'min';
- **(iv)** identify all regions where C' is positive; and
- **(v)** identify all regions where C' is negative.

(c) What is physically happening when C' is:

- **(i)** positive?
- **(ii)** zero?
- **(iii)** negative?

13.4 Finding derivatives

- At school you would have learned how to find derivatives.
- Differentiation techniques are summarised below; make sure you are comfortable with them but don't memorise them!
- Any rules you need will be given on your exam; any derivatives you need to find will be fairly easy.

Derivatives of some common functions

$f(x)$	$f'(x)$
$f(x) = k$, *where k is a constant.*	$f'(x) = 0$
$f(x) = x^n$, *where n is any real number.*	$f'(x) = nx^{n-1}$
$f(x) = \sin x$	$f'(x) = \cos x$
$f(x) = \cos x$	$f'(x) = -\sin x$
$f(x) = e^{kx}$, *where k is a constant.*	$f'(x) = ke^{kx}$
$f(x) = \ln x$ $(x > 0)$	$f'(x) = 1/x$

Some differentiation rules

Let $f(x)$ and $g(x)$ be functions and k be a constant. Then:

- $(kf)' = kf'$ *(Constant multiple rule)*
- $(f \pm g)' = f' \pm g'$ *(Sum/difference rule)*
- $(fg)' = f'g + fg'$ *(Product rule)*
- $(f/g)' = (f'g - fg')/g^2$ *(Quotient rule)*
- $f(g)' = f'(g)g'$ *(Chain rule; alternately, $\dfrac{df}{dx} = \dfrac{df}{dg} \times \dfrac{dg}{dx}$)*

***Question** 13.4.1* For practise, find the derivatives of each of:

(a) $f(t) = 3t^2 + 6t + 4$

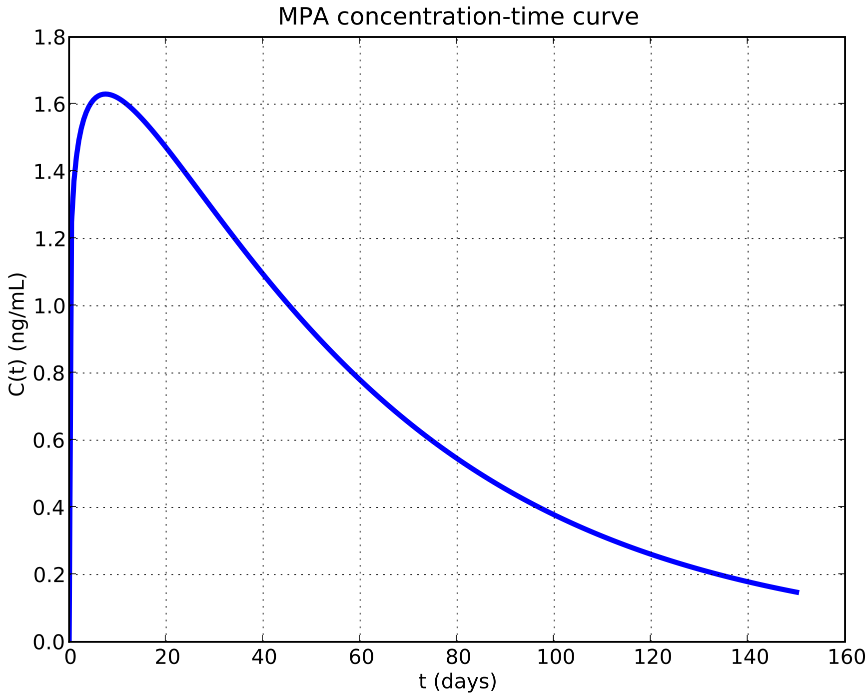
(b) $h(t) = e^{0.2t}$

(c) $j(t) = t^2 e^{0.2t}$

(d) some additional functions of your choice.

13.5 Numerical solutions and Newton's method

***Question** 13.5.1* Later we will see that a function modelling blood-concentration of a long-lasting injection of a female contraceptive (in ng/mL of medroxyprogesterone acetate or MPA) is $C(t) = 1.4t^{0.15}e^{-0.02t}$. The graph of $C(t)$ is:



(a) If the minimum blood-concentration level for reliable contraception is 0.3 ng/mL, estimate from the graph the time at which reliable contraception ceases.

(Injections are given every $12 - 13$ weeks.)

(b) Rewrite Part (a) as an equation to be solved.

(c) How could the equation in Part (b) be solved?

- Often in science we need to solve equations which are difficult or impossible to solve **exactly**.
- An alternative is to find an **approximate** solution, using *root-finding* algorithms. (Remember that *root* is another word for *solution*.)
- Typically, root-finding algorithms involve applying similar steps a number of times; these steps are called *iterations*.
- There is usually a *numerical error* associated with approximate solutions calculated by root-finding algorithms.
- Numerical errors can often be reduced by performing more iterations.
- One iterative root-finding algorithm is called *Newton's method*, which uses an initial estimate of a root and a derivative to find a root of a function.
- Newton's method does not always *converge* to a solution. However, it will usually converge if the initial estimate is 'good enough'.

Newton's method (informal description)

To find a value of x for which $f(x) = 0$, that is a root of $f(x)$, Newton's method proceeds as follows:

1. *Choose an initial estimate of the root.*
2. *Calculate a new estimate of the root using the old estimate and the derivative. (The new estimate is hopefully more accurate than the previous one.)*
3. *Stop if the new estimate is sufficiently accurate or if too many steps have been taken. Otherwise, return to Step 2.*

- Note that Newton's method only solves equations of the form $f(x) = 0$.
- Before Newton's method can be applied the equation may need to rearranged, giving an equivalent equation with 0 on the right hand side.
- For example, in Part (b) of Question 13.5.1, the equation to solve was $C(t) = 0.3$. To use Newton's method we instead solve $C(t) - 0.3 = 0$.

Newton's method (formal description)

To find a value of x for which $f(x) = 0$, that is a root of $f(x)$, Newton's method proceeds as follows:

1 *Let x_0 be an initial estimate of a root of f that is 'sufficiently close' to an actual root of f. At the ith iteration ($i = 0, 1, 2, \ldots$), x_i is the current approximation to the actual root.*

2 *Calculate the next estimate x_{i+1} by the equation:*

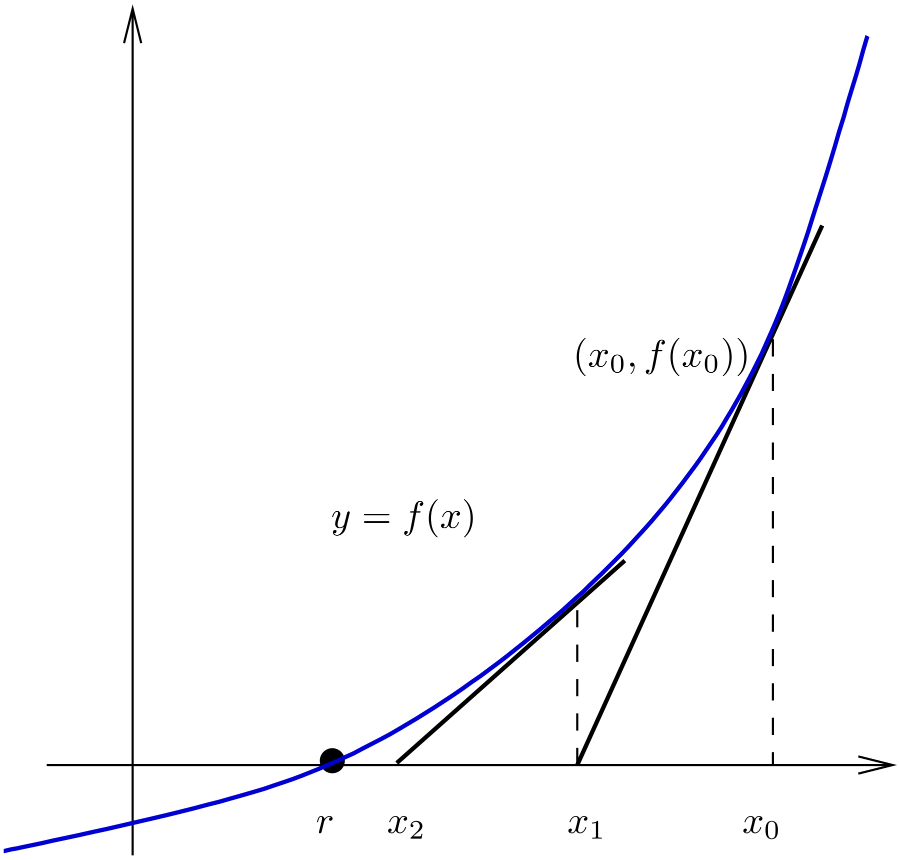
$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$$

3 (a) *If the value of x_{i+1} is sufficiently accurate then stop; x_{i+1} is the estimated root.*

(b) *If too many steps have been taken and x_{i+1} is not sufficiently accurate then stop, as the method is not converging to a solution. Choose a 'better' value for x_0 and start again.*

(c) *Otherwise, return to Step 2.*

- The idea behind Newton's method is not too hard. Assume that $f(x)$ has a root at $x = r$, so $f(r) = 0$. Let the initial estimate of the root be x_0.
- The method calculates the next estimate x_1 by extending a line from the point $(x_0, f(x_0))$ to the x-axis, with the slope of the line equal to the derivative f' at the point x_0.
- Rearranging the formula for the equation of a straight line gives Newton's method (see below).



- If x_0 is sufficiently close to the root then the new approximation x_1 will be closer to the root than was x_0.
- These steps continue until either a good approximation to the root is found, or too many steps have been taken.

(If you are interested in seeing why Newton's method works, consider the straight line joining the points $(x_0, f(x_0))$ and $(x_1, 0)$. This line has gradient equal to $f'(x_0)$, which must also be equal to $\dfrac{f(x_0) - 0}{x_0 - x_1}$.

Thus $f'(x_0) = \dfrac{f(x_0)}{x_0 - x_1}$ and rearranging this gives $x_1 = x_0 - \dfrac{f(x_0)}{f'(x_0)}$.)

Example 13.5.2 Use Newton's method to estimate $\sqrt{12}$.

Answer: First, we need to rewrite the question in the form of an equation to be solved.

Let $f(x) = x^2 - 12$.
Finding $\sqrt{12}$ is the same as solving $f(x) = 0$.

To apply Newton's method, we first need to find the derivative and choose an initial estimate of the root:

- Because $f(x) = x^2 - 12$, we have $f'(x) = 2x$.
- We know that $\sqrt{12}$ is between 3 and 4, so we will use $x_0 = 3$ as the initial estimate of the root. (We could choose other estimates but $x_0 = 3$ is likely to be "close" to the root.)

Now we have everything we need to use Newton's method. Applying three steps gives the following results, with the sequence of approximations to the root in the last column. (Recall that the equation is $x_{i+1} = x_i - \dfrac{f(x_i)}{f'(x_i)}$.)

i	x_i	$f(x_i)$	$f'(x_i)$	x_{i+1}
0	3	-3	6	3.5
1	3.5	0.25	7	3.4642857
2	3.4642857	0.001275	6.92857	3.4641016

After three steps, the estimate of $\sqrt{12}$ is $x_3 = 3.4641016$.

Note that:

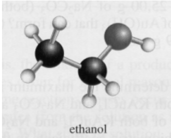
- The estimated root barely changed from x_2 to x_3.
- The estimate of the root is quite accurate; in fact, x_3 is correct to seven decimal places.

13.6 Pleasures of the flesh and derivatives

- Now we will apply derivatives to drug concentration graphs.

Alcohol

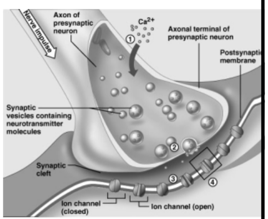
- colourless volatile fluid(s)
- ethanol C_2H_5OH
- obtained by fermentation of sugars
- beer, wine, spirits
- most commonly used drug worldwide



EFFECTS
- acute intoxication
  - slurred speech, motor incoordination, altered behaviour
  - increased self-confidence, impaired judgement/reflexes
- chronic use
  - liver disease (fat deposits, hepatitis, cirrhosis)
  - neuropathy (central and peripheral)
  - cardiovascular (myopathy, hypertension)
  - gastro-intestinal (gastritis, pancreatitis)
  - reproductive (testicular atrophy, foetal alcohol syndrome)

Pharmacodynamics: ethanol

- central nervous system (CNS) depressant (similar to anaesthetics)
- mode of action (unknown)
- ↓ signal transduction in brain
- inhibits:
  - GABA transmitters
  - voltage-gated Ca^{++} channels
  - NMDA receptors
- paradoxically, no specific receptor has been identified
- but chronic use leads to:
  - psychological dependence
  - physical dependence



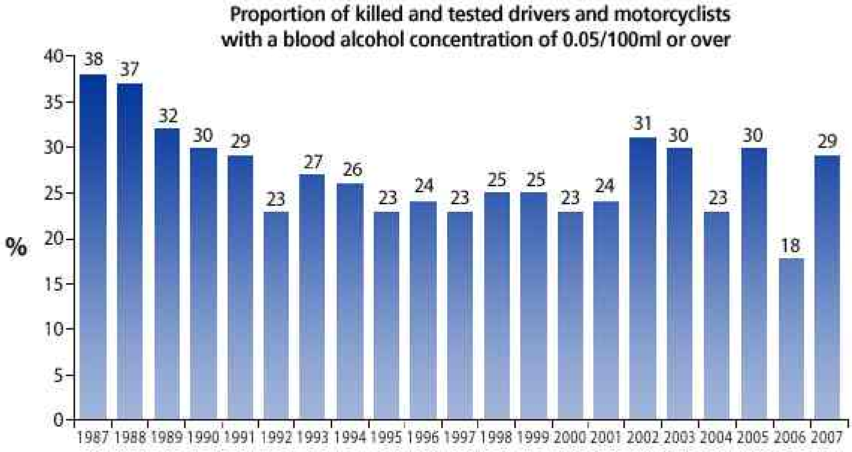
Pharmacokinetics: ethanol

ADME: - variable (age, sex, weight, race, history) (type, amount, activity, diet, etc)

- Absorption
  - 25% stomach, 75% duodenum
  - peaks 0.5-2.0 hours after ingestion
- Distribution
  - rapidly throughout body via bloodstream
- Metabolism
  - 90% in liver (alcohol dehydrogenase, catalase, microsomal ethanol-oxidizing system)
- Excretion
  - 1-5% in breath, 1-3% in urine, 0.5% in sweat

BAC: legal limit = 0.05% = 0.5‰ = 0.5 g/L = 50 mg/dL
0.35% - fatal poisoning (LD_{50} ~ 0.4%)

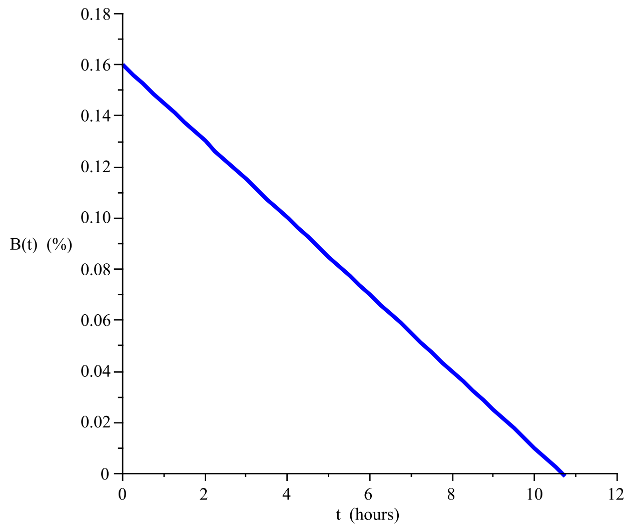
Case Study 20:
Whisky



Statistics for Victoria

- A standard drink contains 10 g of alcohol.
- Blood Alcohol Concentration (BAC) is usually measured as the percentage of total blood volume which is alcohol (or in grams of alcohol per litre of blood). In Australia the legal blood alcohol content for driving is 0.05%, or 0.5 g/L.
- Unlike many other drugs, the rate of metabolising alcohol by the body is roughly constant. (In Chemistry, this is called a *zero-order reaction.*)
- This rate is usually not dependent on the BAC because typical levels of alcohol consumption saturate the capacity of the metabolising enzymes within the liver.
- The exact rate of metabolism varies between individuals, and is influenced by such factors as age, weight and gender.
- A graph of BAC plotted from the time of commencing drinking will show a rapid initial rise during the absorption phase, prior to the elimination phase.
- Because the rate of metabolising alcohol tends to be constant, once a person ceases drinking and alcohol absorption is complete, then a graph of BAC from that time on will be linear (until metabolism is almost complete).

***Question** 13.6.1* After a particularly awful SCIE1000 lecture a student quickly consumes far too much alcohol. At time t in hours **since his last drink** his BAC is $B(t) = 0.16 - 0.015t$ %. This graph is shown below (note that the graph shows the blood concentration **after** the absorption phase):



(a) Find $B'(t)$.

(b) Interpret, in words, what $B'(t)$ represents.

continued...

***Question** 13.6.1 (continued)* The following tables estimate the number of hours required for the BAC of males and females of different weights to return to zero. (These are taken from an American government website; to approximately convert from pounds to kg, divide by 2.2.)

Males:

num. drinks	Weight (pounds)							
	120	140	160	180	200	220	240	260
1	2	2	2	1.5	1	1	1	1
2	4	3.5	3	3	2.5	2	2	2
3	6	5	4.5	4	3.5	3.5	3	3
4	8	7	6	5.5	5	4.5	4	3.5
5	10	8.5	7.5	6.5	6	5.5	5	4.5

Females:

num. drinks	Weight (pounds)							
	120	140	160	180	200	220	240	260
1	3	2.5	2	2	2	1.5	1.5	1
2	6	5	4	4	3.5	3	3	2.5
3	9	7.5	6.5	5.5	5	4.5	4	4
4	12	9.5	8.5	7.5	6.5	6	5.5	5
5	15	12	10.5	9.5	8	7.5	7	6

(c) Using the information in the tables, comment on $B'(t)$ for males versus females, and for different body weights.

End of Case Study 20.

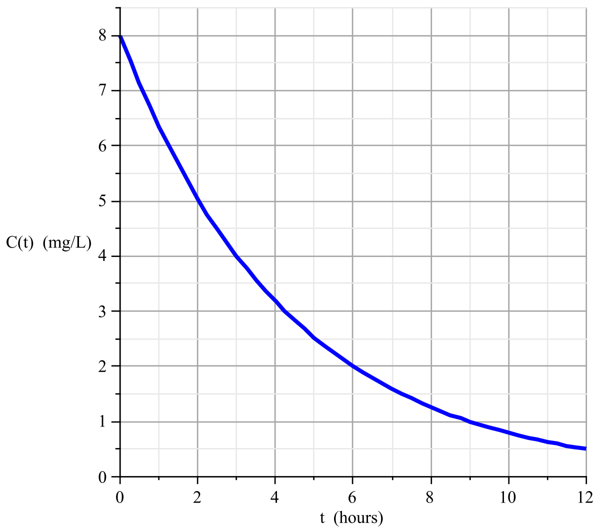
Case Study 21:
Caffeine

- Unlike alcohol (which saturates the enzymes so is metabolised at a constant rate), many other drugs are metabolised by the body at a rate proportional to the current concentration of the drug in the bloodstream. (In Chemistry, this is called a *first-order reaction*.)
- Hence their concentration functions must be exponential .

***Question** 13.6.2* To stay awake in SCIE1000, a student drinks two large, strong cups of coffee. After 30 minutes the caffeine concentration in her blood attains its peak level. At any time t after this (in hours) the concentration of caffeine in her blood in mg/L is given by

$$C(t) = 8e^{-kt}$$

where k is a positive constant (so the power is negative).



continued...

Question *13.6.2 (continued)* Recall that $C(t) = 8e^{-kt}$ mg/L.

(a) Find $C'(t)$.

(b) What do you notice about the functions C and C'? What does this mean? (We will study this in the section on *differential equations*.)

(c) For this student, the half-life of caffeine is 3 hours. Find the value of the constant k.

End of Case Study 21.

Case Study 22:
Wild, wild women

- Depo-subQ Provera 104 is a long-term female contraceptive administered as an injection every 12 – 13 weeks.
- The active ingredient in a standard 0.65 mL does is 104 mg of the artificial female hormone medroxyprogesterone acetate (MPA), which is similar to progesterone.
- The contraceptive works by causing changes to the female reproductive system resulting in both inhibition of egg release and a hostile environment to sperm.
- It is 99.7% effective, which is very high compared to many other forms of contraception.
- Commonly quoted benefits are convenience and reliability.
- As with many drugs, studies have identified potential side effects (including breakthrough bleeding, reduced libido, weight gain and reduced bone density).

Example 13.6.3 Comparison of various forms of contraception.

Percentage of Women Experiencing an Unintended Pregnancy During the First Year of Typical Use and the First Year of Perfect Use of Contraception and the Percentage Continuing Use at the End of the First Year: United States

	% of Women Experiencing an Unintended Pregnancy within the First Year of Use		% of Women Continuing Use at 1 Year*
Method	**Typical Use†**	**Perfect Use‡**	
Chance	85	85	
Spermicides	26	6	40
Periodic Abstinence	25		63
Calendar		9	
Ovulation Method		3	
Symptothermal		2	
Post-ovulation		1	
Cap			
Parous Women	40	26	42
Nulliparous Women	20	9	56
Sponge			
Parous Women	40	20	42
Nulliparous Women	20	9	56
Diaphragm	20	6	56
Withdrawal	19	4	
Condom			
Female (Reality)	21	5	56
Male	14	3	61
Pill	5		71
Progestin only		0.5	
Combined		0.1	
IUD			
Progesterone T	2.0	1.5	81
Copper T 380A	0.8	0.6	78
LNg 20	0.1	0.1	81
Depo-Provera IM 150 mg	**0.3**	**0.3**	**70**
Norplant and Norplant-2	0.05	0.05	88
Female Sterilization	0.5	0.5	100
Male Sterilization	0.15	0.10	100

† Among typical couples who initiate use of a method (not necessarily for the first time), the percentage who experience an accidental pregnancy during the first year if they do not stop use for any other reason.

‡ Among couples who initiate use of a method (not necessarily for the first time) and who use it perfectly (both consistently and correctly), the percentage who experience an accidental pregnancy during the first year if they do not stop use for any other reason.

Source: www.drugs.com/pro/depo-subq-provera-104.html

Example 13.6.4 The following table shows pharmacokinetic parameters of MPA after a single SC injection of Depo-SubQ Provera 104 in healthy women ($n = 42$).

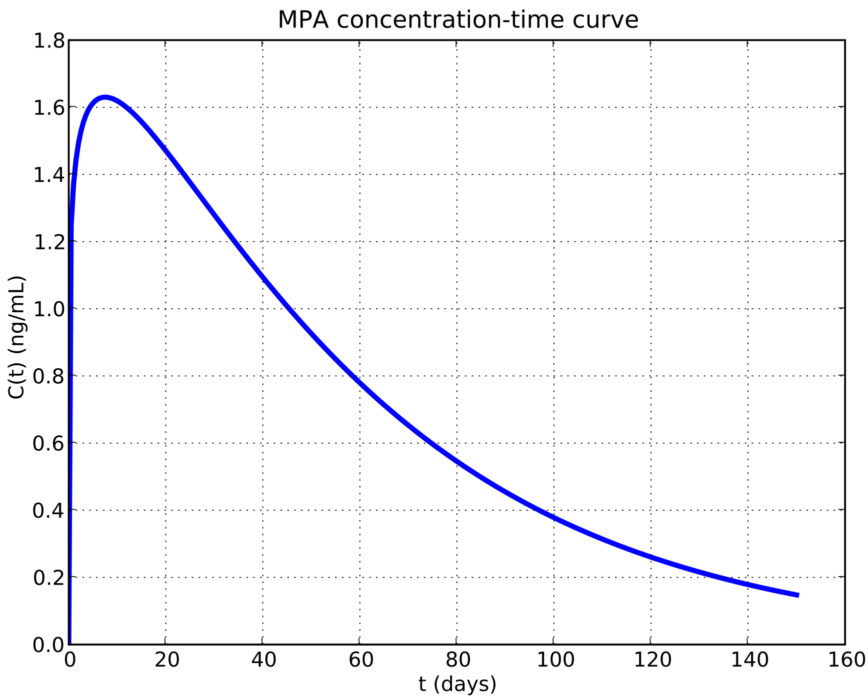
	C_{max} (ng/mL)	t_{max} (day)	C_{91} (ng/mL)	AUC_{0-91} (ng day/mL)	$AUC_{0-\infty}$ (ng day/mL)	$t_{1/2}$ (day)
Mean	1.56	8.8	0.402	66.98	92.84	43
Min	0.53	2.0	0.133	20.63	31.36	16
Max	3.08	80.0	0.733	139.79	162.29	114

www.drugs.com/pro/depo-subq-provera-104.html

- C_{max} = peak serum concentration; t_{max} = time when C_{max} is observed;
- C_{91} = serum concentration at 91 days;
- AUC_{0-91} and $AUC_{0-\infty}$ = area under the concentration-time curve over 91 days or infinity, respectively; and
- $t_{1/2}$ = terminal half-life.

Example 13.6.5 A patient is injected with a dose of Depo-subQ Provera 104. The following function models the concentration of MPA in her blood in ng/mL at time t in days after the dose.

$$C(t) = 1.4t^{0.15}e^{-0.02t}.$$



Surge functions

The concentration function for Depo-subQ Provera 104 is an example of a **surge** *function, so called because the function value initially surges rapidly before falling off exponentially over time. A general equation for a surge function is*

$$f(t) = at^p e^{-bt}$$

where a, p and b are positive constants determined by the characteristics of the particular phenomenon. The function for Depo-subQ Provera 104 is $C(t) = 1.4t^{0.15}e^{-0.02t}$, so $a = 1.4$, $p = 0.15$ and $b = 0.02$.

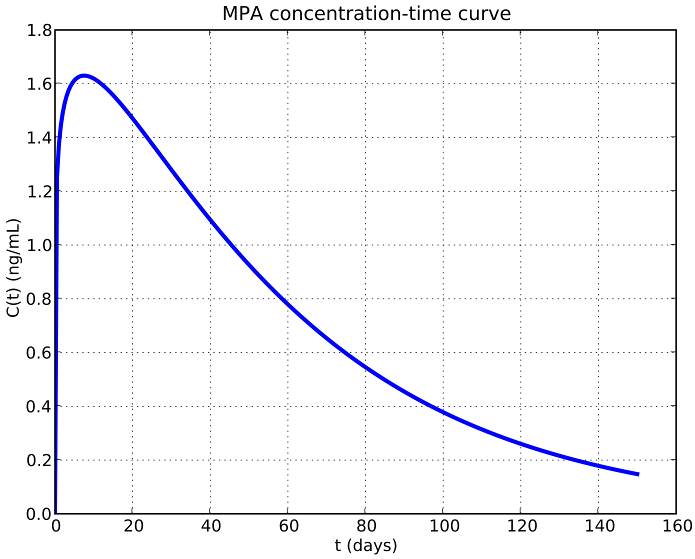
Question *13.6.6* Explain mathematically why surge functions $f(t) = at^p e^{-bt}$ have the general shape as shown in Example 13.6.5.

***Question** 13.6.7* The function modelling the blood concentration of MPA is $C(t) = 1.4t^{0.15}e^{-0.02t}$.

(a) Find C'. (Hint: the derivative of $e^{-0.02t}$ is $-0.02e^{-0.02t}$. You will also need to use the product rule.)

continued...

Question *13.6.7 (continued)* Recall that $C(t) = 1.4t^{0.15}e^{-0.02t}$, with the following concentration graph:



(b) Use your result from Part (a) to find t_{max} and C_{max}, and compare your answers with those in the table in Example 13.6.4. (You may assume that $C' = 0$ only at C_{max}.)

Wild, wild women *(continued)*

- Now we will investigate the timing of a follow-up injection.

Example 13.6.8 If the minimum blood-concentration level for reliable contraception is 0.3 ng/mL, calculate the time at which concentration ceases to be reliable, accurate to 3 decimal places.

Answer: we have $C(t) = 1.4t^{0.15}e^{-0.02t}$. The equation to be solved is $C(t) = 0.3$. Hence if we let $f(t) = C(t) - 4$ then we need to solve $f(t) = 0$. We can do this using Newton's method:

$$\begin{aligned} f(t) &= 1.4t^{0.15}e^{-0.02t} - 0.3, \quad \text{so} \\ f'(t) &= 1.4e^{-0.02t}\left(0.15t^{-0.85} - 0.02t^{0.15}\right) \end{aligned}$$

Finally, we use $t_0 = 50$ as the initial estimate for the root.

Then when we substitute f, f' and t_0 into Newton's method and iterate, on the fifth step the estimate of the root is

$$t_5 \approx 112.440.$$

Further iterations do not change this value significantly, so the time is around 112 days, which is about 16 weeks.

The time recommended by the manufacturer for follow-up injections is 12–13 weeks, which provides a reasonable safety margin.

Then we can develop a computer model.

Program specifications: Write a program which uses Newton's method to find the time at which the concentration of MPA decreases to 0.3 ng/mL.

Python Example 13.6.9

```
# Program to use Newton's method to solve an equation.
from __future__ import division
from pylab import *

# Define the function for Newton's method. Here it is
# the blood-concentration of MPA.
def func(t):
    return 1.4 * t**0.15 * exp(-0.02*t) - 0.3

# Define the derivative of the function for Newton's method.
def funcDash(t):
    return 1.4 * exp(-0.02 * t) * (0.15 * t**-0.85 - 0.02 * t**0.15)

# Initialise variables
ctr = 0
newEst = 50
prevEst = 0
tolerance = 0.001
# Loop through steps of Newton's method.
while abs (newEst - prevEst) > tolerance:
    ctr = ctr + 1
    prevEst = newEst
    newEst = prevEst - func(prevEst) / funcDash(prevEst)
    print ctr, round(newEst,3)
```

Python Example 13.6.10

Here is the output from running the above program:

```
1 89.769
2 108.467
3 112.302
4 112.44
5 112.44
```

End of Case Study 22.

13.7 Forensic toxicology

- *Forensic science* is concerned with applying scientific techniques to gather evidence relevant to legal cases.
- *Forensic toxicology* is the branch of forensic science which investigates drugs, poisons and other substances in the body.
- Many legal systems rely heavily on evidence from forensic science/toxicology units.
- One of the most common drugs of interest is alcohol, in the context of motor vehicle accidents and violent crimes.

Extension 13.7.1 (From www.health.qld.gov.au)

"Forensic Toxicology provides services to confirm or eliminate the possibility that alcohol, drugs or poisons may have contributed to behavioural impairment, a criminal offence, accident or death. This includes analysis of drugs or alcohol in blood or urine in drink or drug driving matters. The main clients of Forensic Toxicology are QPS [Queensland Police Service], the criminal justice system, including the Courts, DPP [Director of Public Prosecutions], LAQ [Legal Aid Queensland] and other defence counsel, the Coronial system, Corrective Services Department, Transport Department and Forensic Pathologists."

Extension 13.7.2 (From www.michigan.gov)

"The Toxicology Unit analyzes biological samples for the presence of alcohol and drugs. Blood, urine, or tissue samples are collected from subjects who have been charged with driving while intoxicated, victims of poisoning or sexual assault, from medical examiners offices, or in other suspicious or unusual circumstances.... Nine forensic scientists analyze over 13,000 alcohol and 2,500 drug cases per year, in addition to providing court testimony on case results."

Extension 13.7.3 (From www.fsni.gov.uk)

"The alcohol team deals with the detection and quantification of alcohol in body fluids and other liquids (for example samples of drinks containing alcohol). Samples are received from drivers suspected of drink driving, and post-mortem samples are submitted by the State Pathologist. In more complex cases such as murder and rape, the team is required to give an opinion on an alcohol concentration in the context of other information supplied with regard to estimating what the level may have been at an earlier time."

Extension 13.7.4 (From www.aifs.gov.au/acssa/pubs/briefing/b2.html)

"To date, there has been only one forensic study conducted in Australia to detect drugs in samples from victims specifically reporting drink spiking to police. Toxicology tests conducted by the Chemistry Centre in Western Australia between June 2002 and February 2003 on 44 cases of alleged drink spiking detected none of the CNS depressants normally associated with drink spiking, such as the benzodiazepines, GHB and ketamine (although it was acknowledged that GHB is extremely difficult to detect, even with early reporting). However, alcohol was present in 75 per cent of samples, with 31 per cent of all cases showing blood alcohol concentration levels in excess of 0.15 per cent. In the majority of cases, the level of alcohol was significantly higher than anticipated, based on the victim's self-assessment of consumption."

Extension 13.7.5 (From www.abc.net.au)

"Research from drug experts and police arrest statistics shows illegal substance abuse at schoolies has dropped, but binge drinking has risen: 90 per cent of schoolies partying in Queensland this week will consume alcohol, 25 per cent will smoke cannabis, and 11 per cent will take ecstasy, trend figures indicate."

***Question** 13.7.6* Reconcile the following two statements:

(i) "The rate of elimination of alcohol by the body is roughly constant in most situations. "

(ii) "Elimination of alcohol from the body follows *Michaelis-Menten* kinetics, where the rate of change of BAC due to elimination is:

$$V = \frac{-V_m B}{K_m + B}$$

where V_m is the maximum rate at which that individual can eliminate alcohol measured in % per time period, B is the BAC at any time, and the *Michaelis constant* K_m is the value of BAC at which the rate of elimination equals one half of V_m. "

(Hint: reasonable estimates are $K_m \approx 0.003$ % and $V_m \approx 0.015$ %/h. Sketch a rough graph of V for a range of values of B.)

***Question** 13.7.7* In practice (particularly in legal cases), BAC is often estimated using the *Widmark* formula (developed in 1932), which states that

$$B = \frac{A}{rW} \times 100\% - Vt$$

where B is the BAC at any time t since commencing drinking, A is the amount of alcohol consumed in g, V is the rate at which the body eliminates alcohol measured in % per time period, W is the body weight in g and r is the *Widmark factor* which estimates the proportion of body weight that is water. The precise value of r depends on factors such as gender, age and percentage body fat. Reasonable estimates are $r \approx 0.7$ for males and $r \approx 0.6$ for females.

(a) What is the physical meaning of the term rW?

(b) Why is the value of r for females typically less than for males?

(c) Verify that the units in the Widmark formula are consistent.

continued...

Question *13.7.7 (continued)* Recall that $B = \dfrac{A}{rW} \times 100\% - Vt$.

(d) Justify Australian government guidelines which suggest that to remain within the legal driving BAC range, within the first hour "men should drink at most two drinks and women at most one".

(e) Justify Australian government guidelines which suggest that to remain within the legal driving BAC range, after the first hour, "men and women should drink at most one drink per hour".

continued...

Question *13.7.7 (continued)* Recall that $B = \dfrac{A}{rW} \times 100\% - Vt$.

(f) Find B' and compare your answer with the answer to Question 13.7.6.

(g) At Schoolies week, a (binge-drinking, Gen Y) female who weighs 60 kg rapidly consumes 10 standard drinks (each with 10 g pure alcohol). Roughly sketch her BAC at any time, and estimate when it will return to 0.

***Question** 13.7.8* In the Widmark formula, the absorption term assumes that alcohol is absorbed by the body **immediately** after drinking. The following variant is given in a paper[a]:

$$B = \frac{A}{rW} \times \left(1 - e^{-k_a t}\right) \times 100\% - Vt$$

where k_a is the rate at which the body absorbs alcohol.

(a) Reconcile the Widmark formula with the variant. (Hint: draw a graph of the revised absorption term.)

(b) If t is measured in hours, what are the units of k_a?

(c) What factors could influence the value of k_a for:

(i) a given person, at different times?

(ii) different people?

continued...

[a]Posey and Mozayani, *The estimation of BAC, Widmark revisited*, Forensic Science, Medicine and Pathology, **3** (2007) 33–39.

***Question** 13.7.8 (continued)* In the units from Part (b), a typical value of k_a is 6. Recall that $B = \dfrac{A}{rW} \times \left(1 - e^{-k_a t}\right) \times 100\% - Vt$.

(d) Find the half-life for the absorption of alcohol.

(e) Find an expression for the time at which the BAC is at its peak value. (Hint: if $y(t) = e^{-k_a t}$ then $y'(t) = -k_a e^{-k_a t}$.)

continued...

Question *13.7.8 (continued)* It has been shown that if alcohol is consumed when the stomach contains food, then a typical value for k_a is 2.3 (compared with $k_a \approx 6$ for an empty stomach).

(f) Compare the maximum BACs and the times at which they occur for an 80 kg male who consumes 4 standard drinks after he has eaten, compared to not having eaten.

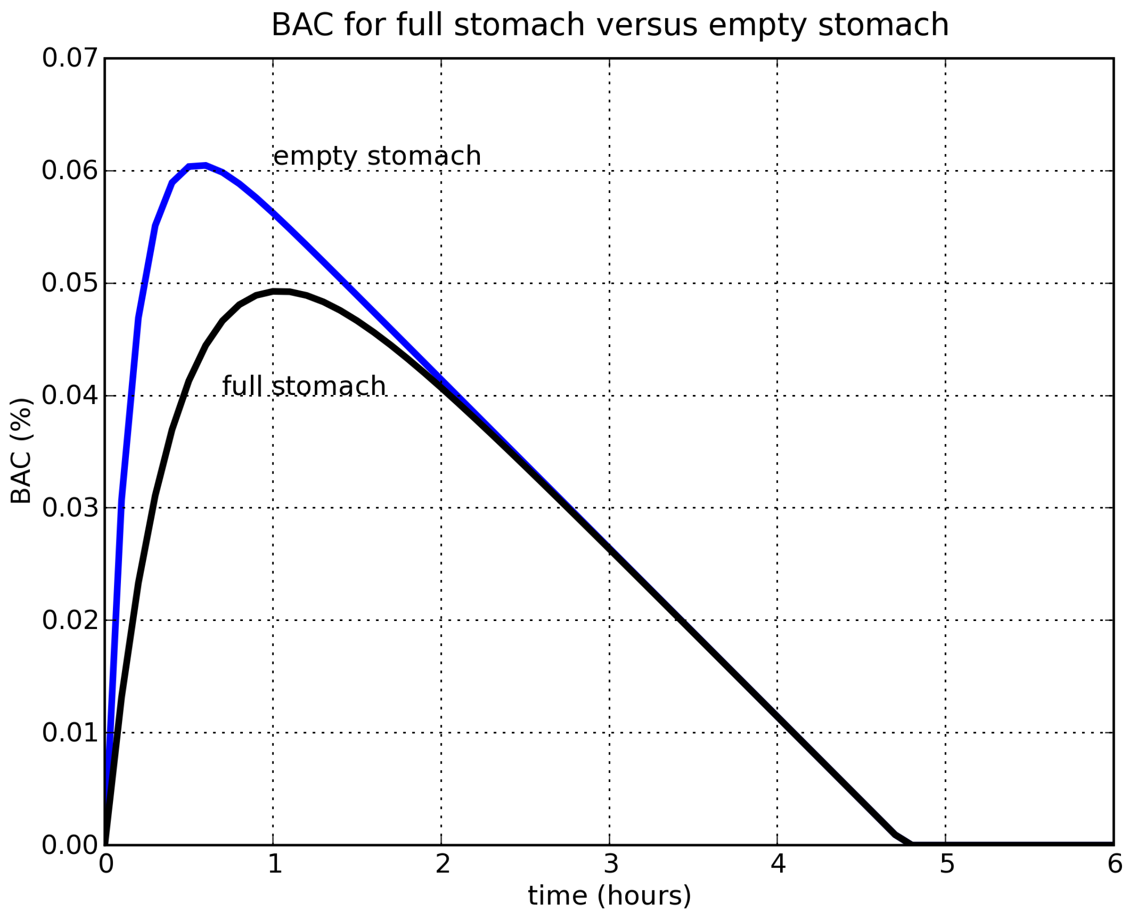
We can also develop a computer model.

Program specifications: Write a Python program which compares the BAC graphs for males or females, of varying weights, having eaten versus not having eaten. Plot graphs of both BACs.

Python Example 13.7.9

```
# Program to compare BACs over 6 hours when drinking
# on a full stomach versus an empty stomach
from __future__ import division
from pylab import *

alcohol = input("How much pure alcohol is consumed (in g)? ")
weight = input("How much does the person weigh (in kg)? ")
gender = input("Type 1 if male, anything else for female? ")
if gender == 1:
    r = 0.7
else:
    r = 0.6
times = arange(0,6.1,0.1)
BAC1 = arange(0,6.1,0.1)
BAC2 = arange(0,6.1,0.1)
ka1 = 6
ka2 = 2.3
mult = alcohol / (r * weight * 1000) * 100

# Apply the equation for the required number of steps.
for i in arange(0,size(times)):
    t = times[i]
    BAC1[i] = mult * (1 - exp(-t * ka1)) - 0.015 * t
    BAC2[i] = mult * (1 - exp(-t * ka2)) - 0.015 * t
    if BAC1[i]<0:
        BAC1[i] = 0
    if BAC2[i]<0:
        BAC2[i] = 0
plot(times,BAC1,'b-',linewidth=3)
plot(times,BAC2,'k-',linewidth=3)
grid(True)
xlabel("time (hours)")
ylabel("BAC (%)")
title("BAC for full stomach versus empty stomach")
text(0.7,0.04,"full stomach")
text(1,0.06,"empty stomach")
show()
```

Here is the output from running the above program for an 80 kg male consuming four standard drinks:



Question *13.7.10* Briefly discuss the previous graph and its implications.

Case Study 23:
CSI UQ

www.schoolies.org.au www.abc.net.au/news/stories/2009/02/11/2488677.htm

both from www.smh.com.au

- In Question 13.7.7 we introduced the *Widmark factor* r, which estimates the proportion of body weight that is water.
- We said that reasonable values for this are $r \approx 0.7$ for males and $r \approx 0.6$ for females.
- Researchers have proposed alternate formulae for more accurate estimation of r for different individuals.

- Below are three methods for estimating the value of r for a female with height H in m and weight W in kg (from, respectively, Watson *et al.*, J Stud Alcohol (1989); Forrest, J Forensic Science Society (1986); Seidl *et al.*, Int J Legal Med (2000)):

(a) $r = 0.29218 + \dfrac{12.666H}{W} - \dfrac{2.4846}{W}$;

(b) $r = 0.8736 - \dfrac{0.0124W}{H^2}$; and

(c) $r = 0.31223 - 0.006446W + 0.4466H$.

Question *13.7.11* In December 2006, American actress Nicole Richie was charged with driving under the influence of alcohol, after driving the wrong way down a highway in Los Angeles. Her police charge sheet shows that she was 1.55 m tall and weighed 38.5 kg.

(a) Would you expect her value of r to be more or less than 0.6 (which is the 'standard' value for females)? Why?

continued...

Question *13.7.11 (continued)*

(b) Using each of the four possible values of r, estimate how many standard drinks she could consume and remain within the legal BAC limit for driving in California (the limit is 0.08%).

continued...

***Question** 13.7.11 (continued)*

(c) Comment on your answers to Part (b).

(d) Nicole Richie had previously been convicted on a similar charge in 2002, after being caught driving at three times the speed limit. On that occasion her BAC was 0.12%, and she told police that all she had eaten that day was some French fries, and all she had drunk was 1 shot of vodka. Assuming she told the truth, and that her vodka contained one standard drink, then the only explanation is that someone must have spiked her French fries with alcohol; estimate the **minimum** amount of alcohol which was in her French fries.

Question *13.7.12* Around midday on August 23 2008, a helicopter crashed near the Mataranka rodeo grounds, 100 km south of Katherine, in the Northern Territory. The pilot died on impact, and his passenger was injured.

The Air Transport Safety Bureau reported that the pilot had attended a social gathering in Katherine on the evening before the accident, and had "drunk an unknown quantity of alcohol". His BAC was 0.254 percent at time of death.

Estimate (at a minimum) how many standard drinks he had consumed the previous evening.

***Question** 13.7.13* The website *www.drinkdrivinglawyer.com.au* quotes a case in which a male finished drinking at 11 pm. The police pulled him over at 11:10 pm, and his roadside BAC reading was 0.097. At 11:40 pm, he underwent a more accurate breath analysis which showed a BAC reading of 0.06.

(a) Comment on this case; assume that he metabolises alcohol at the standard rate. (At trial he was found not guilty.)

continued...

Question *13.7.13 (continued)*

(b) At what time would his BAC have been at a maximum, and what would the maximum value have been?

Question *13.7.14* In a thread about "the most you have ever drunk" on the website *www.schoolies.org.au*, one responsible young man posted "well, im a good 6'3 weigh about 80 ish k'gs so i can hold my liquor pretty well, very well really lol downed a case last night and was all sorts of wasted
records 40.. something, after the 20-30 mark u barely stand up let alone count, ive also managed to down 9 full beers in one beer bong yeah yeah alco i know i know beer is by no way the best place to get pissed tho
spirits and other drinks are a whole nother story lol"

Estimate his peak BAC after drinking 40 beers, and how long after drinking his BAC would return to 0. (Hint: one full-strength beer contains 375 mL and is 5% alcohol by volume. The specific gravity of pure alcohol is 0.789.)

End of Case Study 23.

13.8 Space for additional notes

14 Integrating rockets and drugs

So come and join us all you kids
for lots of fun and laughter
as Roger Ramjet and his men
get all the crooks they're after.
Roger Ramjet, he's our man
hero of our nation
for his adventures just be sure
and stay tuned to this station.

Artist: TV theme song

(www.youtube.com/watch?v=E7SqSNQeAFM)

The Starry Night (1889), Vincent van Gogh (1853 – 1890), Museum of Modern Art, New York.

(Image source: en.wikipedia.org/wiki/Image:VanGogh-starry_night_ballance1.jpg)

Introduction

In this section we will investigate two mathematical approaches which initially appear to be quite dissimilar, but instead are closely related.

The first approach we will cover is *integration*, which is the reverse of differentiation. Previously we studied various quantities and used differentiation to calculate the rate at which they were changing. Suppose instead that we only know the rate at which something is changing: what can we deduce about its value? The mathematical concept that allows us to do this is called an *indefinite integral*, and is an important tool in many applications, such as rocket flight and population dynamics.

The second approach relates to measuring areas. In science, given an equation that models some phenomenon, the area between that curve and the x-axis often has an important and useful physical meaning. For example, if y is an equation for the velocity of an object over time, then the area between the graph of y and the x-axis between two points in time represents the total displacement of the object between those times. Similarly, given an equation for the concentration of a drug in the blood, this area represents the "total exposure" of the body to the drug, which is important in determining whether the drug will have the desired beneficial impact, and whether the dose is potentially toxic.

Finally, we will see how the Fundamental Theorem of Calculus relates the two concepts, and allows indefinite integrals to assist with calculations of areas under curves.

Some of the examples/contexts we will discuss are:

- Simple motion.
- Hypersonic flight.
- Drug concentrations.

Specific techniques and concepts we will cover include:

- Integration and the indefinite integral.
- Areas and definite integrals.
- The Fundamental Theorem of Calculus.

14.1 Integration and the indefinite integral

- All semester we have stressed the importance of studying *change*.
- The *rate at which a function is changing* can be calculated by *differentiating* the function.
- It is often useful to be able to answer the **reverse** question: given the rate at which some quantity is changing, can we find a function for the quantity?
- The process of starting with a rate of change and finding the function is called *integration* .

Integration

A function F is called an indefinite integral *or* antiderivative *of another function f if the derivative of F is f; that is, $F'(x) = f(x)$.*

The process of finding an integral is called **integration**.

- You studied integration at school. In this course we will only expect you to integrate some simple functions.
- It is much more important that you understand *why* integrals are important.
- Note that when a function is differentiated, if the function has a constant term then this term disappears. Hence when finding an indefinite integral you need to include an unknown constant term.

Constant of integration

Indefinite integrals include an arbitrary **constant of integration**, *usually written "$+C$" in the answer.*

Example *14.1.1* The integral of the function $f(x) = 3x^2$ is the function $F(x) = x^3 + C$, where C is an arbitrary constant. (You can check this answer by differentiating F.)

- There is a special notation for integration.

The integral sign

Let $f(x)$ be a function with integral $F(x)$. Then the indefinite integral of f is defined by

$$\int f(x)\,dx = F(x) + C$$

where C is the constant of integration.

The symbol $\displaystyle\int$ *is called the* **integral sign**, *and dx means that the integration is to be performed with respect to the variable x.*

Question *14.1.2* In each case find:

(a) $\int 3x^2 + 6x + 2\,dx$

(b) $\int 2e^x + 10\,dx$

(c) $\int 0.02e^{0.02x}\,dx$

- Sometimes there is extra information that allows a specific value to be assigned to the constant of integration C. This information is often called an **initial condition** or **boundary condition**.

Case Study 24:
Simple motion

In physics, rather than using the terms *distance* and *speed*, the more usual expressions are *displacement* $S(t)$ and *velocity* $v(t)$, each of which has an associated *direction*. Then $v(t) = S'(t)$ and $a(t) = v'(t)$, where $a(t)$ is the *acceleration* at any time t. Thus:

- *velocity* can be found by integrating *acceleration* (possibly also using some initial conditions); and
- *displacement* can be found by integrating *velocity* (again possibly using some initial conditions).

Question *14.1.3* A ball is thrown vertically into the air at time $t = 0$ s from a height 2 m above the ground with an initial velocity of 20 m s^{-1}. The acceleration due to gravity on Earth is approximately -9.8 m s^{-2}. (Ignore air resistance and other similar forces.)

(a) Find the velocity of the ball at any time t.

(b) Find the displacement of the ball at any time t.

continued...

***Question** 14.1.3 (continued)*

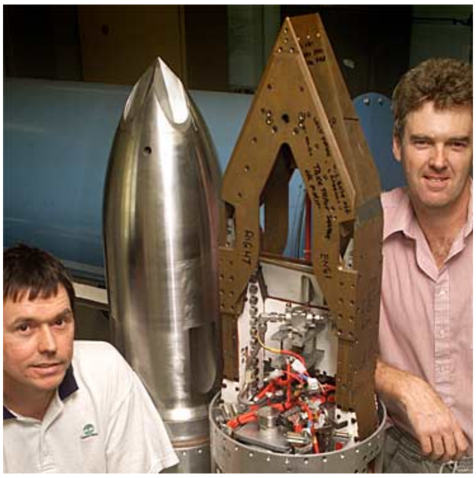
(c) Find the maximum height the ball reaches.

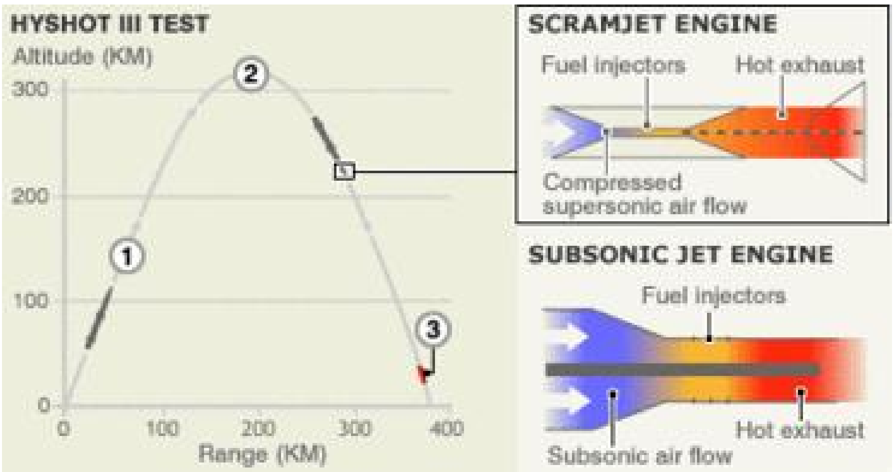
(d) At what time does the ball reach the ground?

End of Case Study 24.

14.2 Hypersonic flight and Newton's laws of motion

Case Study 25:
Hypersonic flight





- The concepts of integration and simple motion can be extended to more complex scientific research projects.
- The University of Queensland is a world-leader in research on modern rocket and jet propulsion systems, working with Boeing, NASA, and the Australian and US Defence Departments.
- The **HyShot** program (initiated at UQ) is developing a new type of jet, known as a scramjet (short for **s**upersonic **c**ombustion **ramjet**).

Hypersonic flight *(continued)*

- Scramjets and ramjets work by using smooth curved surfaces to compress air as it flows into the engine. As the air is compressed it heats up, and by mixing it with some type of fuel (such as hydrogen gas) the two gases will spontaneously ignite, accelerating the scramjet.

- High velocities are typically classified into different categories, relative to the speed of sound:
  - Subsonic: slower than the speed of sound (334 m s^{-1});
  - Sonic: at (or around) the speed of sound;
  - Supersonic: travelling between one and five times the speed of sound; and
  - Hypersonic: more than 5 times the speed of sound.
- (The speed of sound varies depending on humidity, altitude and temperature. The above measurement corresponds to dry air, sea level, and 21° Celsius.)
- High speeds are commonly expressed as a Mach number, which is the multiple of the speed of sound at which the object is travelling. So hypersonic speeds begin at Mach 5.
- A key difference between scramjets and ramjets is that ramjets slow the flow of air to subsonic speeds before combustion takes place. Conversely, inside a scramjet combustion occurs while the air is travelling faster than the speed of sound. Scramjets have the potential to fly as fast as Mach 20.
- At these speeds it would be possible to travel between Sydney and London in less than an hour!
- A limitation is that scramjets need to be travelling at supersonic speeds before they begin to operate, which leads to a host of new scientific and engineering problems.

A typical scramjet test flight

A typical test flight for a scramjet involves attaching the engine to a two-stage rocket, which is fired to a great height. After reaching the peak of its trajectory, gravity accelerates the apparatus back towards Earth. When it reaches a sufficiently high velocity, the scramjet engine fires and the test is conducted. Finally, once the experiment is complete, the apparatus falls back to Earth.

***Example** 14.2.1* Below is a flight log of a HyShot flight at the Woomera Rocket Range, South Australia:

Time (secs)	**Action**
0	Ignition of Stage 1.
0 – 6	Rocket accelerates at a rate equivalent to 22 times that of gravity on Earth.
6 – 15	Rocket coasts until ignition of Stage 2.
15 – 41	Stage 2 accelerates rocket to 8300 km h^{-1}.
46	Nose cone separates and continues upwards, while the remainder falls back to Earth.
46 – 446	Nose cone continues travelling upward while re-aligning itself for re-entry into the atmosphere. Maximum height reached is about 330 km.
446 – impact	The nose cone descends toward Earth using gravity to accelerate it to scramjet ignition velocity, which occurs at 35 km above ground. Once the scramjet ignites it burns until it descends to a height of 23 km, before shutting down and free-falling to ground.

(For all of the following questions we will ignore wind resistance and other similar forces.)

Question *14.2.2* When the rocket reaches a height of 330 km it stops moving up and falls back towards Earth with its only acceleration due to gravity. Assume the acceleration due to gravity is -9.8 m s^{-2}.

(a) Find an expression for the height of the rocket above Earth at any time **after** reaching the maximum height. (For simplicity, let the time of maximum height be $t = 0$ s.)

continued...

Question *14.2.2 (continued)*

(b) Find the velocity of the rocket when the scramjet fires at 35 km.

- In the previous calculation we erroneously assumed that the acceleration due to gravity is a constant -9.8 m s^{-2}.
- However, as the distance from Earth changes, so does the acceleration due to gravity. At low altitudes this change can be ignored, but the difference is substantial at high altitudes.
- In Question 4.4.1 we showed the acceleration due to gravity at height 330 km above the surface of Earth is about -8.87 m s^{-2}.
- A simple way to more accurately calculate the velocity at height 35 km is to find the arithmetic **average** of the acceleration due to gravity at heights 330 km and 35 km, and assume the acceleration equals this average as the rocket falls between these heights.

Question *14.2.3*

(a) Estimate the **average** acceleration as the rocket travels from a height of 330 km to a height of 35 km. (Hint: The acceleration due to gravity at height 35 km is -9.709 m s^{-2}.)

continued...

***Question** 14.2.3 (continued)*

(b) Estimate the velocity of the rocket when the scramjet engine fires at height 35 km. Compare your answer to that in Part (b) of Question 14.2.2.

- The result in Question 14.2.3 is reasonably accurate, but incorrectly assumes that the acceleration due to gravity changes at a constant rate as the rocket descends. In reality, acceleration changes according to the **square** of the distance from the centre of Earth (not linearly with the distance).
- Integration and Newton's Gravitation Law give the following equation for the velocity of the rocket $v(r)$ during its descent from an initial height H, dependent only on the height r of the rocket:

$$v(r) = -\sqrt{2GM_e\left(\frac{1}{r+R_e} - \frac{1}{H+R_e}\right)}$$

***Question** 14.2.4* Substituting values into the previous formula gives the velocity of the rocket at height 35 km as -2340.15 m s^{-1}. Compare this with your answers to Questions 14.2.2 and 14.2.3.

End of Case Study 25.

14.3 Areas and definite integrals

- Given an equation which models some phenomenon, the area between the curve and the x-axis often has an important and useful physical meaning.

Question 14.3.1 Consider a car moving with a constant velocity of $v = 10$ m s^{-1}.

(a) Calculate the displacement of the car between times $t = 0$ s and $t = 5$ s; include units.

(b) Draw a rough sketch of the graph of v between those times.

(c) Calculate the area between the graph of v and the x-axis between those times; include units.

(d) Compare your answers from Parts (b) and (c).

***Question** 14.3.2* In Question 14.1.3, a ball was thrown vertically with velocity $v(t) = -9.8t + 20$ m s^{-1}.

(a) At what time T does the ball reach its maximum height?

(b) Draw a rough sketch of the graph of v between $t = 0$ and $t = T$.

(c) Calculate the area between the graph of v and the graph of the x-axis between those times.

(d) Compare your answers from Part (c) and Question 14.1.3(c).

- This is not a coincidence: given a velocity graph, the area bounded by that graph, the x-axis and two time points on the x-axis, equals the total displacement between those times.
- We will see later that this is also true for graphs of phenomena other than velocity.
- For more complicated graphs, calculating the area can be quite difficult.
- At school you will have approximated areas under curves by summing the areas of rectangles of "narrow" width; this is called the *Riemann sum* .
- You may have also used variants which aim to increase accuracy, such as *middle sums*, *Simpson's rule* or the *trapezoid rule*.
- There is a special notation used to describe the area under a curve.

Definite integrals

Given a function $f(x)$, the area under the curve (AUC) from a point $x = a$ to a point $x = b$ is called the definite integral of $f(x)$ from a to b*, and is written*

$$\int_a^b f(x)\,dx.$$

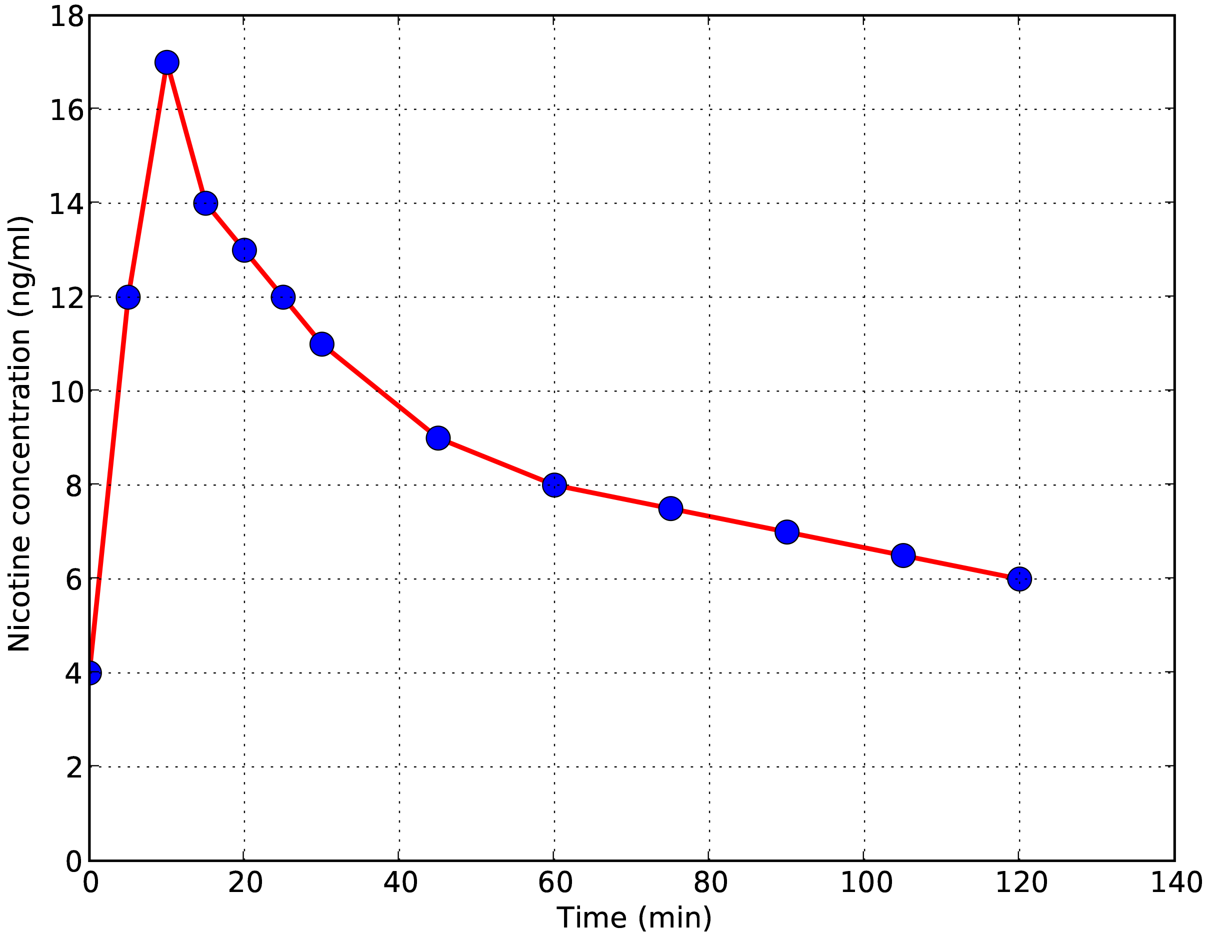
Example *14.3.3* In Question 14.3.2 we used areas to calculate

$$\int_0^T -9.8t + 20\,dt.$$

- Riemann sums are often used to estimate AUCs when an equation is not known but some data values have been measured.
- Indeed, unlike in mathematics practise problems from school, in most cases in real life, Riemann sums are *only* used when an equation is not known.

***Question** 14.3.4* In Example 13.2.3, the measurements of the blood-concentration of nicotine of a person at various time intervals after smoking a cigarette were as follows:

t (min.)	0	5	10	15	20	25	30
$C(t)$ (ng/mL)	4	12	17	14	13	12	11
t (min.)	45	60	75	90	105	120	
$C(t)$ (ng/mL)	9	8	7.5	7	6.5	6	



(a) What are the units of the AUC?

(b) What does the AUC represent?

(c) Why is this significant?

continued...

***Question** 14.3.4 (continued)*

(d) Use Riemann sums to estimate the total AUC of this graph.

Now we can develop a computer model.

Program specifications: Write a Python program which uses left sums, right sums and middle sums to estimate the area under the nicotine concentration curve. The program must output the estimated area, and draw a graph showing the rectangles used in the sums.

Python Example 14.3.5

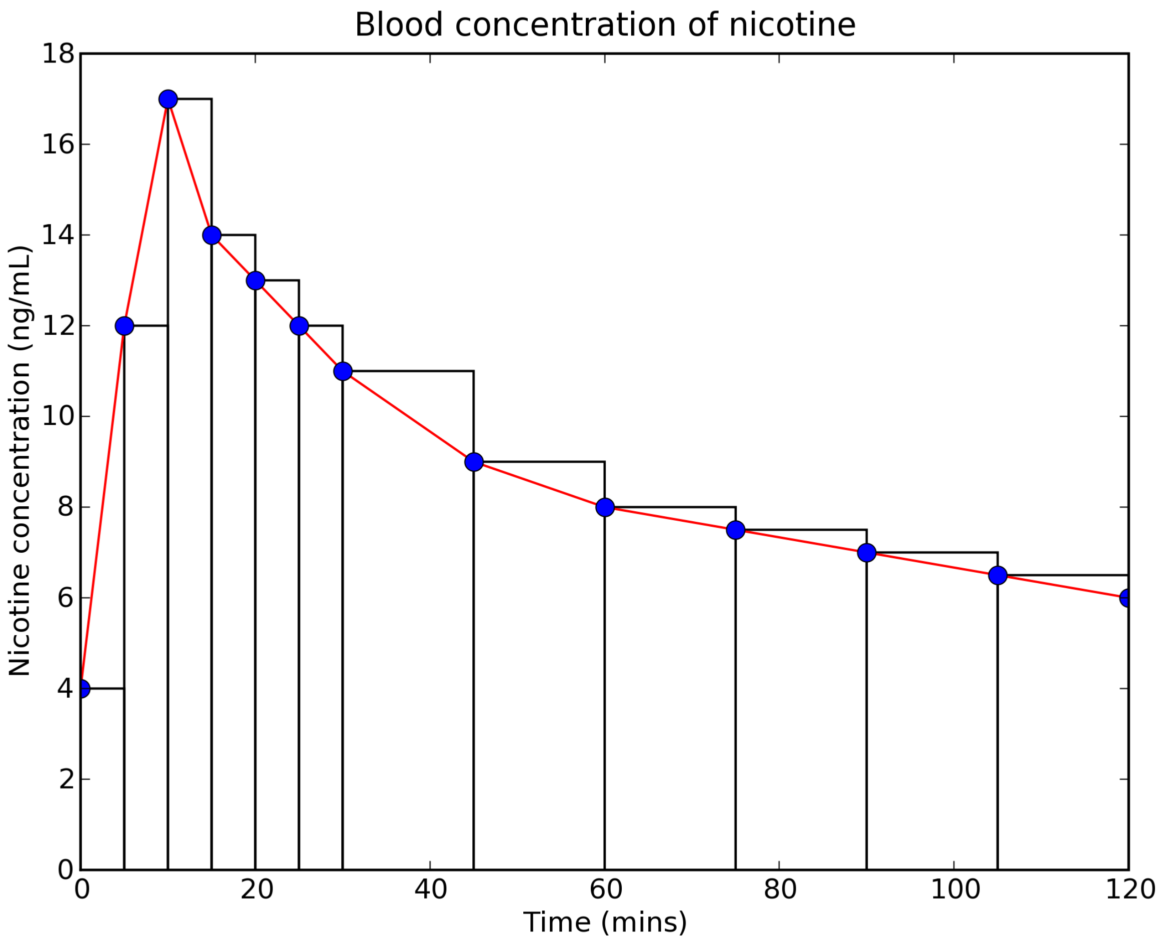
```
# Program to use Riemann sums to calculate
# area under a nicotine concentration curve.

from __future__ import division
from pylab import *

# Initialise variables
type = input("Type: 1 for left sum, 2 for right, 3 for middle: ")
t = array([0, 5, 10, 15, 20, 25, 30, 45, 60, 75, 90, 105, 120])
concs = array([4, 12, 17, 14, 13, 12, 11, 9, 8, 7.5, 7, 6.5, 6])
area = 0

# Sum the areas in each rectangle
for i in arange(1,size(t)):
    width = t[i] - t[i-1]
    if type == 1:
        height = concs[i-1]
    elif type == 2:
        height = concs[i]
    else:
        height = (concs[i-1] + concs[i])/2
    area = area + height * width

# Plot each rectangle
    rectX = array([t[i-1], t[i-1], t[i], t[i]])
    rectY = array([0, height, height, 0])
    plot(rectX, rectY, 'k-')

# Give the output.
print "The estimated AUC is",area,"ng min / mL"

plot(t, concs, 'r-', linewidth=1)
plot(t, concs, 'bo', markersize=8)
xlabel("Time (mins)")
ylabel("Nicotine concentration (ng/mL)")
title("Blood concentration of nicotine")
show()
```

Python Example 14.3.6

Here is the output from running the above program three times:

```
Type: 1 for left sum, 2 for right, 3 for middle: 1
The estimated AUC is 1095.0 ng min / mL

Type: 1 for left sum, 2 for right, 3 for middle: 2
The estimated AUC is 1055.0 ng min / mL

Type: 1 for left sum, 2 for right, 3 for middle: 3
The estimated AUC is 1075.0 ng min / mL
```

Here is the graph for the left sum.



14.4 The Fundamental Theorem of Calculus

- In the last few sections we have covered:
  (1) indefinite integrals, $\int f(x)\ dx$, which are solved using antiderivatives; and
  (2) definite integrals, $\int_a^b f(x)\,dx$, which are calculated by measuring AUCs.
- These two concepts are useful precisely because they represent a range of important physical phenomena. For example:
  - velocity is the antiderivative of acceleration, and displacement is the antiderivative of velocity; and
  - the overall exposure of the body to a drug is measured by the area under the concentration curve.
- Our discussions so far have not demonstrated any apparent links between indefinite integrals and definite integrals. However, a very important theorem shows that there is a very close link.

The Fundamental Theorem of Calculus

The **definite integral** *of the* **rate of change** *of a function F between two points equals the* **net change** *in the* **value** *of F between the two points. That is:*

$$\int_a^b F'(x)\,dx = F(b) - F(a)$$

What this means

The Fundamental Theorem is important for the following reason.

Consider some phenomenon, and let f be a function which models that phenomenon. Then the area under the curve between two points can be calculated without needing to sum the areas of rectangles. Instead, find an antiderivative of f, substitute the values of the points into the antiderivative, and then subtract.

***Example** 14.4.1* Some examples include:

(1) Let $V(t)$ be the volume of water in a reservoir at time t, so $V'(t)$ is the rate of inflow/outflow at any time. Then

$$\int_{t_1}^{t_2} V'(t)\,dt = V(t_2) - V(t_1)$$

is the net change in total volume from time t_1 to time t_2.

(2) If the population size of a bacterial colony changes at a rate of $P'(t)$ (allowing for births, deaths and migration), then

$$\int_{t_1}^{t_2} P'(t)\,dt = P(t_2) - P(t_1)$$

is the net change in population from time t_1 to time t_2.

(3) Let $[C](t)$ be the concentration of the product C of a chemical reaction at time t, so $[C]'(t)$ is the rate of reaction. Then

$$\int_{t_1}^{t_2} [C]'(t)\,dt = [C](t_2) - [C](t_1)$$

is the net change in concentration from time t_1 to time t_2.

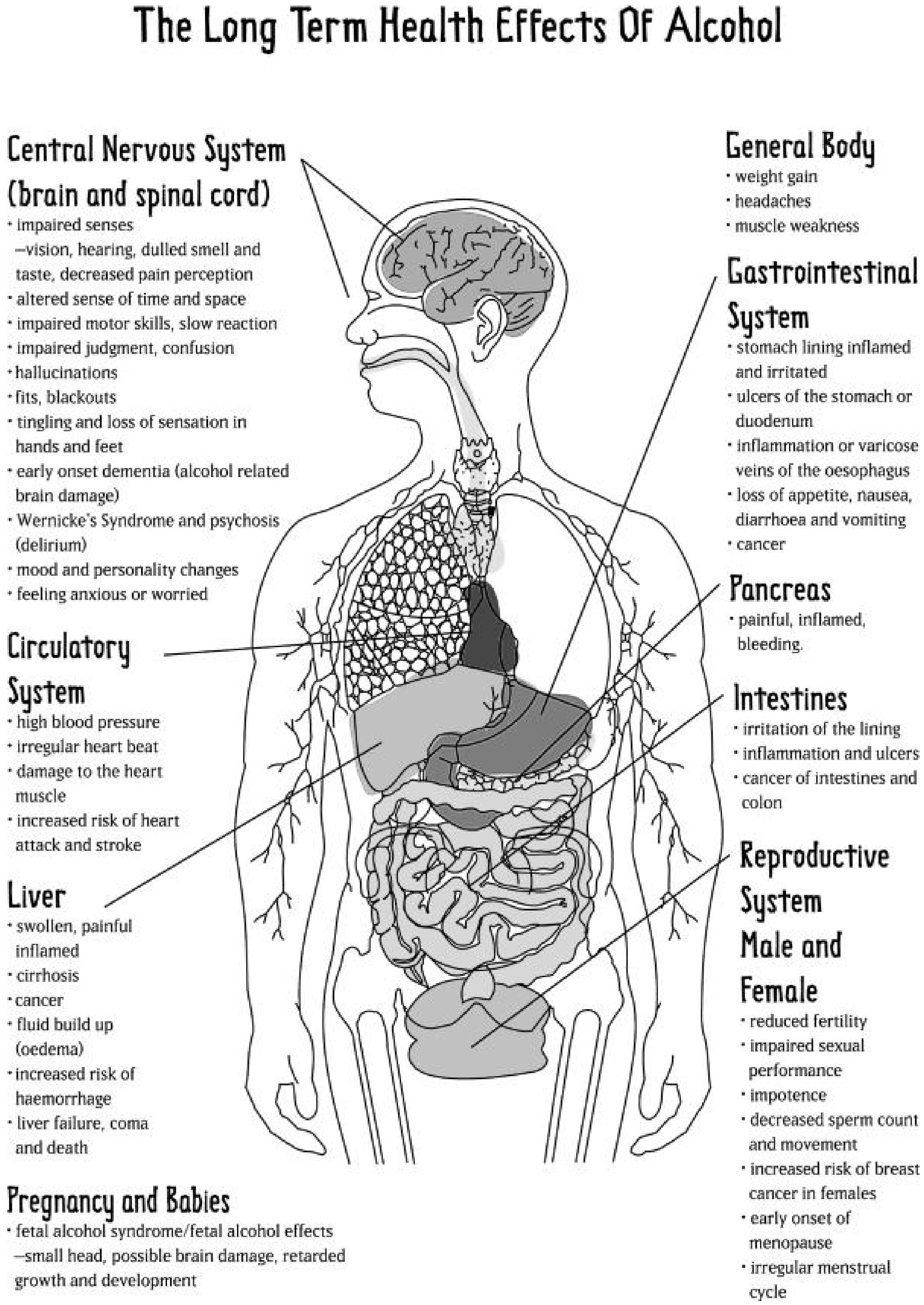
***Question** 14.4.2* In Question 14.3.2 we used areas to calculate

$$\int_0^T -9.8t + 20\,dt$$

where T is the time at which the ball reaches its highest point. Use the Fundamental Theorem to do the calculation.

Case Study 26:
Dying for a drink

- In the previous chapter on derivatives, we considered short-term risks associated with alcohol consumption (such as accidents).
- There are also many negative long-term health effects, with risk increased by both frequency and volume of consumption.



www.nt.gov.au/health

***Question** 14.4.3* In Question 13.7.7, we said that blood alcohol concentrations (BACs) are often estimated using the Widmark formula. For a 70 kg man drinking n standard drinks (each containing 10 grams of alcohol), the formula says that at time t in hours since commencing drinking, his estimated BAC % is

$$B = \frac{10n}{490} - 0.015t.$$

(a) At what time will his BAC return to 0?

(b) Define his *total exposure to alcohol* E as the AUC of B from $t = 0$ until his BAC again reaches 0. Find an expression for E.

continued...

Question *14.4.3 (continued)* Assume that the long-term damage to his internal organs is proportional to his total exposure to alcohol E. (This is simplistic, but not unreasonable.)

(c) Discuss the impact on E of "one extra drink for the road".

(d) One 70 kg man consumes two standard drinks every day, and a second consumes 14 standard drinks once a week, but does not drink at any other time. Estimate the value of E for each.

continued...

Question *14.4.3 (continued)*

(e) Comment on your results to Part (d). What are some ramifications of these results (for example, for binge drinking)?

(f) Earlier we said it was "simplistic but not unreasonable" to assume that long-term organ damage from alcohol is proportional to E. What are some of the simplifying assumptions in this statement?

We can also develop a computer model.

Program specifications: Write a Python program which uses the Widmark formula to graph the total exposure to alcohol of a 70 kg man consuming from 0 to 15 standard drinks, and also prints out the relative exposure to alcohol compared with consuming 2 drinks.

Python Example 14.4.4

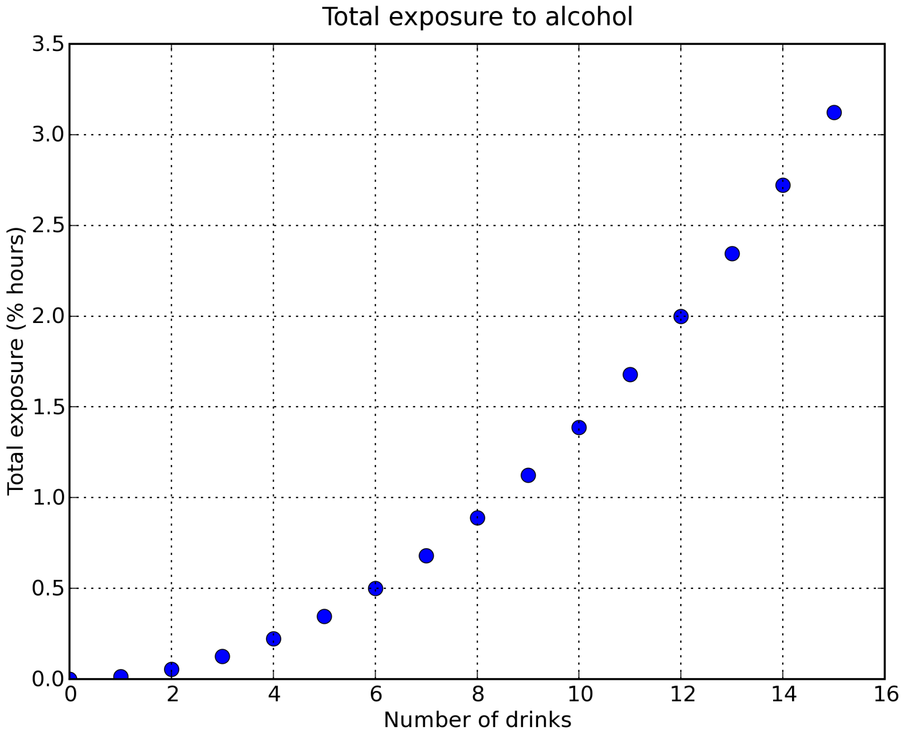
```
# Program to use the Widmark formula to estimate
# the "exposure to alcohol" for a 70 kg man, being the
# total AUC for the BAC curve. The program also prints
# the relative total exposure compared to 2 drinks.

from __future__ import division
from pylab import *

# Initialise variables
drinks = arange(0,16)
areas = 1.0 * arange(0,16)
weight = 70000
water = 100 / (weight * 0.7)

# Estimate E for each number of drinks.
for numd in drinks:
    tBAC0 = 10 * numd / (0.015 * water)
    areas[numd] = 10 * numd * tBAC0 / water - 0.0075 * tBAC0**2

# Output the relative exposure compared with 2 drinks
print "#  Exposure relative to 2 drinks"
for numd in drinks:
        ratio = areas[numd] / areas[2]
        print numd,"   ",round(ratio,1)

# Draw graph
plot(drinks, areas, 'bo', markersize=8)
grid(True)
xlabel("Number of drinks")
ylabel("Total exposure (% hours)")
title("Total exposure to alcohol")
show()
```

Dying for a drink *(continued)*

Python Example 14.4.5

Here is the output from running the above program:

```
#  Exposure relative to 2 drinks
0     0.0
1     0.3
2     1.0
3     2.3
4     4.0
5     6.3
6     9.0
7     12.3
8     16.0
9     20.2
10     25.0
11     30.3
12     36.0
13     42.3
14     49.0
15     56.3
```



End of Case Study 26.

Case Study 27:
Sweet Peas

bbc.co.uk

www.thedailygreen.com

dsc.discovery.com

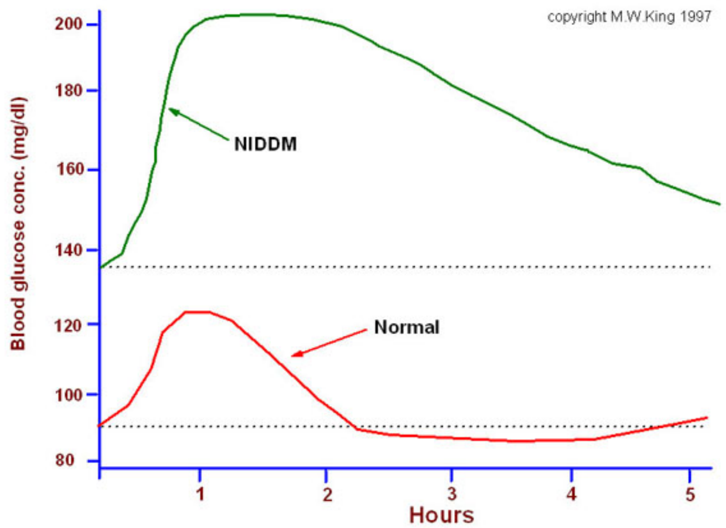
- *Diabetes mellitus* is a chronic disease, increasingly afflicting societies with a "western lifestyle"; once contracted it is typically permanent.
- Data from the Framingham study (which we saw early in semester) shows that "among those aged 50 and older, diabetic men lived an average of 7.5 years less than men without diabetes, and diabetes reduced women's life expectancy by an average of 8.2 years".
- There is a close relationship between diabetes and AUCs!

Example *14.4.6* (From access.health.qld.gov.au.) "Diabetes mellitus is a condition where the body cannot maintain normal blood glucose levels. Glucose is the main source of fuel for the body. Glucose is made by the breakdown of carbohydrate.

Insulin is a hormone that helps glucose move from the blood into the cells. When the body does not produce enough insulin, the cells cannot use glucose and the blood glucose level rises. Three main types of diabetes affect Australians - type 1 (previously known as insulin-dependent diabetes), type 2 (previously known as non-insulin-dependent diabetes) and gestational diabetes mellitus.

Diabetes affects an estimated 940,000 Australians, and about half of these are not aware they have the disease. If undetected or poorly controlled, diabetes can lead to blindness, kidney failure, lower limb amputation, heart attack, stoke and impotence."

- An *Oral Glucose Tolerance Test* (OGTT) is a common test for diabetes.
- Prior to taking the test, patients fast for around 12 hours, then a measured oral dose of glucose is administered.
- Blood-glucose levels are measured immediately prior to ingestion of the glucose and at various intervals for 2 hours afterwards.
- The following graph shows glucose tolerance curves for a normal person and one with non-insulin-dependent diabetes mellitus (NIDDM; Type 2 diabetes). The dotted lines indicate the range of glucose concentrations expected in a normal individual.



themedicalbiochemistrypage.org/diabetes.html

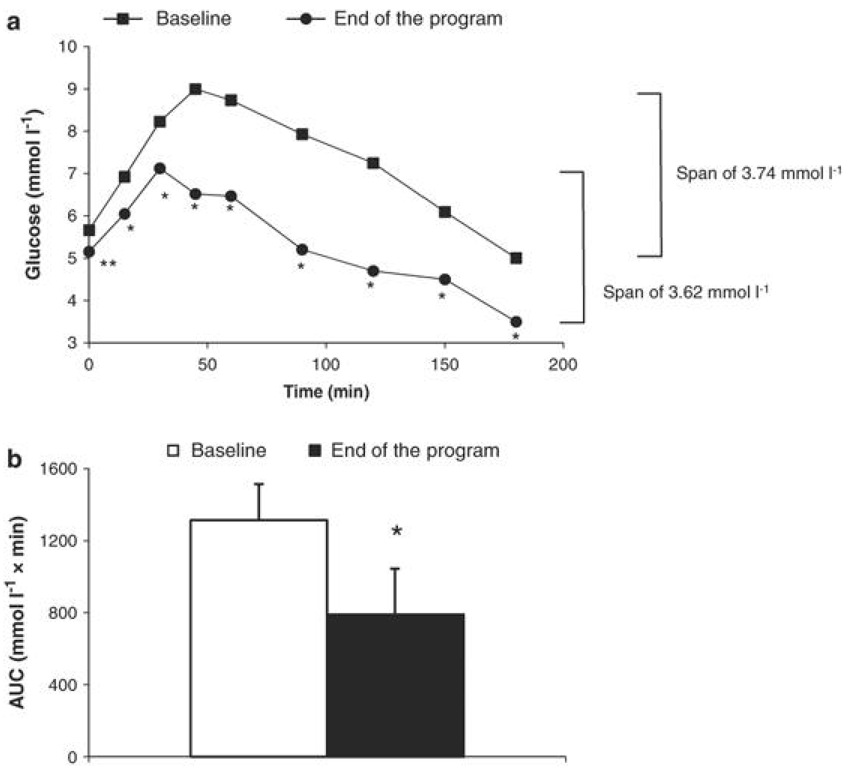
- The following table shows blood-glucose levels adopted by the World Health Organisation as indicators of: Impaired Fasting Glycaemia (IFG); Impaired Glucose Tolerance (IGT; sometimes called *pre-diabetes*); and Diabetes Mellitus (DM).

	Normal		IFG		IGT		DM	
Levels	$t = 0$	$t = 2$	$t = 0$	$t = 2$	$t = 0$	$t = 2$	$t = 0$	$t = 2$
mmol/L	< 6.1	< 7.8	≥ 6.1, < 7	< 7.8	< 7.0	≥ 7.8	≥ 7.0	≥ 11.1
mg/dL	< 100	< 140	≥ 100, < 126	< 140	< 126	≥ 140	≥ 126	≥ 200

- Many researchers believe AUC for a glucose tolerance curve is closely linked to the amount and frequency of food consumption, and is an indicator of general diet-related health.

***Example** 14.4.7* A paper[a] investigated links between blood-glucose levels, appetite and weight gain, and states:

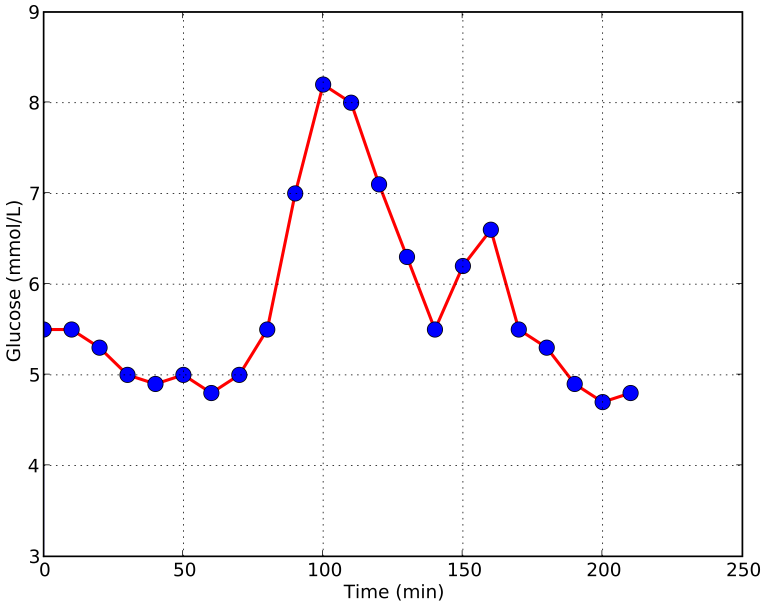
"Weight losses, even modest, have repeatedly been associated with an improvement of the metabolic profile of the obese. Indeed, [the graph] shows the curves and areas under the curve (AUC) of plasma glucose in response to an OGTT in male obese participants before and after a weight-loss programme up to a state of plateau consisting of a supervised diet and exercise clinical intervention. A mean loss of 11.5 kg of body weight (93.9% from fat stores) was achieved over 7 months of intervention. As expected, the AUC to the oral glucose challenge was considerably reduced at the end of the programme. Even if the metabolic fitness of individuals who underwent this intervention was substantially improved, it is of importance to note the impact of this strategy on blood glucose at the end of the oral glucose challenge. Indeed, at the 180th minute of this test, the glycemia was significantly lower than that before treatment."



www.nature.com/ijo/journal/v33/n1/full/ijo2008221a.html

[a] Chaput and Tremblay, *The glucostatic theory of appetite control and the risk of obesity and diabetes*, International Journal of Obesity **33** (2009) 46–53.

***Question** 14.4.8* Peter took 22 measurements of his blood-glucose levels at ten minute intervals from 6 am until 9:30 am, having not eaten for the previous 10 hours. At 7:10 am he commenced eating breakfast. A graph of his measurements is as follows:



(a) Comment on the graph and the measured values.

(b) Estimate the total mass of glucose (molar mass 180.16 g/mol) in Peter's blood at the time of peak concentration.

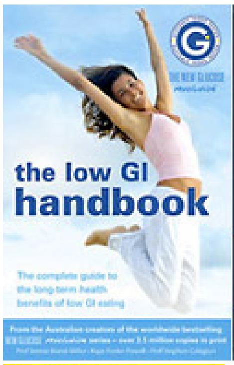
End of Case Study 27.

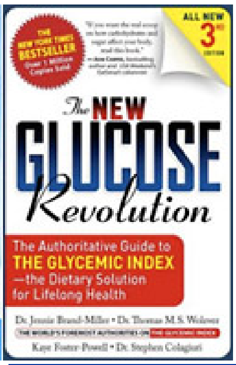
Case Study 28:
Hi GI!

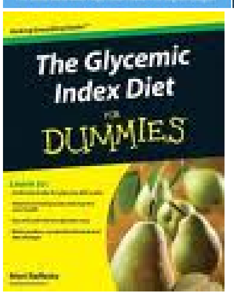
- The *Glycaemic Index* or GI of foods is often mentioned in marketing campaigns and in association with dietary health claims. GIs are defined in terms of AUCs for blood-glucose curves.

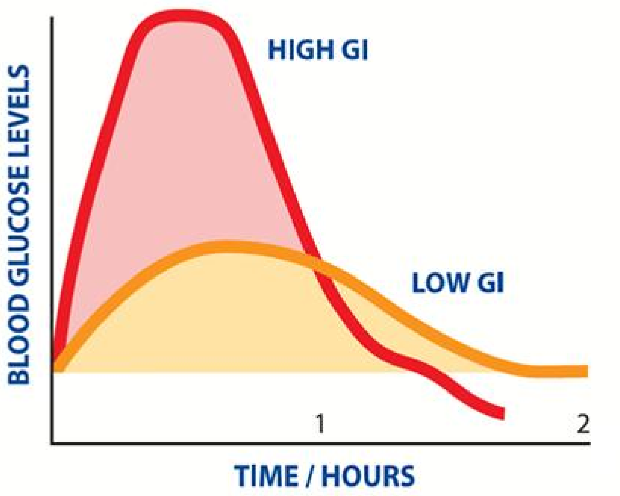
***Example** 14.4.9* (From www.glycaemicindex.com.)
"The glycaemic index (GI) is a ranking of carbohydrates on a scale from 0 to 100 according to the extent to which they raise blood sugar levels after eating. Foods with a high GI are those which are rapidly digested and absorbed and result in marked fluctuations in blood sugar levels. Low-GI foods, by virtue of their slow digestion and absorption, produce gradual rises in blood sugar and insulin levels, and have proven benefits for health. Low GI diets have been shown to improve both glucose and lipid levels in people with diabetes (type 1 and type 2). They have benefits for weight control because they help control appetite and delay hunger. Low GI diets also reduce insulin levels and insulin resistance.

To determine a food's GI rating, measured portions of the food containing 10 - 50 grams of carbohydrate are fed to 10 healthy people after an overnight fast. Finger-prick blood samples are taken at 15-30 minute intervals over the next two hours. These blood samples are used to construct a blood sugar response curve for the two hour period. The area under the curve (AUC) is calculated to reflect the total rise in blood glucose levels after eating the test food. The GI rating (%) is calculated by dividing the AUC for the test food by the AUC for the reference food (same amount of glucose) and multiplying by 100. The use of a standard food is essential for reducing the confounding influence of differences in the physical characteristics of the subjects. The average of the GI ratings from all ten subjects is published as the GI of that food."



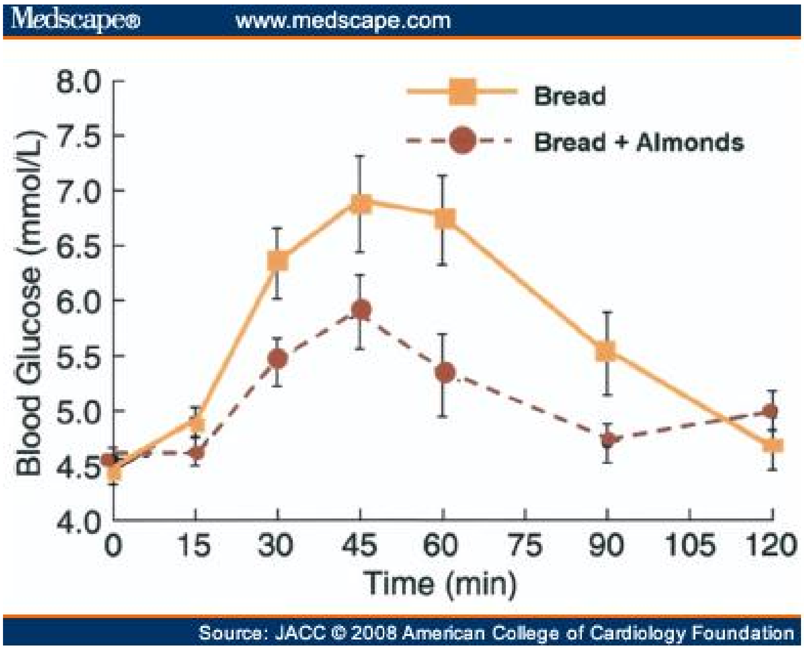






The amount of carbohydrate in the reference and test food must be the same.

Question *14.4.10* The following graph shows measured blood-glucose levels after consuming meals of: 'bread only'; and 'bread and almonds' The GI of 'bread only' is about 71. Calculate the (approximate) GI of 'bread and almonds'.



End of Case Study 28.

14.5 Space for additional notes

15 Populations and differential equations

All things bright and beautiful,
All creatures great and small,
All things wise and wonderful,
The Lord God made them all.
Each little flower that opens,
Each little bird that sings,
He made their glowing colours,
He made their tiny wings.

𝓊Artist: Cecil Alexander (www.youtube.com/watch?v=KLfkL8uDuc8)

The Entry of the Animals into Noah's Ark (1613), Jan Brueghel the Elder (1568 – 1625), The J. Paul Getty Museum, Los Angeles. (Image source: www.getty.edu)

Anthonie van Leeuwenhoek (1670), Jan Verkolje (1650 – 1693), Rijksmuseum, Amsterdam. (Image source: commons.wikimedia.org)

Introduction

Throughout semester we have investigated how change is a fundamental part of many systems, and the importance of being able to represent and model change. Differentiation and integration allow us to do this.

Of course, modelling change is often more complex than we have considered so far. Most of the time, the phenomenon will be described by one or more equations that include the value of the phenomenon, its derivatives, and sometimes other factors. These equations are called *differential equations* or *DEs*. A number of the techniques and phenomena we have studied already are in fact closely related to DEs.

You will need to understand how to formulate and describe DEs, and how to interpret their solutions. This section covers an introduction to DEs and their solutions, and how they can be applied to modelling a number of phenomena.

Some of the examples/contexts we will discuss are:

- Unconstrained growth of algae and bacteria.
- Newton's Law of Cooling.
- Alcohol.
- Constrained growth of a fish population.
- Modelling growth of cancer tumours.

Specific techniques and concepts we will cover include:

- Exponential DE.
- Stable points.
- Logistic DE.
- Euler's method.

15.1 Introduction to differential equations

- Understanding how objects and processes change allows predictions to be made about the future.
- In many cases, it is possible to measure or make inferences about the rate at which some phenomenon is changing.
- If an equation can be written representing the rate at which a phenomenon is changing, then it is often possible to use mathematical techniques to solve those equations and make predictions about the future values.

***Example** 15.1.1* If a ball is dropped from a building at time $t = 0$, then the rate of change of its velocity is -9.8 m/s^2 (recalling that the rate of change of velocity is acceleration).

If $v(t)$ is the unknown velocity at any time t then

$$v'(t) = -9.8.$$

We can use integration to solve for v, giving $v(t) = -9.8t$ m/s at any time t in seconds.

- In Example 15.1.1, we started with an equation for the rate at which the function v is changing, and used integration to find the value of the function.
- This was easy to do, because **the rate at which v is changing is only dependent on the value of t.**
- This is (probably) true of every integration question you have ever studied or solved: you will always have integrated functions of a single variable x or t.

- In science (and many other disciplines including engineering, business and the social sciences), models are not always this simple.
- Many phenomena do not just change according to the time. For example, their rate of change may be influenced by the **value they currently have**, or to the **value that some other phenomenon has**, or even the rate at which the other phenomenon is changing.
- Equations that relate rates of change to the value of a function (and possibly other properties) are called *differential equations*.

Differential equation

If y is an unknown function of t, then a **differential equation** *or* **DE** *is an equation that involves a combination of t, y and/or the derivatives of y.*

If the DE is true when a particular function y and its derivative(s) are substituted into the DE then y is called a **solution** *to the DE.*

Some DEs can be solved analytically, giving an exact solution. Many other DEs cannot be solved exactly, and instead require numerical methods to give approximate solutions.

- Make sure you understand what a DE actually is. In all of the examples we will study, the DE will be of the form $y' = \ldots$.
- Then a **solution** to the DE will be **another function** which, when **substituted** into the DE, makes the DE **true**.
- We will study some important DEs. In each case we will:
  - describe the phenomenon being modelled;
  - discuss how to represent the phenomenon with a DE;
  - understand what the DE is saying;
  - solve the DE and interpret its solution.

15.2 DEs and exponential growth and decay

- Earlier we studied exponential growth and decay. On Page 231 we said "Any phenomenon which changes at a rate proportional to the current amount follows an exponential function".
- This occurs precisely because such phenomena satisfy simple DEs whose solutions are exponential functions.

***Question** 15.2.1* In Question 11.2.2 we studied an algae population growing at 2% per hour. If $N(t)$ is the population of algae per mL of water at time t in hours then the population size satisfies the DE $N' = 0.02N$.

(a) Explain carefully, in words, what this DE is saying.

(b) Show that $N(t) = Ae^{0.02t}$ is a solution to the DE, where A is a constant.

(c) If we know that the population at time $t = 0$ hours is 500 algae per mL of water, find the population at any time t.

DE for exponential growth and decay

Any function $N(t)$ with rate of change at any time proportional to the value of N, with change constant r per time period, is modelled by the DE $N' = rN$.

The solution to this DE is $N(t) = N_0 e^{rt}$ *, where N_0 is the value of N at time 0.*

***Question** 15.2.2* Demonstrate mathematically *why* the solution to the DE $N' = rN$ is the exponential function.

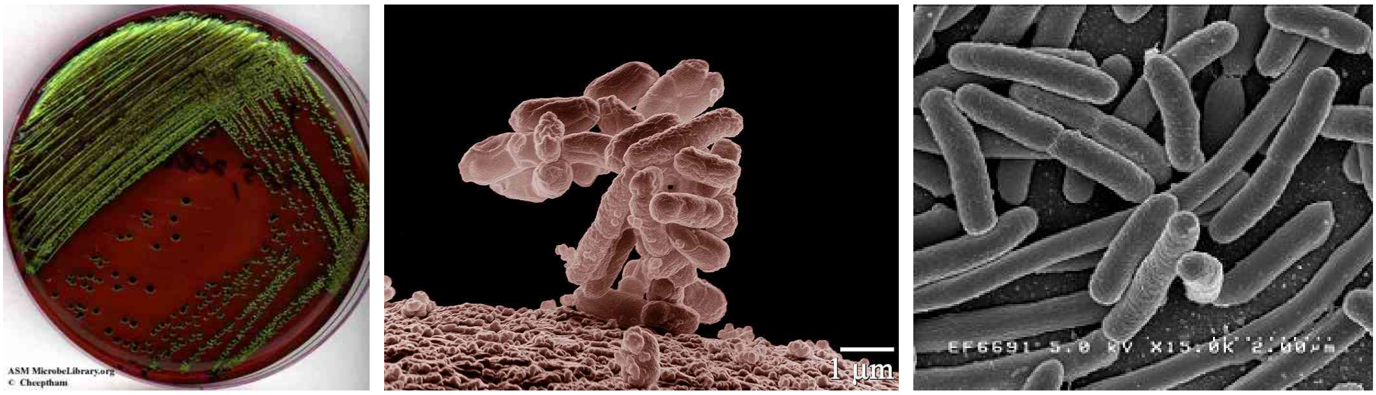
***Example** 15.2.3* Every exponential function we have studied during semester arises from this DE, including:

- the growth during an algal bloom in Question 11.2.2;
- radioactive decay of Strontium-90 in Question 11.2.6;
- radiocarbon dating in Question 11.2.8;
- the cooling of hot water in Question 11.2.11; and
- the concentration of caffeine in the blood in Question 13.6.2.

Other phenomena which arise from very similar DEs include:

- *learning curves*, used by psychologists to model the rate at which an individual learns new material; and
- *Newton's law of cooling*, which models the rate at which the temperature of an object changes to match the temperature of its surroundings.

Case Study 29: Poo



From: http://emu.arsusda.gov/default.html

- *Escherichia coli* (usually shortened to *E. coli*) is a bacterium commonly found in the lower intestine of warm-blooded animals, including humans.
- Most strains of *E. coli* are harmless in the digestive system, or even beneficial to the host individual.
- However, some strains do produce toxins, and can cause food poisoning, gastrointestinal infections and urinary tract infections.
- One such strain is *O157:H7*; this was linked to illness outbreaks in Washington and California in 1994, from contaminated salami.
- Because *E. coli* can survive outside the body for some time, tests for *E. coli* are often used to indicate the presence of faecal contamination in environmental samples or in food hygiene checks.
- Under simplifying assumptions (such as comparatively unlimited resources) the rate of increase of a population of *E. coli* at any time is proportional to the population size at that time.
- Hence the population follows an exponential function, and it makes sense to discuss the *doubling time* of the population.
- Under favourable conditions, the doubling time for a population of *E. coli* may be an hour, or even shorter.
- This rapid growth rate is one reason why good hygiene standards are important in food preparation.

- When studying populations of bacteria, microbiologists commonly count *colony-forming units* (CFU), which is the number of viable (live) bacterial cells present.
- This method differs from direct counts of individuals, which include both dead and living cells.

***Question** 15.2.4* A population of *E. coli* in a contaminated food sample changes with growth constant $r = 1$ per hour; assume that the sample contains 10^3 CFU per g at time 0.

(a) Write a DE for the population size $E(t)$ in CFU per gram at any time t in hours.

(b) Solve the DE in Part (a).

(c) Estimate the population size after 6 hours.

- A recent paper[a] investigates *E. coli* contamination of pre-cooked meat products (specifically ham) during the slicing process.
- The study models two sources of contamination:
  - from a slicing blade infected with *E. coli* to clean ham; and
  - from ham infected with *E. coli*, to a clean slicing blade, then to clean ham.

[a] Sheen and Hwang, *Mathematical modelling the cross-contamination of E. coli O157:H7 on the surface of ready-to-eat meat product while slicing*, Food Microbiology **27** (2010) 37–43.

Poo *(continued)*

One of the research experiments involved:

- inoculating (infecting) ham with "7 log CFU of O157:H7 *E. coli*" (that is, 10^7 CFU);
- using a clean blade to slice the inoculated ham;
- using that blade to cut 100 slices of clean ham; and
- counting the number of CFU on each of the 100 slices.

***Question** 15.2.5* If x is the number of the slice from 1 to 100, then $\log_{10}$ of the number of CFU on each slice $Y(x)$ is modelled by

$$Y = 2.793 \times e^{-0.0105x}.$$

(a) Roughly how many CFU were on Slice 1 and on Slice 100?

(b) Find an expression for the number of CFU on any slice of ham after any number of hours, assuming the slices are stored under ideal growing conditions for *E. coli*.

Extension 15.2.6 (From www.lshtm.ac.uk, 15/10/2008.)

"The further north you go [in the UK], the more likely you are to have faecal bacteria on your hands, especially if you are a man, according to a preliminary study conducted by the London School of Hygiene & Tropical Medicine.

But women living in the South and Wales have little to feel smug about. In London, they are three times as likely as their men folk to have dirty hands, and in Cardiff, twice as likely. The men of London registered the most impressive score among all those surveyed, with a mere 6% found to have faecal bugs on their hands. Overall more than one in four commuters have bacteria which come from faeces on their hands...

The results indicated that commuters in Newcastle were up to three times more likely than those in London to have faecal bacteria on their hands (44% compared to 13%)...Commuters in Liverpool also registered a high score for faecal bacteria, with a contamination rate of 34%. In Newcastle and Liverpool, men were more likely than women to show contamination (53% of men compared to 30% of women in Newcastle, and 36% of men compared to 31% of women in Liverpool)...

The bacteria that were found are all from the gut, and do not necessarily always cause disease, although they do indicate that hands have not been washed properly.

Dr Val Curtis, Director of the Hygiene Centre at the London School of Hygiene & Tropical Medicine, comments: 'We were flabbergasted by the finding that so many people had faecal bugs on their hands. The figures were far higher than we had anticipated, and suggest that there is a real problem with people washing their hands in the UK. If any of these people had been suffering from a diarrhoeal disease, the potential for it to be passed around would be greatly increased by their failure to wash their hands after going to the toilet'. "

Poo *(continued)*

- Consider a DE which models some phenomenon. The general solution to the DE (together with initial conditions) predicts the values of the phenomenon at various times.
- Scientists are often interested in *stable points*.

Stable points

The general solution y to a DE **may** *have one or more* stable points *(which are also called* fixed points *or* equilibrium values*), which are points at which* $y' = 0$ *. If the phenomenon ever reaches one of these values, it will indefinitely* *remain equal to that value.*

Question *15.2.7* Why are stable points scientifically important?

Question *15.2.8* In Question 15.2.4 we considered a population of *E. coli* bacteria which satisfied the DE $E' = E$.

(a) Find all stable population sizes.

(b) Interpret your answer to Part (a).

End of Case Study 29.

- Many other phenomena satisfy the exponential DE. Here are two examples.

Question *15.2.9* When an object with one temperature is moved to an environment with a different temperature, the temperature of the object changes according to *Newton's Law of Cooling*. Assume a small object is placed in a room with temperature equal to a constant T. Let $y(t)$ be the temperature of the object at any time t.

(a) Derive a DE for the rate of temperature change of the object.

(b) Your equation should include a constant, say k. What physical factors would determine the value of k?

continued...

Question *15.2.9 (continued)* In Question 11.2.11 we considered hot water placed in a room with temperature 25 °C. The temperature $y(t)$ in °C at any time t in minutes was modelled by:

$$y(t) = 60e^{-0.05t} + 25.$$

(c) Show that this is the solution to the DE $y' = -0.05(y - 25)$ and relate this to Newton's Law of Cooling.

(d) Find all stable solutions and explain your answer.

Question *15.2.10* When alcohol is consumed, most of it is absorbed into the bloodstream via the small intestine. The rate of absorption is proportional to the amount which is in the digestive tract at any time.

(a) Assume an individual consumes A grams of pure alcohol. Write a DE for the rate of change of the amount of alcohol D *in the digestive system* at any time, and solve the DE.

(b) Find an expression for the total amount of alcohol *that has been absorbed by the body at any time*, ignoring elimination.

continued...

***Question** 15.2.10 (continued)*

(c) Find an expression for blood-alcohol content (BAC) if the drinker weighs W kg, and a fraction r of their weight is water. (Hint: ignore elimination, and remember to convert BAC to a percentage.)

(d) If the body can eliminate alcohol at a constant rate of V % per hour, find an expression for the BAC at any time t in hours.

(e) Compare your answer to the equation given in Question 13.7.8.

15.3 DEs and constrained logistic growth

- Any phenomenon which always changes at a rate proportional to its value follows an exponential function.
- Exponential growth functions are *unconstrained* ; that is, they continue growing indefinitely.

***Question** 15.3.1* Let $N(t)$ be the size of a fish population in a certain lake at any time t in months. If the natural rate of increase of the fish population is 10% per month, then $N(t)$ satisfies the differential equation $N' = 0.1N$. Assume that at time 0 there are 30 fish.

(a) Draw a rough sketch of the population over time predicted by the given DE.

(b) Environmental analysis has shown that the maximum fish population the lake can support is 1000. Given this, what do you think is a more realistic rough sketch of $N(t)$ over time?

***Question** 15.3.2* Give some reasons why the exponential DE is often inaccurate (and even impossible) in modelling, particularly over long time periods.

- During unconstrained exponential growth, the proportional rate of increase is constant at all times, irrespective of the population size.
- This is often quite accurate over some time periods.
- However, in most cases populations cannot continue to show unconstrained growth: there is a *maximum* population size that can be supported by the conditions and resources.

Carrying capacity

The **carrying capacity** *of an ecosystem for a particular organism is the maximum population that can be supported by the resources within the ecosystem. Resources may include food, water, shelter and sunlight.*

A population size below the carrying capacity will typically increase towards the carrying capacity, whereas a population size above the carrying capacity will typically decrease to the carrying capacity.

- The carrying capacity for a particular organism often changes over time; for simplicity, we will assume it remains constant.

- In more sophisticated population models than the exponential model, the **rate of change** in the population will:
  - **increase** as the population size gets bigger and there are more individuals who can reproduce; and
  - **decrease** as the population size gets closer to the carrying capacity and individuals compete for scarce resources.
- One such model that reflects these features is the *logistic model*.
- The power of the logistic model is the way in which the two opposing growth and competition factors interact.

***Question** 15.3.3* The logistic DE is

$$N' = r\,N\left(\frac{K-N}{K}\right)$$

where $N(t)$ is an unknown function (such as a population), r is the unconstrained growth rate and K is the carrying capacity. Explain carefully, in words, what this DE is saying.
In particular, what is the significance of the term $\left(\dfrac{K-N}{K}\right)$?

- Just as it is possible to solve the exponential DE, it is also possible to find a solution to the logistic DE.

Solution to the logistic DE

Any function $N(t)$ that changes at a rate proportional to the value of the function (with unconstrained growth rate r), **and also** *in reverse proportion to how close the value is to a carrying capacity K, is modelled by the logistic DE*

$$N' = r\,N\left(\frac{K-N}{K}\right).$$

If N_0 is the value of N at time 0 then the solution to this DE is

$$N(t) = \frac{K\,N_0}{N_0 + (K-N_0)e^{-rt}}$$

Question *15.3.4* From the equation for N', explain why the solution to the logistic DE displays the following properties. If the initial population is:

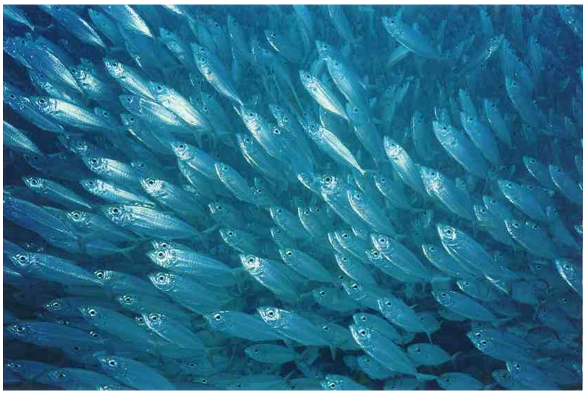
(a) much less than the carrying capacity, then the population initially grows approximately exponentially.

(b) close to the carrying capacity, then the population grows slowly towards the carrying capacity.

(c) more than the carrying capacity, then the population declines exponentially towards the carrying capacity.

Case Study 30:

Fish and the logistic model



- The logistic model applies to many types of population. It is commonly used to model fish populations, and can be extended to model fish harvest rates and stock management.

***Example** 15.3.5* A certain species of fish with an unconstrained population growth rate of 10% per month is living in a lake with a carrying capacity of K=1000 fish. Assume that this species follows the logistic model, and that the initial population is $N_0 = 30$ fish.

The function for the fish population $N(t)$ at time t in months satisfies the DE

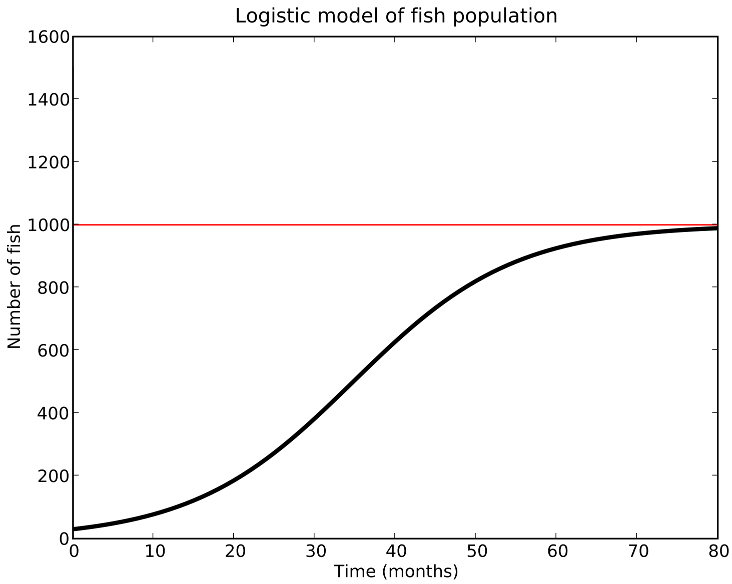
$$N' = 0.1\, N\left(\frac{1000 - N}{1000}\right).$$

Substituting for N_0, r and K in the solution for the logistic DE gives the following function for the number of fish at time t months:

$$\begin{aligned} N(t) &= \frac{1000 \times 30}{30 + (1000 - 30)e^{-0.1t}} \\ &= \frac{30000}{30 + 970e^{-0.1t}} \end{aligned}$$

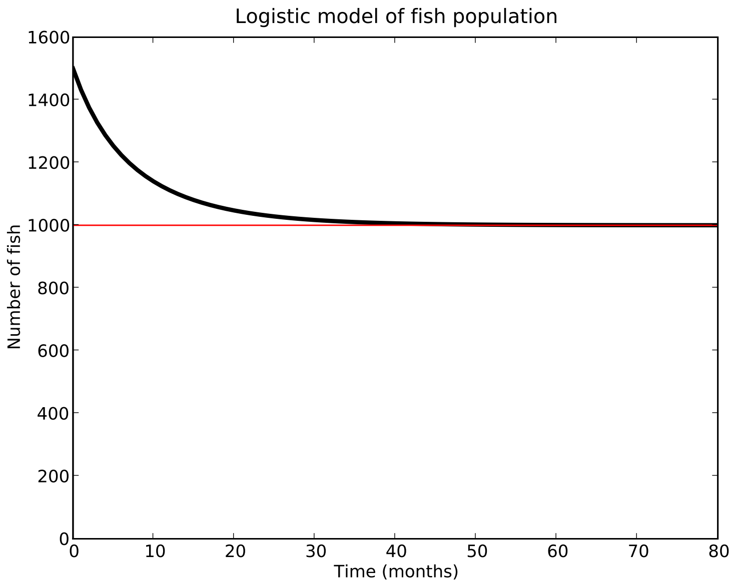
continued...

***Example** 15.3.5 (continued)* The population over 80 months is shown in the following graph.



- The initial population is much less than the carrying capacity, so as expected the population initially rises close to exponentially, then the growth rate reduces and the population gradually approaches the carrying capacity.
- The graph shows the *sigmoidal* "S"-shaped logistic curve.

For comparison, the following graph shows the fish population over time if the initial population is $N_0 = 1500$.



***Question** 15.3.6* Recall that $N' = 0.1\,N\left(\dfrac{1000 - N}{1000}\right)$.

(a) Find all stable population sizes.

(b) Interpret your answer to Part (a).

(c) The government allows limited fishing, with 9 fish caught per month. Write a new DE for $N(t)$, and explain your answer.

(d) Find all new stable population sizes.

continued...

***Question** 15.3.6 (continued)*

(e) Interpret your answer to Part (d).

(f) A business proposes harvesting 30 fish (in total) per month. Comment on the sustainability of this proposal.

continued...

Question *15.3.6 (continued)*

(g) What is the largest number of fish harvested per month which can be maintained indefinitely?

(h) Briefly make some recommendations to assist government with long-term stock management.

End of Case Study 30.

15.4 Euler's method

- Many DEs can be solved *analytically*; that is, using integration and algebra, it is possible to find an exact solution to the equation.
- All of the DEs we have seen so far can be solved in this way.
- However, for more complex cases, especially with systems of DEs, it is not possible to find exact solutions.
- Approximate solutions can be found using numerical algorithms (this is a similar concept to the use of Newton's method for approximately solving equations).
- One of the simplest techniques for solving DEs approximately is *Euler's method* .
- We will describe how to use Euler's method to solve a simple DE (which you would not do in practice as this equation can be solved exactly) as an illustration of how the method works.

Euler's method (informal description)

To approximate an unknown function y:

1. *Choose a small* step size *h, and start at the given initial point.*
2. *Use the DE to calculate the (estimated) slope of the function at the current point.*
3. *Approximate the unknown function as a short* **straight line**, *starting from the current point, with:*
   - **width** *equal to the step size h;*
   - **slope** *equal to the estimated slope of the function calculated using the expression for the derivative; and hence*
   - **height** *equal to width multiplied by slope.*
   - *Advance the current point to the end point of the straight line.*
4. *If finished then stop, otherwise return to Step 2.*

Euler's method (semi-formal description)

Given a DE $y' = \dots$ and an initial value (x_0, y_0):

1. *Choose a small* step size *h, and start at $(x, y) = (x_0, y_0)$.*
2. *Substitute the current values of x and y into the DE to estimate an approximate value for y'.*
3. *Set $y = y + h \times y'$* and *$x = x + h$.*
   The new point (x, y) is the next approximate function value.
4. *Stop when x has advanced sufficiently far. Otherwise, return to Step 2.*

***Question** 15.4.1* Draw a diagram illustrating Euler's method.

Example 15.4.2 Use Euler's method to find an approximate solution to the DE $y' = 0.1y$, with initial condition $y_0 = 100$ when $x_0 = 0$. Estimate y when $x = 5$, using a stepsize of $h = 1$.

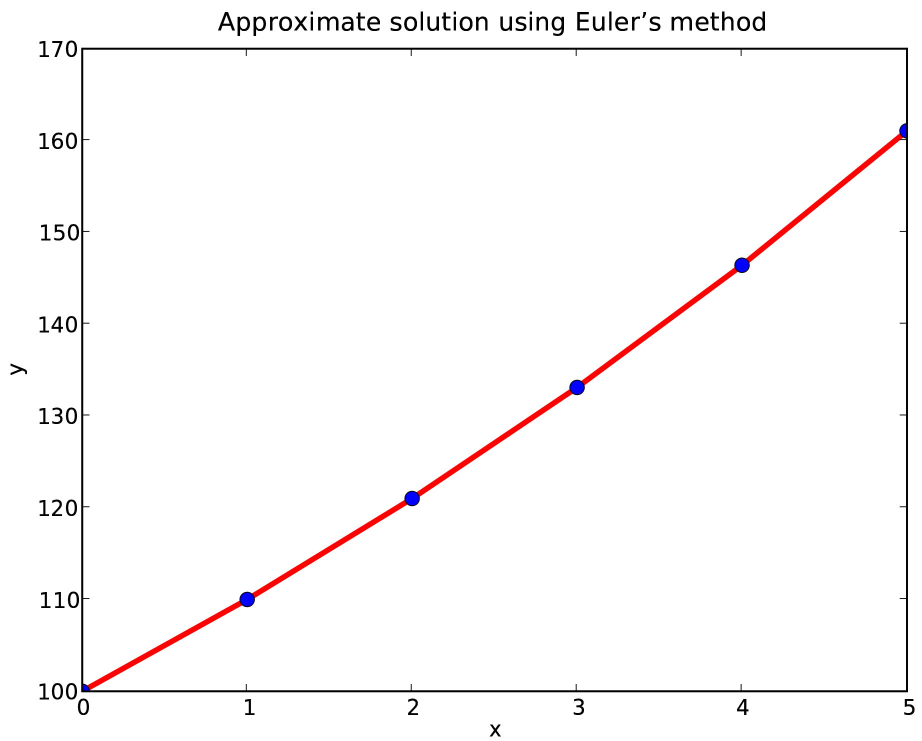
(Note that this is an exponential DE, which we can solve exactly. In practice we would not need to use Euler's method to solve it; this is just a demonstration.)

Answer: With a stepsize of $h = 1$, to find the approximate value of y when $x = 5$ we proceed as follows. (Remember that at each step, the new value of x equals the previous value of x plus h.)

Step	x	y	$y' = 0.1y$	$h \times y'$	new x	new y
0	0	100	10	10	1	110
1	1	110	11	11	2	121
2	2	121	12.1	12.1	3	133.1
3	3	133.1	13.31	13.31	4	146.41
4	4	146.41	14.641	14.641	5	161.051

So when $x = 5$, $y \approx 161.051$.

A graph of the approximate solution is shown below. The five y values from the last column of the above table are marked as circles, with straight lines approximating the function between these points.



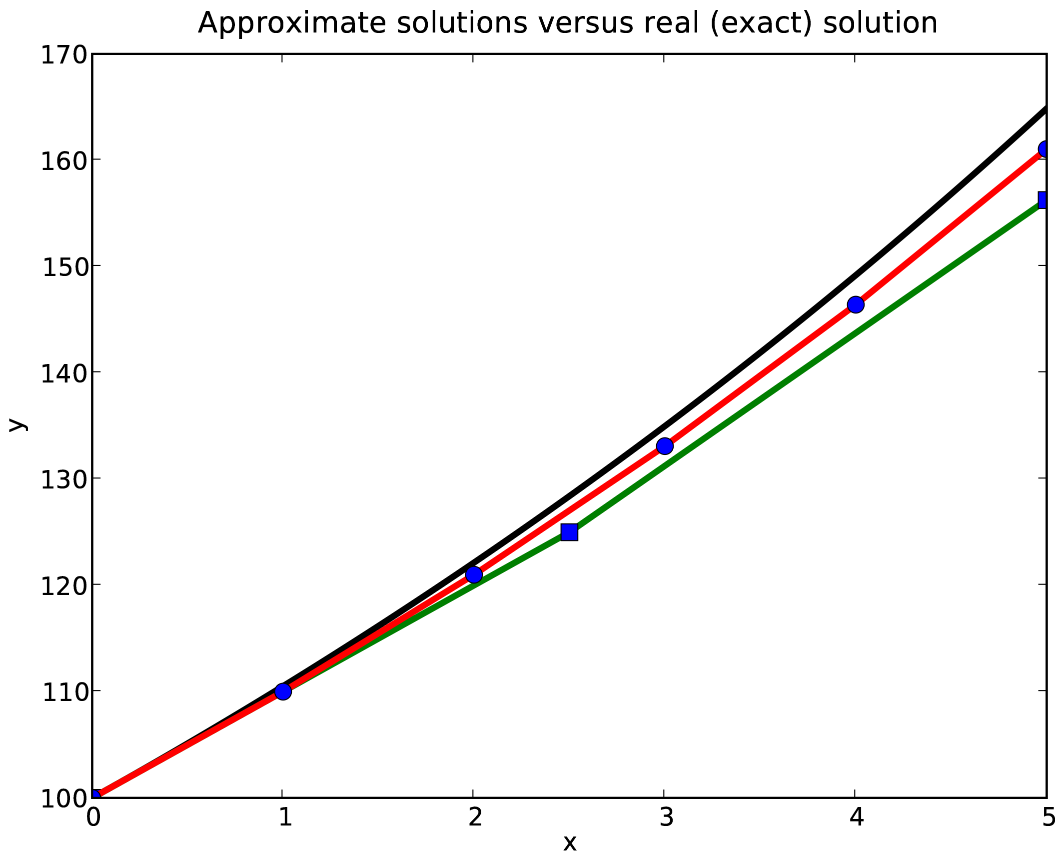
There are some important things to know about Euler's method.

- It gives an **approximate** solution, not an exact solution. There will be numerical inaccuracies in the answer.
- The choice of stepsize is very important: smaller values will give a more accurate answer, but take longer to calculate.
- The method can result in large numerical inaccuracies if it is used over a very large range of x values.
- Despite these limitations, the method can give very good approximate solutions to quite difficult problems.

***Example** 15.4.3* In Example 15.4.2, we used a stepsize of $h = 1$ to approximately solve $y' = 0.1y$.

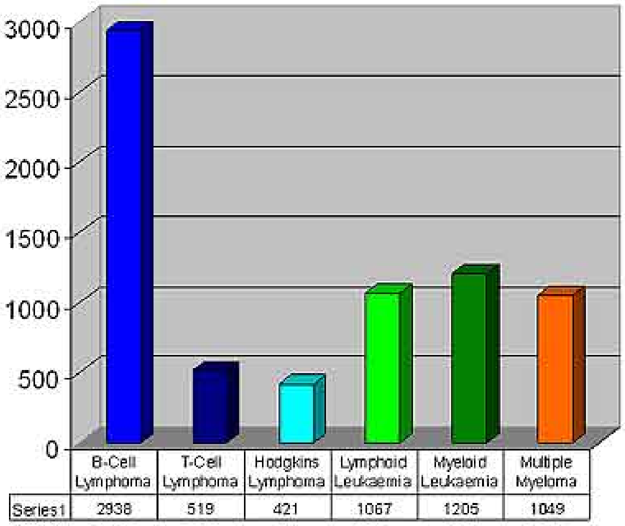
The following graph shows the approximate solution with a stepsize of $h = 2.5$ (bottom curve), $h = 1$ (middle curve) and the exact solution (top curve).

As h becomes smaller, the solution becomes more accurate (that is, moves closer to the top curve).



- In addition to modelling populations in ecology, the logistic equation has also proved to be a valuable model of cell growth in cancerous tumours.

Case Study 31:
Medicine, Maths and Multiple Myeloma



Australian Blood Cancer Incidence: Year 2000; see www.lymphoma.org.au/content/?id=25

- Cancer is a leading cause of death in humans.
- The health website *www.healthinsite.gov.au/topics/Cancer* states "Cancer is a diverse range of diseases where abnormal cells grow rapidly and generally spread uncontrolled throughout the body. These cancerous cells can invade and destroy surrounding tissue and spread (metastasise) to distant parts of the body."
- *Multiple myeloma* is a cancer of the plasma cells, which are an integral part of the immune system.
- It is one of the more common blood cancers, affecting around 4 people per 100,000.
- Average age at diagnosis is around 60. No cause or clear risk factors have been identified.
- Multiple myeloma is incurable, but treatment via steroids or chemotherapy has extended life expectancy (which is currently around 60 months if diagnosis is early).

- A large amount of ongoing research is undertaken in order to understand different forms of cancer, including the search for better methods of management, treatment and cure.
- An important component of this is developing better models of tumour growth and treatment.
- For example, a paper[a] discusses various models of tumour growth, including modelling multiple myeloma tumour growth using the logistic equation.
- Tumours cannot grow indefinitely: their maximum size is determined by the physiology of the sufferer and by the need for tumour cells to receive nutrients (such as oxygen).
- The maximum tumour size corresponds to the carrying capacity K in the logistic DE.
- *Chemotherapy* is a medical treatment involving the infusion of highly toxic chemicals into the body, killing rapidly dividing cells. (Rapid division is a common characteristic of cancerous cells.)
- High-dosage chemotherapy and stem-cell grafts are the primary treatments for multiple myeloma.
- Determining the precise chemotherapy dosage involves a trade-off between the beneficial impact of reducing tumour size and the (often severe or life-threatening) side-effects resulting from the highly toxic drugs.

[a] Swan, *Cancer Chemotherapy: optimal control using the Verhulst-Pearl [logistic] equation*, Bulletin of Mathematical Biology, **48:4** (1986) 381–404.

***Question** 15.4.4* A newly diagnosed, early-stage tumour will typically have: a size of around 10^9 cells; a doubling time of about 61 days so the growth rate is $r \approx 0.0114$ per day; and a maximum size of about 4×10^{12} cells.

(a) Write a DE for the rate of change of the size $C(t)$ of this tumour.

(b) Assume that the rate at which chemotherapy kills cancerous cells is proportional to the tumour size. Write a new DE for the rate of change of the size $C(t)$ of a tumour undergoing treatment.

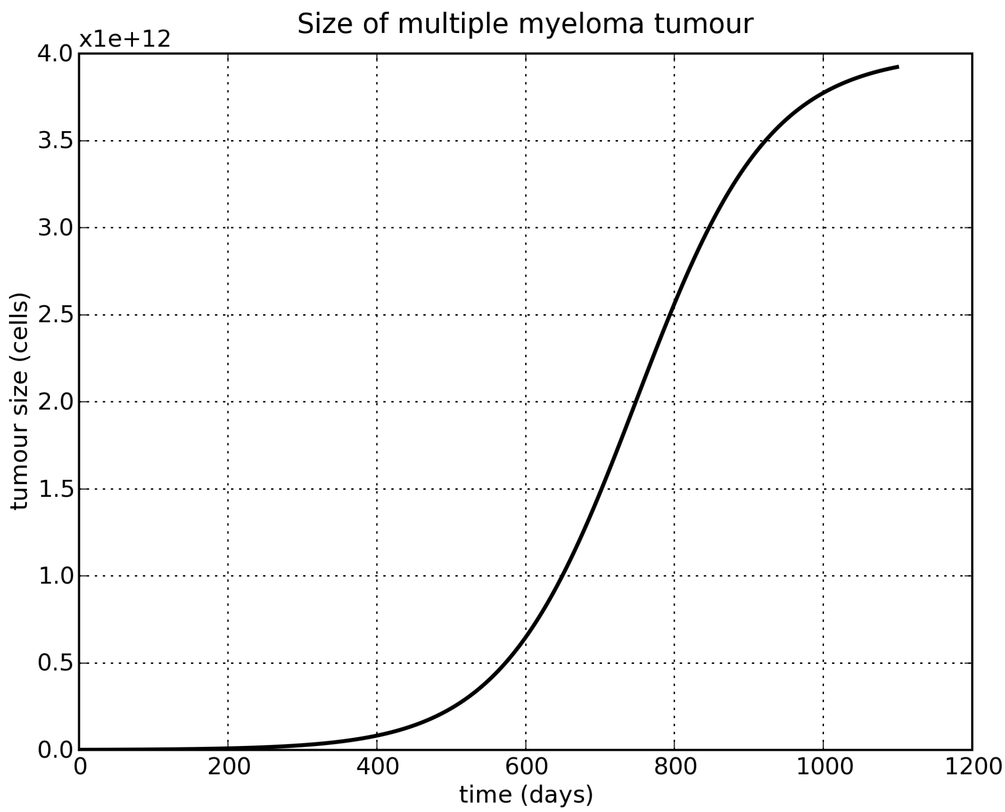
- One treatment regime for multiple myeloma involves administering chemotherapy for each of days 1 to 4, on 4 to 6 week cycles, for a period of more than a year.
- We can develop a computer model to investigate the potential impact of this treatment on tumour size.

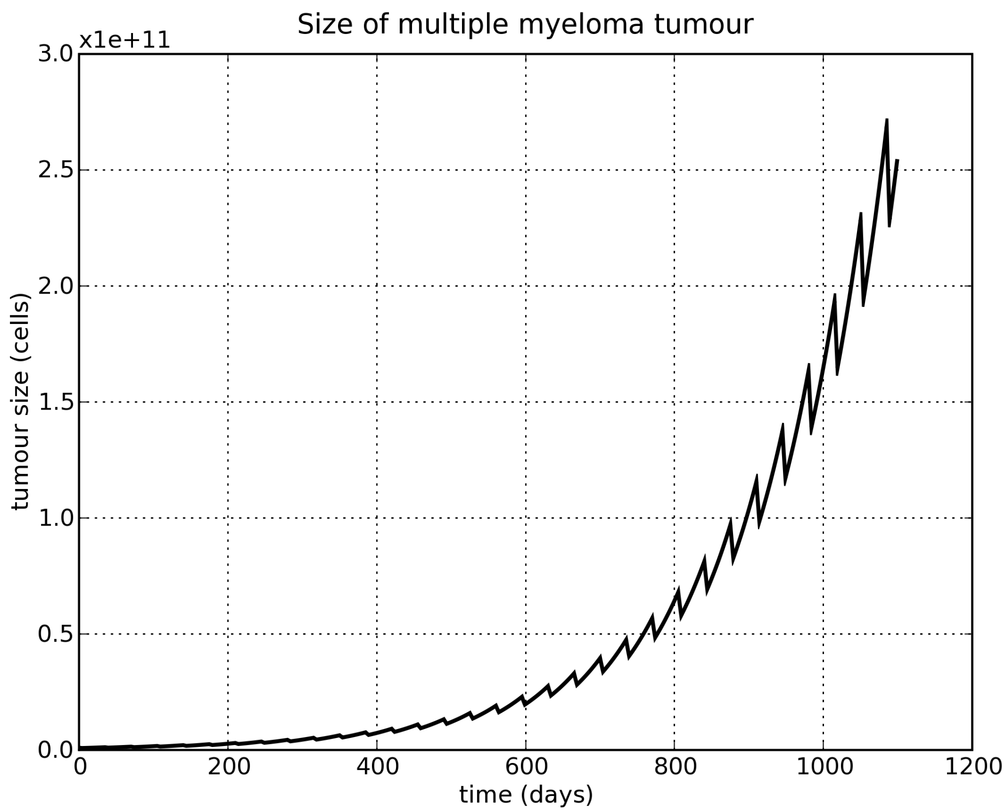
Program specifications: Write a Python program which uses Euler's method to plot the predicted tumour size over a chosen number of days. The program must model chemotherapy treatment as described, with the user able to choose the proportion of cells killed on each treatment day. Use a step size of one day and cycles of five weeks.

Python Example 15.4.5

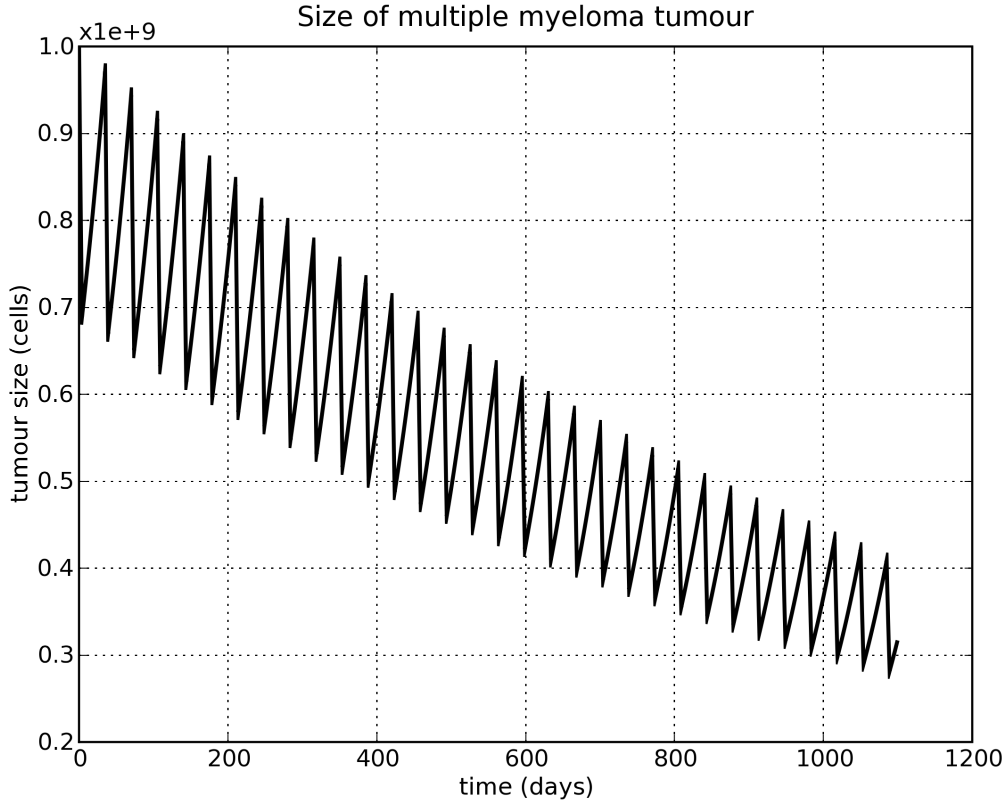
```
# A program to model the effect of chemotherapy on
# a multiple myeloma tumour.

from __future__ import division
from pylab import *

kill =input("What proportion of cells does chemo kill each day:")
duration = input("For how long should the model run in days? ")

# Initialise variables
days = arange(0, duration)
sizes = 1.0 * arange(0,duration)
r = 0.01114
stepSize = 1
cells = pow(10,9)
maxSize = 4 * pow(10,12)

# Complete each step of Euler's method.
for i in days:
    sizes [i] = cells
    Cdash = r * cells * (1 - cells/maxSize)

# Apply the effect of chemotherapy if it is a treatment day;
# cycles occur every 5 weeks; treatment is on days 1 to 4.
    if i % 35 < 4:
        Cdash = Cdash - kill * cells
    cells = cells + Cdash * stepSize

plot(days, sizes, 'k-', linewidth = 2)
grid(True)
xlabel("time (days)")
ylabel("tumour size (cells)")
title("Size of multiple myeloma tumour")
show()
```

The graphs show modelled tumour sizes with: no treatment (top; note that median overall survival time after diagnosis is around 3 years); and 5% of cells killed per day during treatment (bottom).





The following graph shows the modelled tumour size with 10% of cells killed per day during treatment. Note the difference in trend in the tumour sizes in this graph and in the previous two graphs.



Question *15.4.6* The previous model of cancer treatment is **VERY** rough. What are likely to be some of the largest errors?

End of Case Study 31.

15.5 Space for additional notes

16 Systems of DEs

On the farm, every Friday
On the farm, it's rabbit pie day.
So, every Friday that ever comes along,
I get up early and sing this little song
Run rabbit - run rabbit - Run! Run! Run!
Don't give the farmer his fun! Fun! Fun!
He'll get by
Without his rabbit pie
So run rabbit - run rabbit - Run! Run! Run!

Artist: Flanagan and Allen

(www.youtube.com/watch?v=SVdoZNxtL8k)

(www.youtube.com/watch?v=lEqtcmn-ePU)

The wild hunt: Åsgårdsreien (1872), Peter Nicolai Arbo (1831 – 1892), Nasjonalgalleriet, Oslo. (Image source: en.wikipedia.org)

Introduction

In the previous section we introduced DEs, and showed how they are important tools for modelling a range of phenomena, including populations.

Rather than being isolated entities, many natural phenomena involve interactions between multiple factors. For example, in predator/prey relationships, movements in the populations of both predators and prey are interlinked.

In this section we extend the use of DEs, showing how a *system* of DEs can be used to model more complex phenomena.

Some of the examples/contexts we will discuss are:

- Organisms with distinct life stages.
- Behaviourism.
- Interacting species.
- Predator/prey relationships.

Specific techniques and concepts we will cover include:

- Life-cycle diagrams.
- Systems of DEs.
- Using Euler's method to solve systems of DEs.
- Lotka-Volterra equations.

16.1 Introduction to systems of differential equations

- The DEs studied so far have all involved modelling a single, distinct phenomenon.
- Often there are multiple factors which interact, requiring more sophisticated models.
- For example:
  - in a predator-prey relationship, the changes in the population sizes of *two* species are interrelated;
  - in a species with multiple distinct life stages, changes in the population sizes of each stage depend on the populations in other stages; and
  - the rate at which an epidemic spreads through a population is influenced by the number of infected individuals and the number of susceptible individuals.
- These more complex situations are typically modelled using a system of DEs; that is, more than one DE.
- Just as with single DEs, sometimes a system of DEs can be solved analytically, and other times the system needs to be solved using approximate techniques.
- Euler's method can be applied to a system of equations in a very similar way to solving a single equation: simply apply one step of Euler's method to each equation in turn, then apply subsequent steps to all equations in turn.

16.2 Going through a difficult stage

- Earlier we modelled populations using exponential and logistic DEs.
- In all cases, the populations were assumed to be *homogeneous*; that is, every individual in the population is identical in terms of its impact on population growth.
- Many organisms have substantial differences in typical survival rates and reproduction rates between different life stages.
- For example, in many species, small juveniles have a low survival rate and do not reproduce, whereas mature breeders have a high survival rate and do reproduce.
- Hence, for more advanced organisms, particularly those with a long life-span, a simple model based on a single DE will be inaccurate.
- In such cases, systems of DEs give rise to better models.
- In one model, populations are divided into groups based on their *life stages*, such as *juvenile* or *breeding adult*.
- Rather than applying a constant growth rate to every individual in the population, a system of DEs:
  - considers the *distribution* of the population within the distinct groups;
  - allows different rates of reproduction and death within different groups; and
  - includes the transitions of individuals between groups.
- To assist with writing the equations in a system of DEs, it is sometimes useful to draw a diagram showing the rates of *transition* between stages.
- When modelling a population, this is called a *life-cycle diagram*.

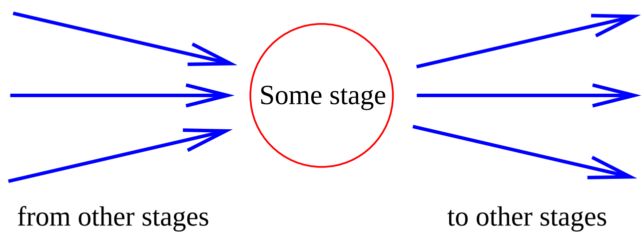
Life-cycle diagram

A **life-cycle diagram** *for an organism describes the transitions between the stages that define its life cycle.*

Each stage in the life cycle of the organism is represented as a circle, with a directed arrow joining Stage A to Stage B whenever it is possible for there to be a transition from Stage A to Stage B.

Each arrow from A to B has a number associated with it, which is the rate *of transition from Stage A to Stage B.*

- The general form of a stage in a life-cycle diagram is shown below. Not all stages will have all of these arrows, as some particular transitions may not occur.



- To draw the life-cycle diagram for an organism, you need to know:
  - the number of stages;
  - all possible transitions from/to each stage, including:
    * reproduction;
    * transitions due to the passage of time;
    * transitions due to other factors; and
    * deaths.
  - the number associated with each transition.
- From a life-cycle diagram, it is easy to write a system of DEs for the number of individuals in each stage.

Question *16.2.1* An idealised fish species has two distinct life stages: juvenile and adult. Each month, on average:

- Juveniles do not breed, nd have a 0.5 probability of surviving to adulthood, and a 0.5 probability of dying.
- Adults have a fertility of 5, and will all die.

(a) Draw a life-cycle diagram for this fish, with two stages.

(b) If the populations of juveniles and adults at any time are $J(t)$ and $A(t)$, write a system of DEs for these populations.

(c) At time 0 a population comprises 20 juveniles and 2 adults. Use Euler's method and a step size of one month to estimate the number of fish in each stage at time $t = 2$ months.

continued...

Question *16.2.1 (continued)* Sometimes it is convenient to include death as a stage in a life-cycle diagram.

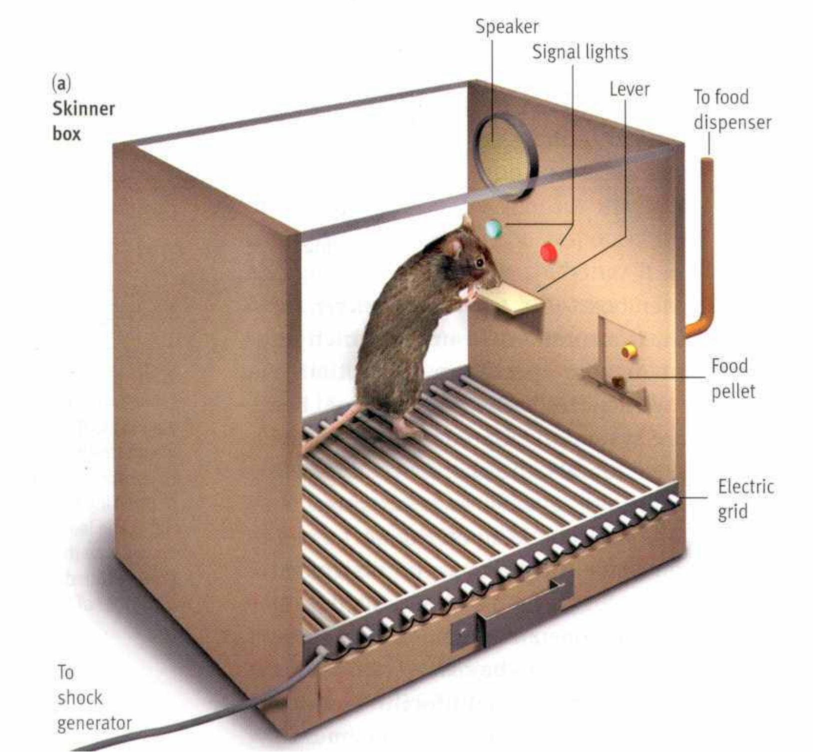
(d) Draw a life-cycle diagram for this fish, with three stages, including death.

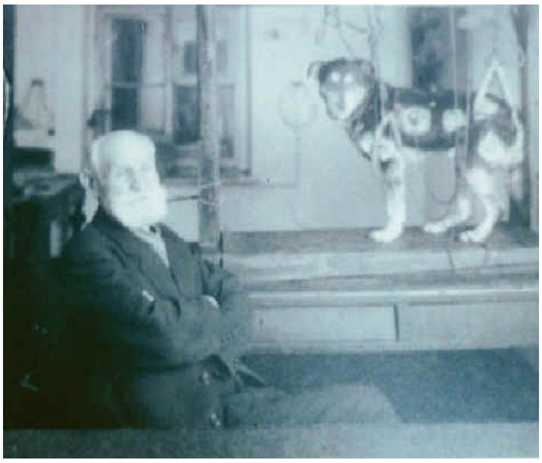
(e) Let $D(t)$ be the total number of dead fish at any time. Write a system of DEs for $J(t)$, $A(t)$ and $D(t)$.

(c) At time 0 a population comprises 20 juveniles, 2 adults and no dead fish. Use Euler's method and a step size of one month to estimate the number of fish in each stage at time $t = 2$ months.

- This approach can be used to model other phenomena.

Case Study 32:
Behaviourism, rats and mazes.





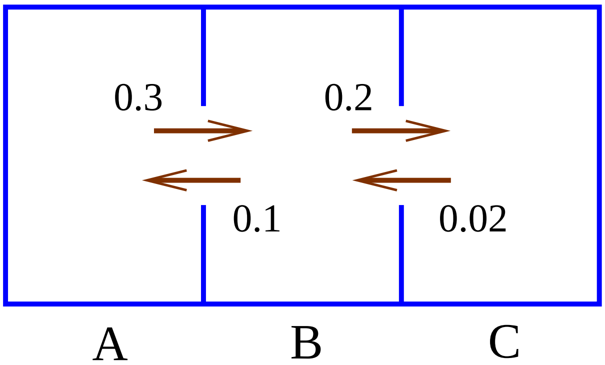
- In psychology, *behaviourism* is a theory of learning based on the proposition that everything that an organism does is a behaviour acquired through *conditioning*, which is the interaction of the organism with its environment.
- According to this theory, behaviour can be studied in a scientific, systematic manner.
- Three of the most famous researchers in behaviourism are Pavlov, Skinner and Watson.

- Over the last century, psychologists have conducted many behavioural experiments on rats (also on pigeons and students!).
- Some such experiments involved observing movement patterns of rats in mazes, and measuring any impact on these patterns arising from applying different stimuli to the rats.

Question *16.2.2* Consider an experiment analysing the movement of a rat through a three-stage maze. During each time step the rat will either:

- remain within the same stage in the maze; or
- move forwards to the next stage (if any); or
- move backwards to the previous stage (if any).

A stylised representation of the maze is shown, with the probabilities that a rat in a stage will move to an adjacent stage in each time step.



(a) Let $A(t)$, $B(t)$ and $C(t)$ be the probabilities that a rat will be in each corresponding stage of the maze at time t. Write a system of DEs for $J(t)$, $A(t)$ and $D(t)$.

continued...

Question *16.2.2 (continued)*

(b) If a rat is placed in Stage A at time 0, use Euler's method and a step size of 1 to estimate the probability that the rat will be in each stage at time $t = 2$.

- If the experiment runs for many time steps, it is convenient to use a Python program to implement Euler's method.

Program specifications: Develop a Python program which uses Euler's method with a stepsize of one to estimate the probabilities that the rat will be in each stage, from $t = 0$ to $t = 30$. Draw a graph of these probabilities.

Python Example 16.2.3

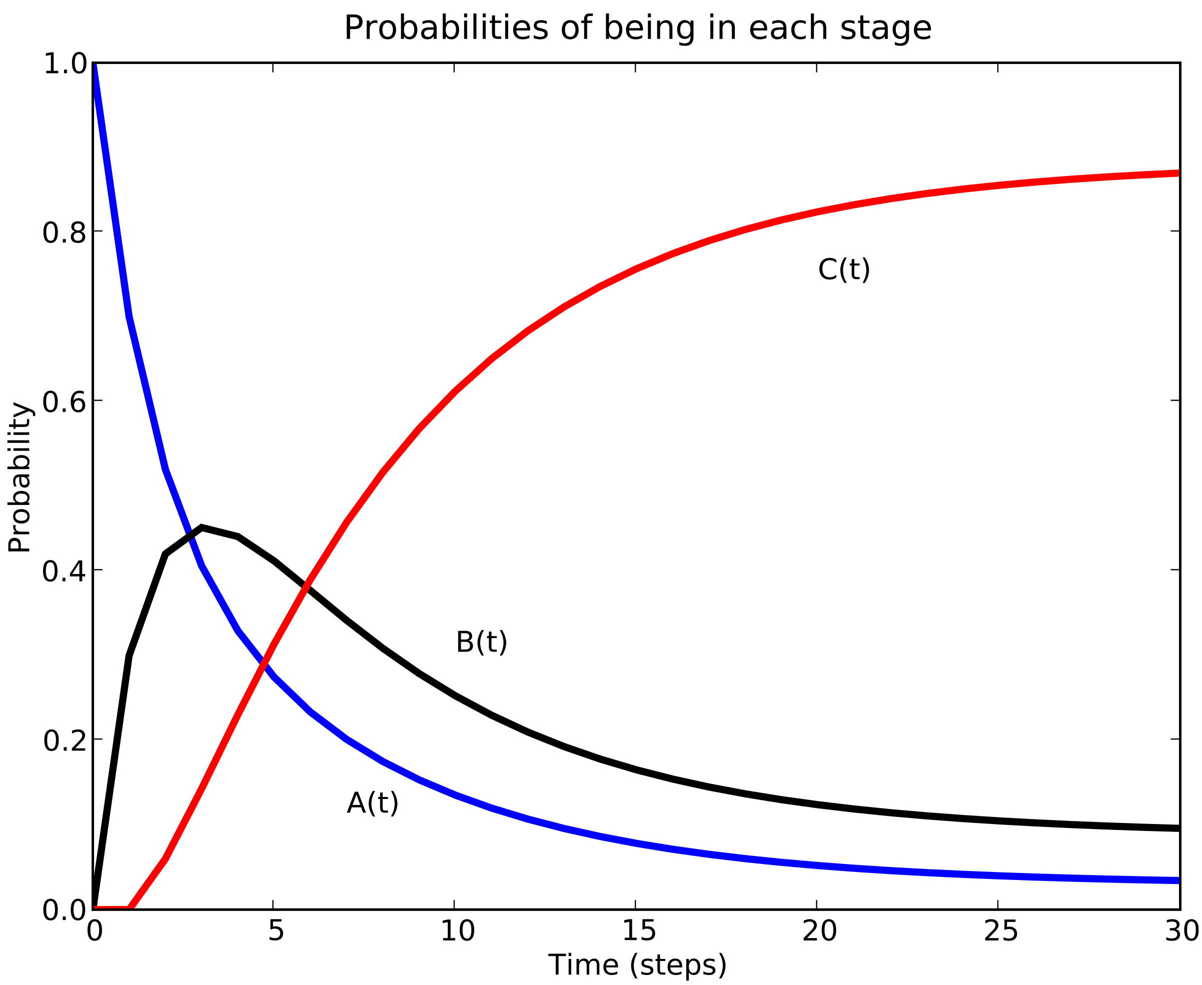
```
# Uses Euler's method to model rat movements in a maze.
from __future__ import division
from pylab import *

# Initialise variables: apply Euler's method for 30 steps.
maxt = 30
# The rat is initially in Stage A.
A = 1
```

Python Example 16.2.4

```
B = 0
C = 0
AProb = zeros(maxt+1)
BProb = zeros(maxt+1)
CProb = zeros(maxt+1)
AProb[0]=1
stepsize = 1

# Step through Euler's method.
for i in arange(1, maxt+1):
    dA = -0.3 *A + 0.1 * B
    dB = -0.3 * B + 0.3 *A + 0.02 * C
    dC = -0.02 * C + 0.2 * B
    A = A + stepsize * dA
    B = B + stepsize * dB
    C = C + stepsize * dC
    AProb[i] = A
    BProb[i] = B
    CProb[i] = C

# Output the graphs.
times = arange(0, maxt+1)
plot(times, AProb, 'b-', linewidth=3)
plot(times, BProb, 'k-', linewidth=3)
plot(times, CProb, 'r-', linewidth=3)
xlabel('Time (steps)')
ylabel('Probability')
title('Probabilities of being in each stage')
text(20, 0.74, 'C(t)')
text(10, 0.3, 'B(t)')
text(7, 0.11, 'A(t)')
show()
```

Behaviourism, rats and mazes. *(continued)*

- Here is the output from running the program.



- Psychologists might conduct a series of experiments in which they apply some stimulus to rats in the maze and investigate how closely the observed positions match the expected positions, and hence investigate whether the stimulus causes a behavioural change.
- The calculations can easily be modified to reflect changes in the experiment, including: the difficulty of traversing the maze; the number of stages in the maze; the strengths of any positive or negative stimuli; or the initial location of rats in the maze.

End of Case Study 32.

16.3 Interacting species

- Systems of DEs can also be used to model interactions between multiple species.

Question *16.3.1* Consider a controlled laboratory experiment simulating the effects of immigration, emigration, births and deaths on populations of Assassin bugs (predators) and caterpillars (prey). Initially there are 40 Assassin bugs and 400 caterpillars. Each day:

- 15 caterpillars are introduced into the experiment (modelling immigration and birth of caterpillars);
- one quarter of the Assassin bugs each eat a caterpillar (death of caterpillars);
- 12 Assassin bugs are removed (modelling emigration and death of Assassin bugs); and
- for each 25 caterpillars eaten, one new Assassin bug is introduced (modelling birth of Assassin bugs).

Let $A(t)$ and $C(t)$ be the populations of Assassin bugs and caterpillars at any time t in days.

(a) Write a DE for the rate of change of **each** of the populations.

continued...

Question *16.3.1 (continued)*

(b) Show that the following equations are solutions to the DEs in Part (a).

$$\begin{aligned} A &= 40\sin 0.1t + 60 \\ C &= 100\cos 0.1t + 300. \end{aligned}$$

(c) Draw a rough sketch of the populations over time, and briefly interpret the graph.

continued...

Question *16.3.1 (continued)*

(d) Ecologists might use the phrase *stable populations*. What does this mean, and why is it important?

(e) How are stable populations represented mathematically? Why?

(f) Find all pairs of population sizes of Assassin beetles and caterpillars which represent stable populations. Interpret your answer.

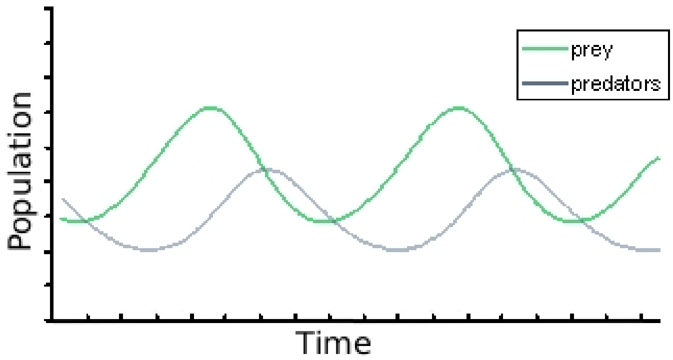
- This model of interactions is very simple, but it is not unreasonable.
- It is well-known that many pairs of phenomena show linked, periodic behaviour over time, including:
  - populations of predator/prey species in isolated ecological systems;
  - economic conditions and employment opportunities in "cyclic" industries such as geology; and
  - levels of affection in relationships.

16.4 Lotka-Volterra model

- Question 16.3.1 modelled interactions between two species in a controlled environment.
- In general, inter-species interactions are not controlled.
- A classical problem in ecology is that of *predator/prey* relationships. Given two species, with one a predator of the other, various models can be used to predict population changes over time.

Case Study 33:

Seals and polar bears



- Consider a simple ecosystem in which a population of seals is preyed upon by a population of polar bears.

Seals and polar bears *(continued)*

Standard assumptions for this type of model are that:

- the prey species has no other predators, and the predator species has no other prey; and
- the prey species breeds rapidly and individuals do not compete with each other, but the predator species breeds more slowly and individuals compete with each other.

***Question** 16.4.1* Let $P(t)$ and $S(t)$ be the populations of polar bears and seals (respectively) at time t in years. What factors would influence the *rate of change* of each of S and P? In each case, identify whether the factor leads to an increase or decrease in the corresponding population.

(a) Factors influencing the rate of change of the seal population:

(b) Factors influencing the rate of change of the polar bear population:

- The best-known predator/prey model is the **Lotka-Volterra** model.

Lotka-Volterra model

Let $P(t)$ and $S(t)$ be the sizes of populations of a predator and prey species respectively, at any time t. The Lotka-Volterra model *represents the population movements in the following system of DEs:*

$$\begin{aligned} S' &= aS - bSP \\ P' &= -cP + dSP \end{aligned}$$

where a, b, c and d are positive constants whose values depend on the particular species being modelled.

Question *16.4.2* Explain carefully what each of the terms in each of the equations in the Lotka-Volterra model represents. In particular, explain the physical relevance of the term SP.

- Unlike the system of equations in Question 16.3.1, it is not possible to find a general solution to the Lotka-Volterra equations. Instead, approximate solutions can be found using Euler's method.

Question *16.4.3* Let $P(t)$ and $S(t)$ be the populations of polar bears (predators) and seals (prey) respectively. Recall that

$$S' = aS - bSP \qquad\qquad P' = -cP + dSP$$

(a) How would the statement "Polar bears become extinct" be written mathematically?

(b) If all polar bears died suddenly from disease, what does the model predict will happen to the population of seals? Explain your answer carefully.

(c) Is your answer to Part (b) biologically realistic? What would probably happen in reality?

continued...

Question *16.4.3 (continued)*

(d) If $a = 0.05$ year^{-1}, $b = 0.001$ year^{-1}, $c = 0.05$ year^{-1} and $d = 0.0001$ year^{-1}, find all pairs of stable population sizes.

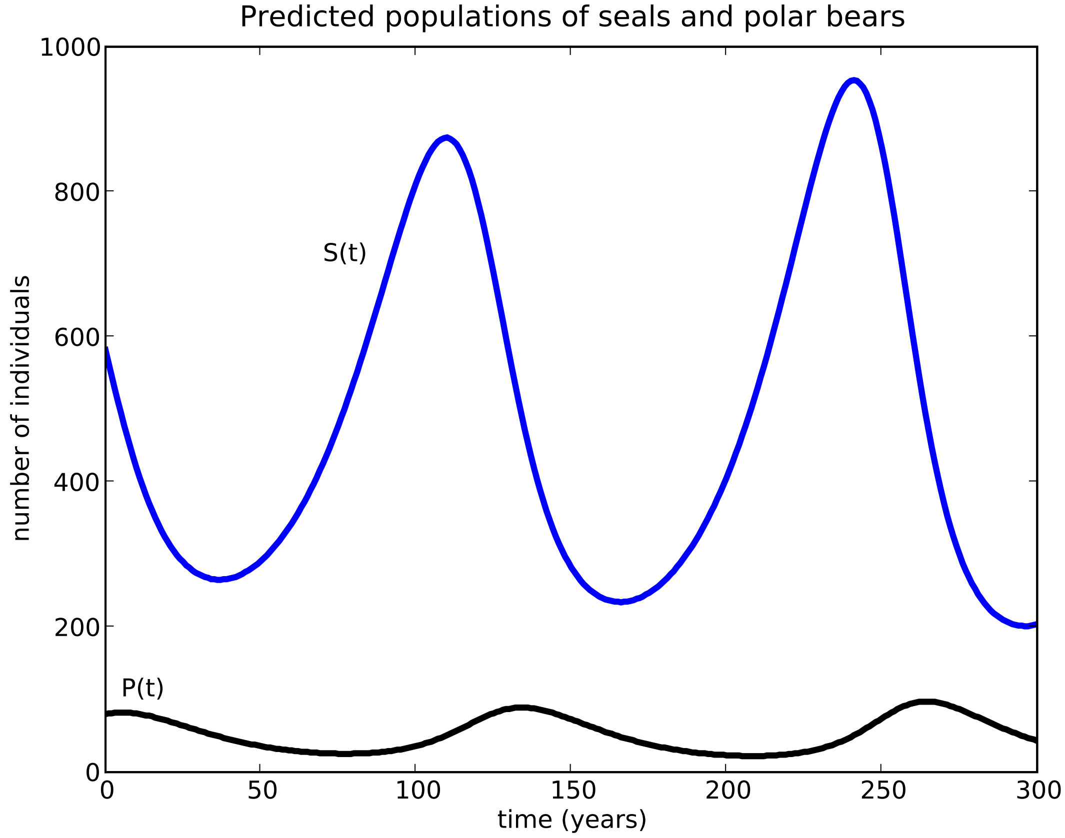
(e) Interpret your answer to Part (d).

(f) **Program specifications**: Develop a Python program which uses Euler's method with a stepsize of one year to solve the Lotka-Volterra equations.

Python Example 16.4.4

```
# Euler's method to model populations of seals and polar bears.
from __future__ import division
from pylab import *

# Initialise variables.
maxt = 300
S = 600
P = 80
a = 0.05
b = 0.001
c = 0.05
d = 0.0001
SA = arange(0,maxt+1)
PA = arange(0,maxt+1)
SA[0] = S
PA[0] = P

# Step through Euler's method with stepsize 1
for i in arange(0, maxt+1):
    dS = a*S - b*S*P
    dP = -c*P + d*S*P
    S = S + dS
    P = P + dP
    SA[i] = S
    PA[i] = P
# Output graphs.
times = arange(0, maxt+1)
plot(times, SA, 'b-', linewidth=3)
plot(times, PA, 'k-', linewidth=3)
xlabel('time (years)')
ylabel('number of individuals')
title('Predicted populations of seals and polar bears')
text(70, 700, 'S(t)')
text(5, 100, 'P(t)')
show()
```

***Example** 16.4.5* Assume at time $t = 0$ years there are 600 seals and 80 polar bears. Running the above program predicts the following movements in population sizes over 300 years.



***Question** 16.4.6*

(a) Comment on the comparative population changes over time.

continued...

Question *16.4.6 (continued)*

(b) Critically evaluate the following possible media statement:

> *A survey has shown that the populations of both species are in decline. Hence we need to act promptly, otherwise one or both species will become extinct.*

End of Case Study 33.

16.5 Space for additional notes

17 Fully sick

From New Delhi to Darjeeling
I have done my share of healing,
and I've never yet been beaten or outboxed.
I remember that with one jab
of my needle in the Punjab
how I cleared up beriberi
and the dreaded dysentery,
but your complaint has got me really foxed.
Oh doctor, touch my fingers.
Well, goodness gracious me.
You may be very clever
but however, can't you see,
my heart beats much too much
at a certain tender touch,
it goes boom boody-boom boody-boom boody-boom
boody-boom boody-boom boody-boom-boom-boom.

Artist: Peter Sellers and Sophia Loren
(www.youtube.com/watch?v=gKMy15O1tCw)

The Triumph of Death (1562), Pieter Bruegel the Elder (c. 1525 – 1569), Museo del Prado, Madrid.
(Image source: commons.wikimedia.org/wiki/Image:Thetriumphofdeath.jpg)

Introduction

Throughout history, infectious diseases have claimed many human lives. The effects of diseases on humans and other species remain a major challenge for the international community, so it is important to understand what causes diseases, how they spread, how their impact can be minimised and what mechanisms are effective for prevention and cure.

Various aspects and impacts of disease are managed by a diverse group of individuals and organisations. Health practitioners spend much of their professional lives treating people with disease, parents attempt to prevent their children from catching diseases, governments organise mass vaccination campaigns, countries expend a large proportion of their national income on health, the World Health Organisation is preparing contingency plans for pandemics, and researchers are always working on finding new cures.

An important approach to developing effective responses to possible pandemics is understanding how a disease might spread throughout a population. Differential equations are one of the most commonly used modelling tools to enable such predictions to be made. In this section we will study several DE-based models of disease spread.

Some of the examples/contexts we will discuss are:

- Epidemics.
- Rubella.
- Catastrophes, Spanish flu and avian influenza.

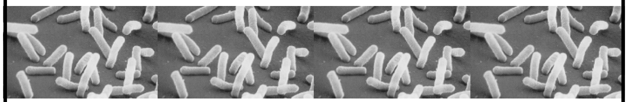
Specific techniques and concepts we will cover include:

- The SIR model.
- The SIRD model.

17.1 Epidemiology and epidemic models

Epidemiology?

Like ecologists, epidemiologists seek to understand:
- species richness (biodiversity)
- species abundance (populations/communities)
- species distribution (temporal, spatial)



Study human pathogens = epidemiology
Study animal pathogens = epizootiology

Epidemiology/Epizootiology

Study of occurrence, spread and control of diseases
(descriptive) (analytical) (experimental)

- Prevalence (number infected)
- Incidence (change in prevalence over time)
- Distribution (density, intensity, concentration,..)

exhibit longitudinal fluctuations (esp. seasonal)

influenced by many factors:
- demographic, socioeconomic, behavioural
- geographic, climatic

Epidemiological studies

Four main types:	Maths
• Case series (descriptive) – index, incidental, miscellaneous	not quantitative
• Case control studies (retrospective) – cases + controls interviewed	statistics Odds Ratio
• Cohort studies (prospective) – cohort followed forward in time	statistics Relative Risk
• Outbreak studies (predictive) – rate of change in population	calculus Differential Equations

- In this section we will discuss some methods for using DEs to model the large-scale spread of infectious disease through a population over time.

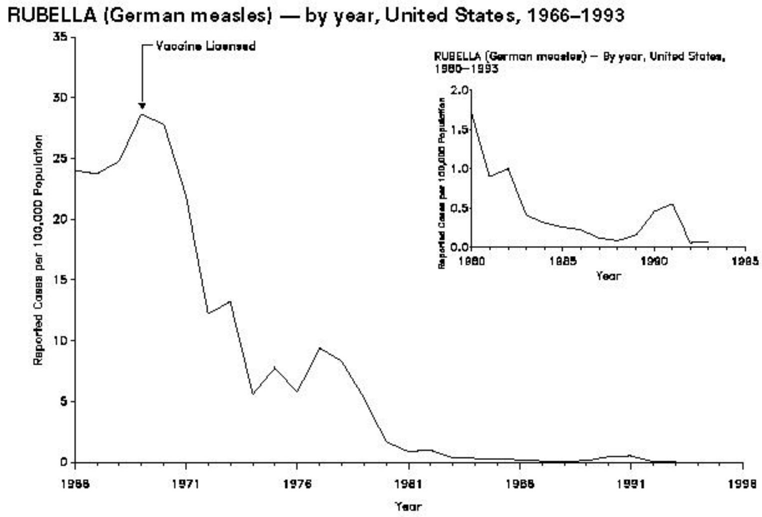
Epidemic

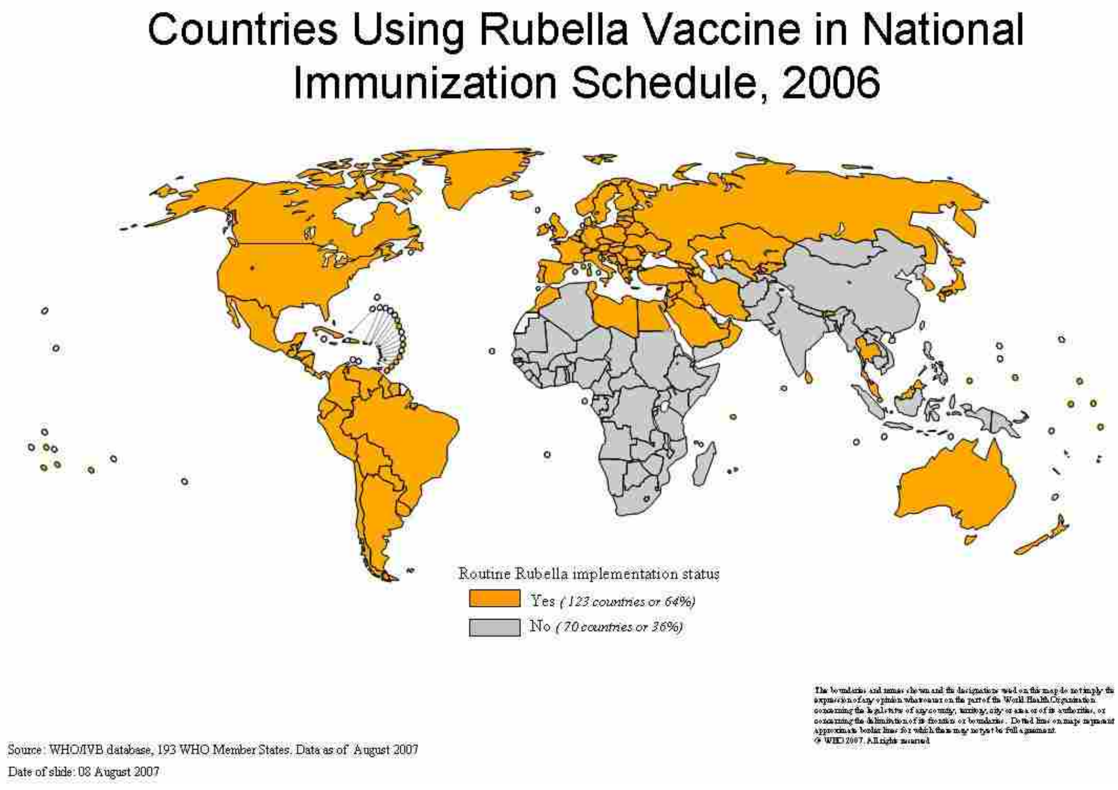
A large-scale occurrence of disease in a human population is called an **epidemic** *if new cases of the disease arise at a rate that "substantially exceeds what is expected" in a given time period.*

Localised occurrences are called **outbreaks**, *and global occurrences are often called* **pandemics**.

- Modelling epidemics and pandemics is an important aid to understanding how they spread and how they can be controlled through various techniques such as quarantine and immunisation.
- Many epidemic models are based on systems of DEs (as was the case for the predator/prey relationship).
- We will commence our study of epidemics with a simple model, known as the SIR (**S**usceptible, **I**nfected, **R**emoved) model.
- We will study the SIR model in the context of the disease *rubella*, but this type of model can be applied to many different diseases (such as measles, cholera, swine flu and bubonic plague).
- Researchers use a variety of models when studying epidemics, including numerous variations of the basic SIR model.
- Later we will study Avian influenza using the SIRD model, which includes an additional category: **D**ead.

Case Study 34:
Rubella





- **Rubella** (or **German measles**) was (and in some countries, is) a common disease, particularly in childhood.
- The primary mechanism for transmission is via airborne droplets.

Rubella *(continued)*

- In most cases rubella has very mild symptoms, which may even pass unnoticed.
- However, if a woman is infected during the first 20 weeks of pregnancy then spontaneous abortion can occur (in about 20% of cases), or the child may be born with congenital rubella syndrome (CRS), which is a range of incurable conditions including deafness, blindness and mental retardation.
- There was a rubella epidemic in the USA between 1962 and 1965. It is estimated that there were well over 10 million infections, around 30,000 still births and 20,000 children were born with CRS.
- A rubella vaccine was introduced in 1969 and is routinely administered in many countries, including Australia. For example, the Queensland Department of Health recommends all children have a combined MMR (measles, mumps and rubella) vaccine at ages 12 months and 4 years. (Previously a rubella vaccine was administered to early-teenage girls.)
- Vaccination campaigns have greatly reduced the incidence of rubella and the frequency of outbreaks. In 2004, it was announced that rubella has been eliminated from the USA.
- (In January 2008, at least four babies in Sydney became infected with rubella. All were less than 12 months old, so were under the age for administering the MMR vaccine.)
- Some individuals and groups are opposed to vaccination campaigns in general (not just the MMR vaccine), claiming that associated risks outweigh likely benefits.
- However, consider the following news item from the BBC.

Extension 17.1.1 (From news.bbc.co.uk, August 8th 2008.)

"Measles fears prompt MMR campaign

The government has launched a campaign to raise MMR vaccination rates in England amid growing concerns about a measles epidemic. The Department of Health has asked primary care trusts to offer the jab to all children up to the age of 18 not already fully protected…

An epidemic of measles - which can be fatal - could potentially affect up to 100,000 young people in England alone.

Experts say MMR is perfectly safe, but vaccination rates dipped following controversy about its safety.

A study which raised the possibility that MMR was linked to autism has since been dismissed by the vast majority of research, but levels of public confidence in the jab have still not fully recovered…

The number of cases of measles in England is rising following a decade of relatively low vaccine uptake…In 2006 and 2007 there were 1,726 confirmed cases in England and Wales - more than the previous 10 years put together. From 1996 to 2005 there was a total of 1,621 confirmed cases.

It is estimated that around three million children aged 18 months to 18 years have missed either their first or second MMR vaccination.

Scientific advice from both the Department of Health and the Health Protection Agency suggests vaccination levels need to be increased as a matter of urgency…Around 95% of the population need to be vaccinated to protect against widespread outbreaks of measles. The current vaccination rate across England and Wales is around 10 percentage points lower…'If we continue to accumulate unvaccinated children, measles will spread among them - at some point there will be a measles epidemic.' "

Rubella *(continued)*

- We will now introduce the SIR epidemic model and apply it to possible outbreaks of rubella.

SIR model of epidemics

The SIR *model of epidemics divides a population into three distinct* **compartments** *or groups. At any time t:*

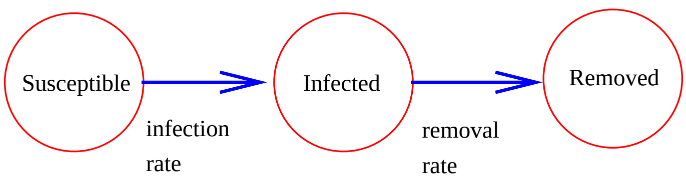
(1) *The susceptible compartment $S(t)$ is the group of people who are susceptible to the disease.*

(2) *The infective compartment $I(t)$ is the group of people who have the disease and can infect susceptible people.*

(3) *The removed compartment $R(t)$ is the group of people who cannot catch the disease, either because they have permanently recovered, are naturally immune, or have already died from the disease.*

The SIR model models the changes in the number of people in each compartment over time.

- The only possible movements *between* compartments are:
  - A susceptible person can become infected; and
  - An infected person can become removed.



- The model also assumes that:
  - there are no births, or deaths from other causes, so the population size is constant (apart from disease-related deaths); and
  - the population mixes homogeneously, so susceptible, infected and removed individuals mix equally.

- For any given disease there can be significant variation between how long different individuals take to recover, and how many other people they will infect. However, it is usually possible to estimate representative or "average" values for each of these quantities.

Basic reproduction number

The **basic reproduction number** *of a disease, written R_0, is the average number of secondary infections caused by a single infected individual in a completely susceptible population, in the absence of any preventive interventions.*

The value of R_0 is determined by such factors as how infectious the disease is, how homogeneously the population mixes and the duration of the infectious period.

***Example** 17.1.2* For rubella, the infectious period is typically 2 weeks and on average an infected individual will infect five other people in a completely susceptible population, so $R_0 \approx 5$.

- When developing the equations for the SIR model, it is useful to define two additional concepts:
  - the **infection rate** is defined to equal the basic reproduction number divided by the infectious period; and
  - the **recovery rate** is defined to equal 1 divided by the infectious period.

***Example** 17.1.3* For rubella, the infection rate is 2.5 people per week and the recovery rate is 0.5 per week.

These concepts make sense. For rubella, on average an infected person will infect 5 additional people in 2 weeks. Hence this individual infects 2.5 people per week on average while they are sick, and each week they "half recover".

The equations for the SIR model

If a population of N people at time t is divided into three compartments, susceptible $S(t)$, infected $I(t)$ and removed $R(t)$, then the SIR model states:

$$
\begin{aligned}
S' &= -\frac{a}{N}\,SI \\
I' &= \frac{a}{N}\,SI - bI \\
R' &= b\,I
\end{aligned}
$$

where a is the infection rate and b is the recovery rate.

Question *17.1.4* Explain carefully, in words, what each of the terms in each of the SIR equations represents.

***Question** 17.1.5* Assume that everyone in a population of 10000 people is susceptible to rubella. Ten people become infected on a group vacation and return while infective. Recall that the infectious period for rubella is 2 weeks and $R_0 \approx 5$.

(a) Draw a rough sketch of your prediction of the shapes of the graphs of $S(t)$, $I(t)$ and $R(t)$ over a period of 30 weeks.

(b) What do you think is the peak number of infected people at any time, and when will this occur?

(c) How many people do you think will be in each compartment S, I and R after 30 weeks?

- Note that the SIR equations keep the same total population size at all times (because the rate of movement between compartments all balance).
- An epidemic occurs if introducing a group of infected people to a population causes the number of infectives to increase.
- The SIR model predicts that an epidemic will occur if at $t = 0$, $I' > 0$ (that is, the number of infectives is increasing).
- Simple algebra shows that $I' > 0$ at time 0 if the fraction of the total population that is susceptible is more than b/a.
- (This is identical to saying that the proportion of susceptibles in the population is more than $1/R_0$, where R_0 is the basic reproduction number.)

***Example** 17.1.6* For rubella,

$$\begin{aligned} \text{the infection rate } a &= 2.5 \text{ week}^{-1}; \text{ and} \\ \text{the recovery rate } b &= 0.5 \text{ week}^{-1}. \end{aligned}$$

The fraction $b/a = 0.5/2.5 = 0.2$. (Alternately, $1/R_0 = 1/5 = 0.2$.)

Hence if more than 20% of an initial population is susceptible to rubella and infected individuals enter the population then we expect an epidemic to occur.

***Question** 17.1.7* Explain intuitively **why** an epidemic will occur if a fraction of more than $1/R_0$ of a population is susceptible.

***Question** 17.1.8* What is the purpose of a vaccination campaign? (This question may be a little less obvious than it looks.)

***Example** 17.1.9* Now we can write equations for modelling a rubella epidemic. Using the values of a and b from above, and taking the population of 10000 susceptible people with 10 infectives from Question 17.1.5, the SIR equations are:

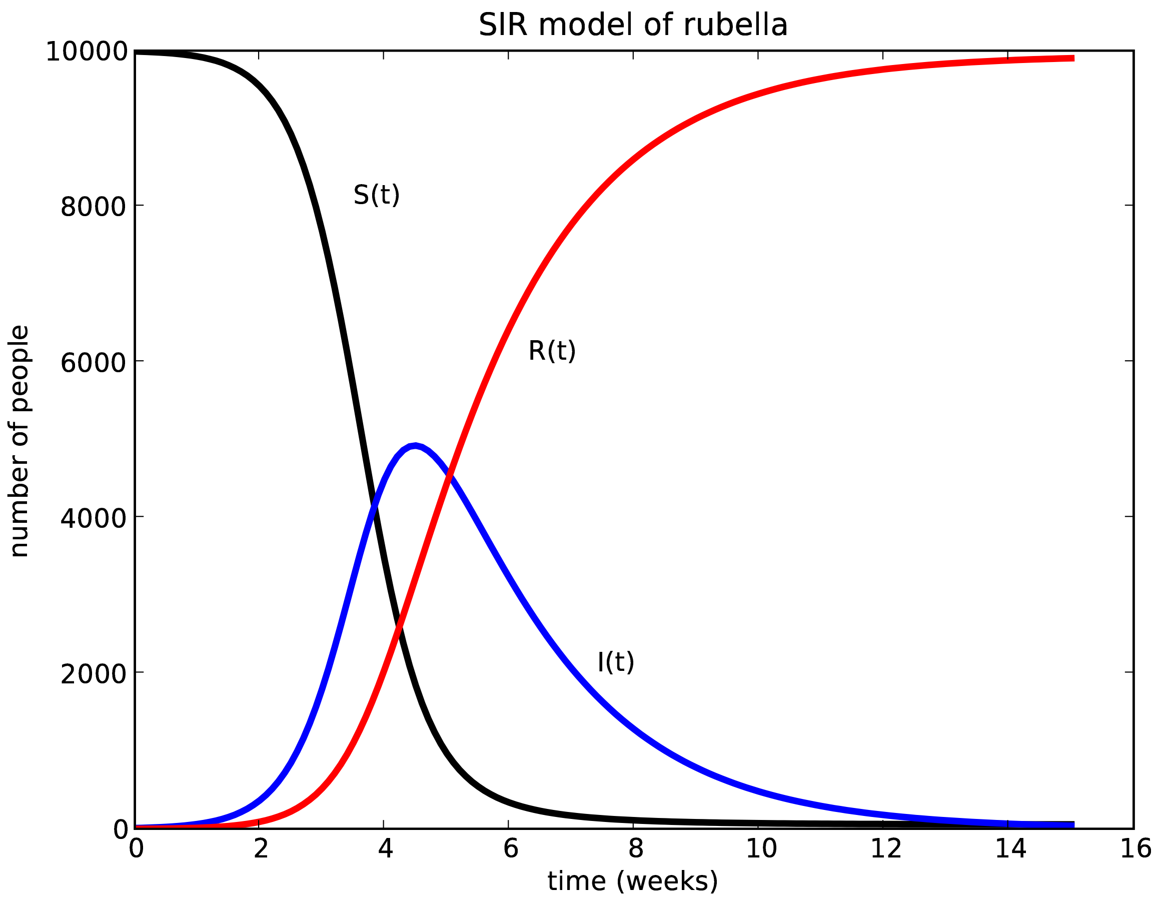
$$\begin{aligned} S' &= -\frac{2.5}{10000} SI \\ I' &= \frac{2.5}{10000} SI - 0.5I \\ R' &= 0.5I \end{aligned}$$

where $I(0) = 10$, $S(0) = 9990$ and $R(0) = 0$.

Because the proportion of susceptibles is more than 0.2, in this case we would expect an epidemic to occur.

- Just as with the Lotka-Volterra equations, it is not possible to find a general solution to the SIR equations. However, we can use Euler's method to find an approximate solution.

***Example** 17.1.10* Consider the population of 10000 people, with 10 infectives. Euler's method was used to predict the spread of rubella through the population over 16 weeks, commencing when the 10 infected individuals entered the population. The graph shows the predicted numbers of susceptibles $S(t)$, infectives $I(t)$ and removed people $R(t)$.



From the graph we notice that:

- An epidemic occurs, and lasts for about 14 weeks.
- The peak number of infectives at any time is 4925 individuals, which occurs at time 4.4 weeks.
- Almost everybody becomes infected over time, although a small number never become infected.

Question *17.1.11* The SIR model predicted that 56 people **never** become infected.

(a) Does this accurately reflect what happens in practice?

(b) This leads to an interesting question: what causes the end of an epidemic, a lack of infectives or a lack of susceptibles?

(c) Earlier, we said that the SIR model predicts an epidemic will occur whenever the proportion of susceptibles in a population is greater than b/a, where b is the recovery rate and a is the infection rate. Suggest some strategies which might be used to prevent an epidemic or reduce its severity or duration.

- The SIR model can also be applied when some individuals have been vaccinated against a disease, so are not susceptible.
- The model is applied by placing such people in the removed compartment at time 0, rather than in the susceptible compartment.
- Applying the model with different parameters allows predictions to be made about the impact of different vaccination rates on the potential spread of disease in an outbreak.

***Example** 17.1.12* Consider a population of 10000 people with 10 infectives.

If no people are vaccinated, then we saw in Example 17.1.10 that:

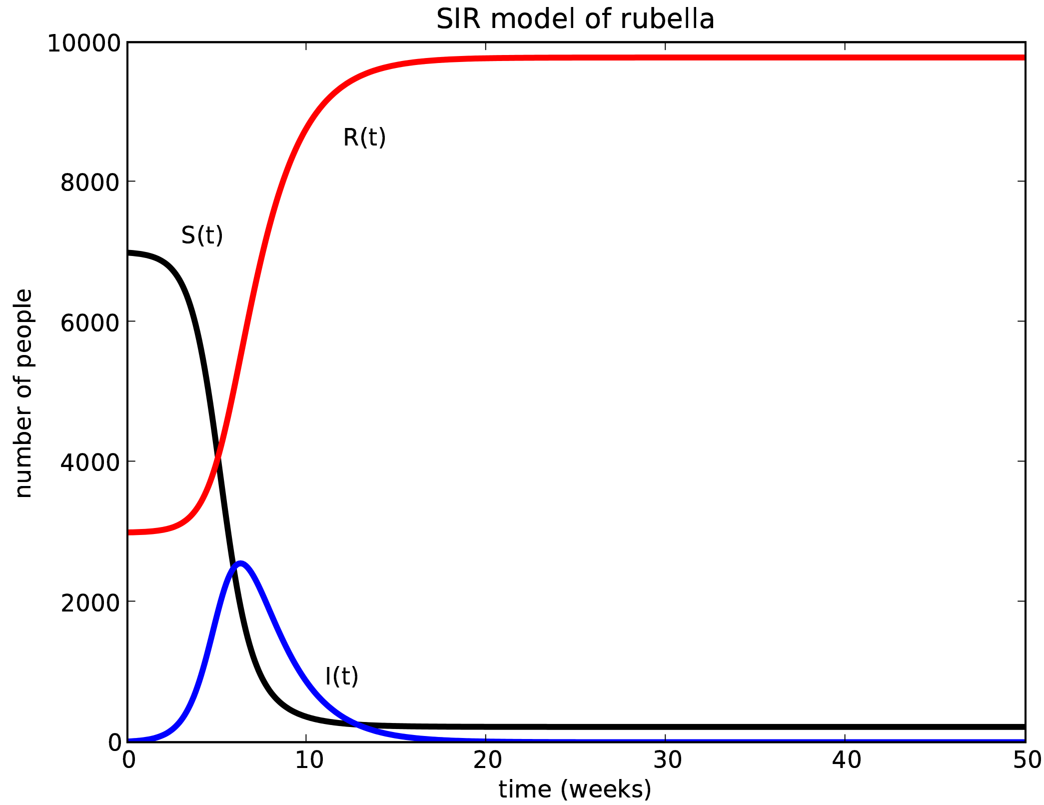
- the peak number of people infected at any time, I_{peak}, is 4925;
- the time in weeks at which this occurs, t_{peak}, is 4.4 weeks after the infectives entered the population;
- the total number of people infected by the outbreak, I_{tot}, is 9944; and
- the number of susceptible people who never become infected, S_{final}, is 56.

Euler's method was used to predict the impact of different population-wide rubella vaccination rates. The following graphs show the predicted values of $S(t)$, $I(t)$ and $R(t)$ for vaccination rates of 30% (first graph) and 70% (second graph).

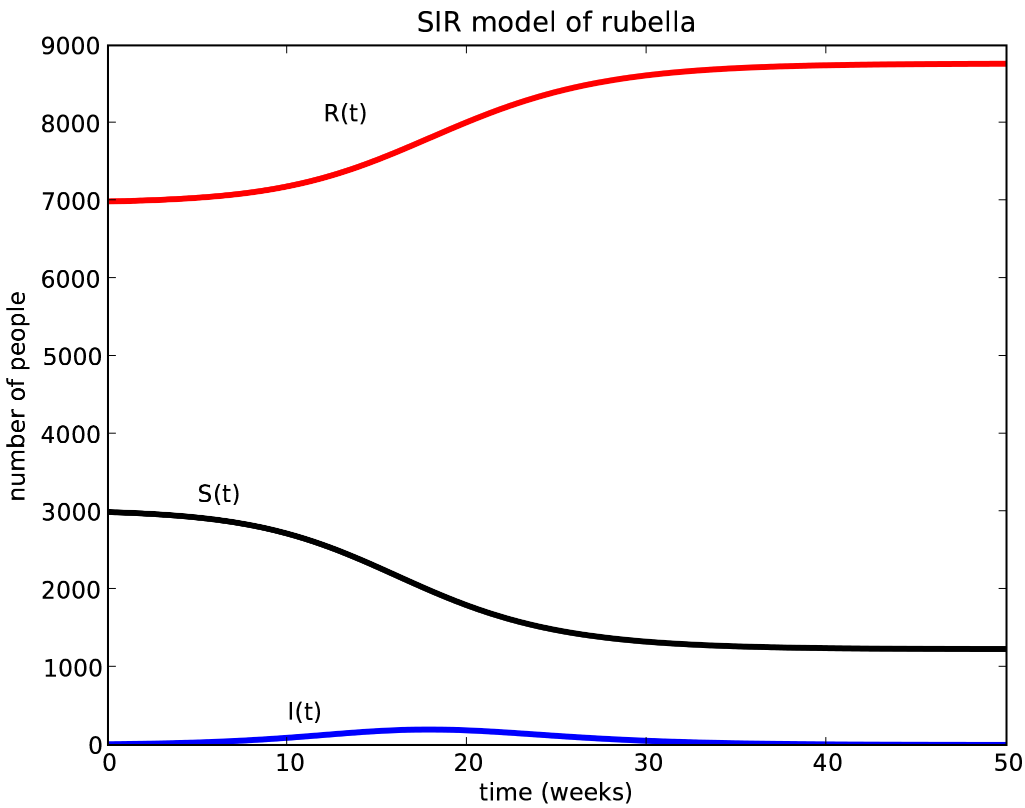
continued...

Example *17.1.12 (continued)*

30% vaccination rate:



70% vaccination rate:



Question *17.1.13* With respect to the predictions about rubella outbreaks with no vaccinations (Example 17.1.10), 30% vaccination rates and 70% vaccination rates (Example 17.1.12):

(a) Describe the key differences between the predictions.

(b) What would be the practical benefits of achieving high vaccination rates?

Example 17.1.14 Some additional predictions about possible rubella outbreaks are shown in the following table, again for a population of 10000 individuals with 10 infectives.

In each case, V is the percentage of the population vaccinated, I_{peak} is the peak number of infected people at any time, t_{peak} is the time in weeks at which this occurs, I_{tot} is the total number of people who become infected over the 50 week period, and S_{final} is the number of susceptible people who never become infected.

V (%)	I_{peak} (people)	t_{peak} (weeks)	I_{tot} (people)	S_{final} (people)
0	4925	4.4	9944	56
10	4102	4.8	8911	89
20	3300	5.4	7860	140
30	2550	6.2	6782	218
40	1844	7.3	5663	337
50	1193	8.9	4482	518
60	629	11.7	3204	796
70	199	17.8	1766	1234
80	10	0	170	1830

Recall that the recovery rate for rubella is $b = 0.5$ week^{-1} and the infection rate is $a = 2.5$ week^{-1}. Hence $b/a = 0.2$, so we would expect an epidemic to occur while more than 20% of the population is initially susceptible.

As the table shows, epidemics of varying severity occurred until the vaccination rate reached 80%, at which point no epidemic occurred.

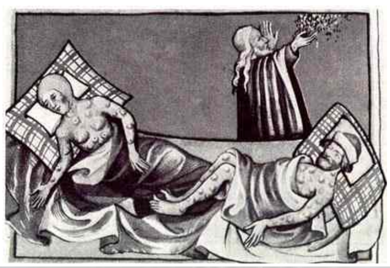
End of Case Study 34.

17.2 Catastrophes

- Many governments around the world conduct *catastrophe planning*, which uses sophisticated scientific and mathematical models to predict the potential impact(s) of disastrous events.
- Catastrophes typically include large-scale events such as nuclear explosions in major cities, severe terrorist strikes, giant tsunamis or earthquakes, and the widespread outbreak of serious disease.
- Much of this work is highly secret, partly for security reasons, but also because the scenarios and some of the outcomes predicted by the models are too frightening to release publicly.
- Recall that a *pandemic* is an epidemic that spreads over a very large area, such as multiple countries or even the whole world. There have been many severe (and famous) pandemics; the most recent one was swine flu in 2009, which was comparatively mild.

Example 17.2.1 In the 1300s, the bubonic plague or *Black Death* killed around 20 million Europeans in six years; this was about one third of the total population. In the worst-affected urban areas, around half the population died.

The plague returned regularly for around 400 years, with around 100 epidemics occurring in that time. The social, economic, humanitarian and psychological costs and disruption arising from these pandemics are incalculable and unimaginable today.



Example 17.2.2 The Spanish Flu, which occurred in 1918–1919, spread to become a global pandemic. Within six months, 25 million people were dead, statistical life expectancy in the USA dropped by 10 years and it is generally accepted that more people died from the disease than from combat in the First World War. The flu was so virulent and deadly that it 'burnt itself out', disappearing completely within 18 months.

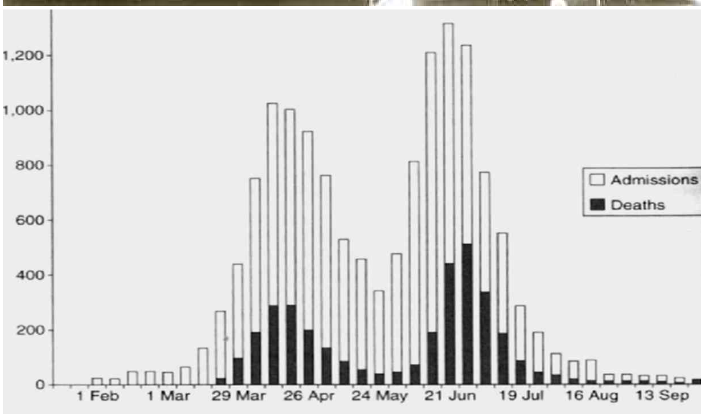
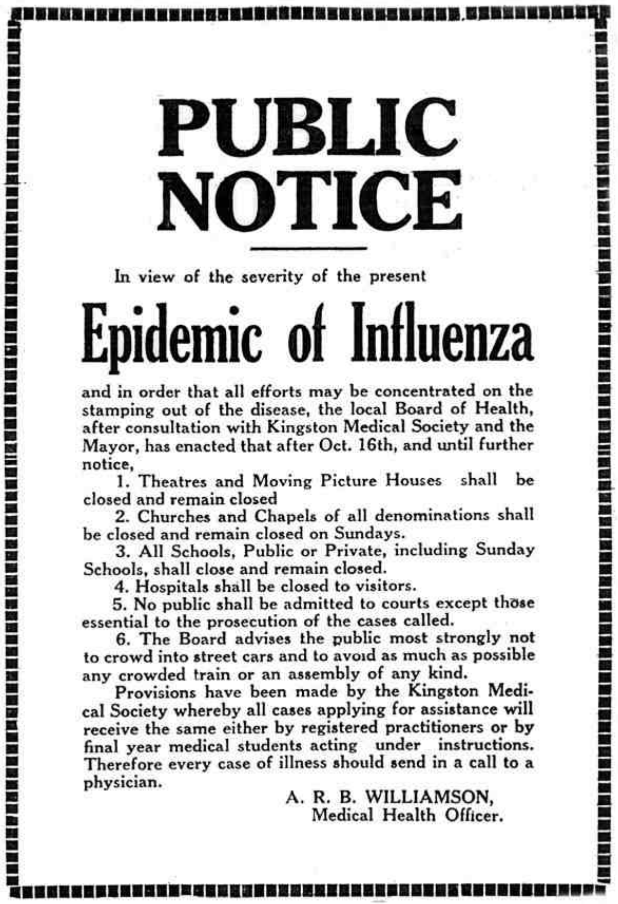


Figure 8.2 Hospital admissions and deaths from influenza, Sydney, 1919.



PUBLIC NOTICE

In view of the severity of the present

Epidemic of Influenza

and in order that all efforts may be concentrated on the stamping out of the disease, the local Board of Health, after consultation with Kingston Medical Society and the Mayor, has enacted that after Oct. 16th, and until further notice,

1. Theatres and Moving Picture Houses shall be closed and remain closed
2. Churches and Chapels of all denominations shall be closed and remain closed on Sundays.
3. All Schools, Public or Private, including Sunday Schools, shall close and remain closed.
4. Hospitals shall be closed to visitors.
5. No public shall be admitted to courts except those essential to the prosecution of the cases called.
6. The Board advises the public most strongly not to crowd into street cars and to avoid as much as possible any crowded train or an assembly of any kind.

Provisions have been made by the Kingston Medical Society whereby all cases applying for assistance will receive the same either by registered practitioners or by final year medical students acting under instructions. Therefore every case of illness should send in a call to a physician.

A. R. B. WILLIAMSON,
Medical Health Officer.

Extension 17.2.3 (From a letter written by Professor N R Grist in a camp infected by the disease, 29 September 1918.)

> "These men start with what appears to be an ordinary attack of LaGrippe or Influenza, and when brought to the Hosp. they very rapidly develop the most viscous type of Pneumonia that has ever been seen. Two hours after admission they have the Mahogany spots over the cheek bones, and a few hours later you can begin to see the Cyanosis extending from their ears and spreading all over the face, until it is hard to distinguish the coloured men from the white. It is only a matter of a few hours then until death comes, and it is simply a struggle for air until they suffocate. It is horrible."

Extension 17.2.4 (From ABC news, 30 December 2008)

"Study finds genes for 1918 'Spanish flu' pandemic

A US-Japanese research team has announced it had isolated three genes that explain why the 1918 Spanish flu, believed to be the deadliest infectious disease in history, was so lethal.

The pandemic killed between 20 and 50 million people - more than in all of World War I, which ended in November 1918 - and spread around the world.

The genes allowed the virus to reproduce in lung tissue, according to research published in the Proceedings of the National Academy of Sciences.

"Conventional flu viruses replicate mainly in the upper respiratory tract: the mouth, nose and throat," said University of Wisconsin-Madison virologist Yoshihiro Kawaoka, who co-authored the study along with Masato Hatta, also of UW-Madison.

"The 1918 virus replicates in the upper respiratory tract, but also in the lungs," causing primary pneumonia among its victims," Mr Kawaoka said.

"We wanted to know why the 1918 flu caused severe pneumonia," he added.

Autopsies of Spanish flu victims often revealed fluid-filled lungs severely damaged by massive haemorrhaging.

Virologists linked the virus' ability to invade the lungs with its high level of virulence, but the genes that conferred that ability were unknown, the researchers wrote.

The discovery of the three genes and how they help the virus infect the lungs is important because it could provide a way to quickly identify the potential virulence factors in new pandemic strains of influenza, Mr Kawaoka said.

The genes could also lead to a new class of antiviral drugs, which is urgently needed as vaccines are unlikely to be produced fast enough at the outset of a pandemic to blunt its spread, he added."

- The threat of pandemics has not disappeared; for example, the recent swine-flu outbreak was declared a global pandemic by the World Health Organisation.

Extension 17.2.5 (From ABC Radio program PM, 2/9/2008)

"**Worried scientists set up Australian biosecurity centre**

In the last few years we've had scares about SARS and bird flu, and the United States went through months of fear, in the wake of September 11th, that terrorists were spreading anthrax spores. Hendra virus has killed people and horses in Queensland, and horse flu did massive economic damage last year. It all comes under the umbrella of biosecurity.

Now a group of scientists is so concerned about Australia's potential vulnerability that they've joined forces to establish a National Centre for Biosecurity. They say advances in viral technology are way ahead of regulators. That means real threats which leave countries like Australia vulnerable to attacks and outbreaks…

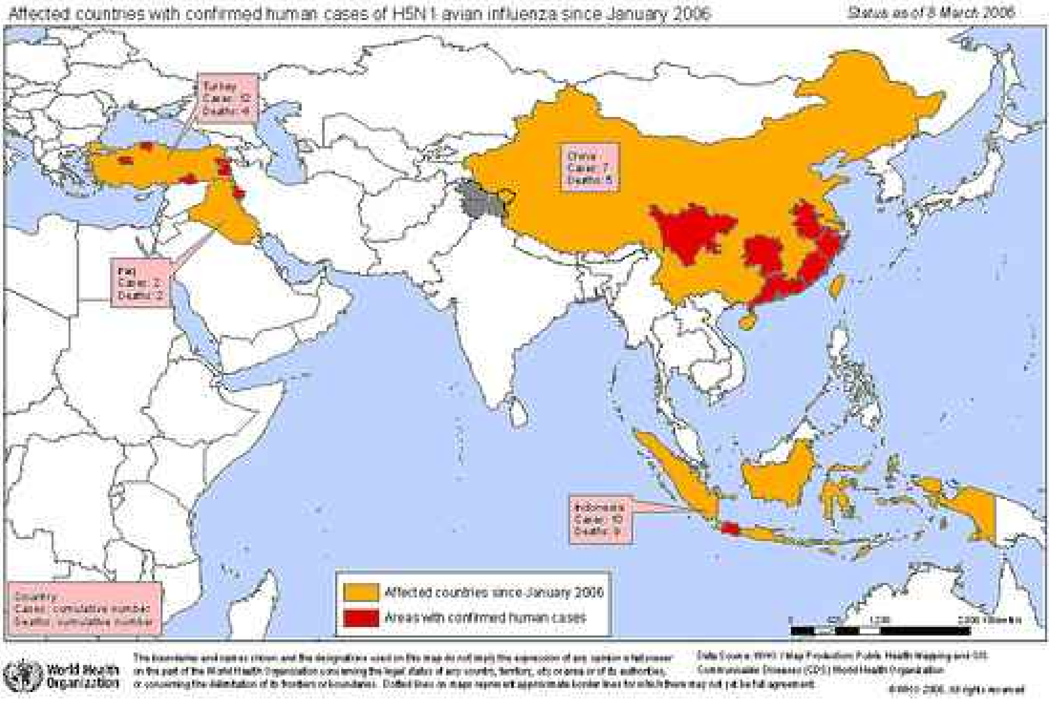
Remember SARS? There was an outbreak five years ago, several hundred people died, there was a wave of dire warnings about the possibility of a global disease outbreak. But then it just faded away and all those concerns seemed to dissipate…Sydney University professor of population and security, Peter Curson, was involved in the effort at the time and says it showed just how poorly prepared Australia is…

Professor Ian Ramshaw, from the Australian National University, says there'll be a broad range of specialists.

"So we have epidemiologists looking at spread, we've got mathematical modellers and so you know what happens when there's a pandemic. Research scientists, ethicist, we have a whole host of different disciplines with the centre, and that's what's required for biosecurity. No one discipline owns biosecurity. We need this variation, this think tank, this ability to research all these different areas to understand…

We'll know what happens if you model what happens with the pandemic influenza. We know whether to close schools or open them or isolate ourselves. We know in terms of bio-terrorism, what the bio-terrorists may want to use…' "

Case Study 35:
Avian influenza



- So far there have been no verified cases of human-to-human transmissible avian influenza. However, a focus of international catastrophe planning relates to the *possibility* of a pandemic occurring.

Extension *17.2.6* (From World Health Organisation publications.)

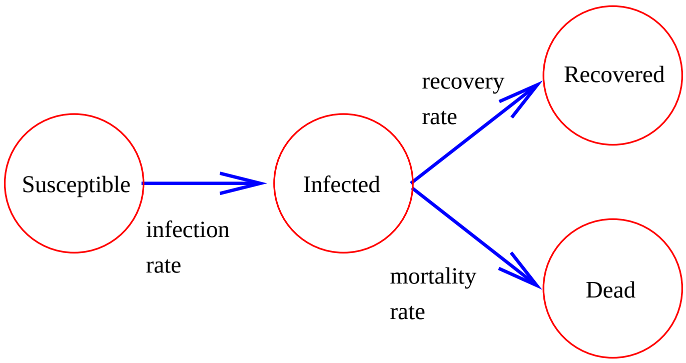
"WHO is coordinating the global response to human cases of H5N1 avian influenza and monitoring the corresponding threat of an influenza pandemic...

Since the last pandemic in 1968/69, the risk of an influenza pandemic has never been considered greater than at the present time. As of the date of this document, H5N1 is endemic in birds in many parts of the world. The widespread persistence of H5N1 in bird populations poses two main risks to human health. The first is the risk of infection when the virus spreads directly from birds to humans. The second risk, which is of even greater concern, is that there will be increased possibilities for the widely circulating virus to infect humans and possibly reassort into a strain that is both highly infectious for humans and spreads easily from human to human. Such a change could mark the start of a pandemic."

- Assume that the Australian government wants to prepare for a possible human-transmissible avian influenza pandemic.
- They require a model that predicts how the disease would spread over time in a city of one million people (such as Brisbane), including how many people will be infected over time, and how many people are likely to die.
- For catastrophe planning we will build a model which divides the population into **four** distinct compartments:

(1) Susceptible, $S(t)$	(2) Infected, $I(t)$
(3) Recovered, $R(t)$	(4) Dead, $D(t)$

- The only possible movements *between* compartments are:
  - a susceptible person can become infected; and
  - an infected person can either recover or die.



- When building a hypothetical model such as this, it is important to choose realistic values for the model parameters.
- For this example, we will use the following values; these are the estimated values for the Spanish Flu pandemic in 1918–1919:

$$\begin{aligned} a &= \text{the infection rate} \\ &= 1.9 \text{ week}^{-1}; \end{aligned}$$

$$\begin{aligned} b &= \text{the recovery rate} \\ &= 1.4 \text{ week}^{-1}; \text{ and} \end{aligned}$$

$$\begin{aligned} c &= \text{the flu-induced mortality rate} \\ &= 0.065 \text{ week}^{-1}. \end{aligned}$$

Example 17.2.7 Then the equations of the catastrophe model are:

$$S' = -a \frac{S}{(N-D)} I \tag{1}$$

$$I' = a \frac{S}{(N-D)} I - (c+b) I \tag{2}$$

$$R' = b I \tag{3}$$

$$D' = c I \tag{4}$$

where N is the total initial population size, so $N = S + I + R + D$.

Question 17.2.8 Explain the differences between the equations in Example 17.2.7 and the equations in the (standard) SIR model.

(1)

(2)

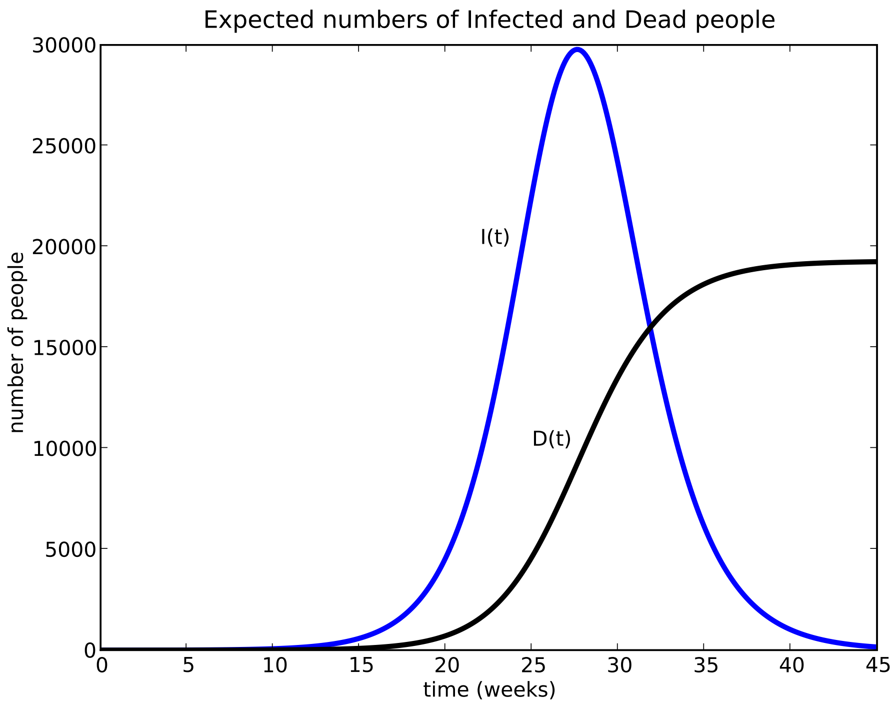
(3)

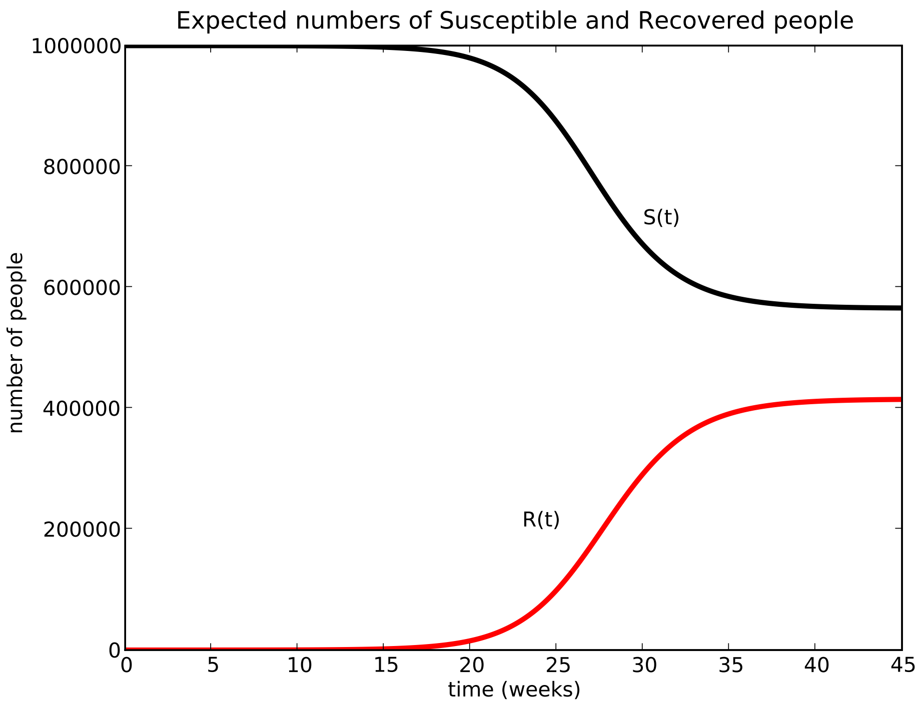
(4)

- Having formulated a model, we can use Euler's method to computationally simulate various scenarios in a city such as Brisbane with $N = 10^6$.

Example 17.2.9 One infected person arrives in a city in which $N = 10^6$ and everyone is susceptible.

Results: For this scenario, the model predicts that the disease outbreak will last for about 45 weeks, around 435,000 people will become ill, the largest number of infected people at any time is about 29,800, and that approximately 19,200 people will die.





- When studying rubella, we calculated that if a sufficient fraction of the population were vaccinated then no epidemic occurs. A similar approach can be used here.

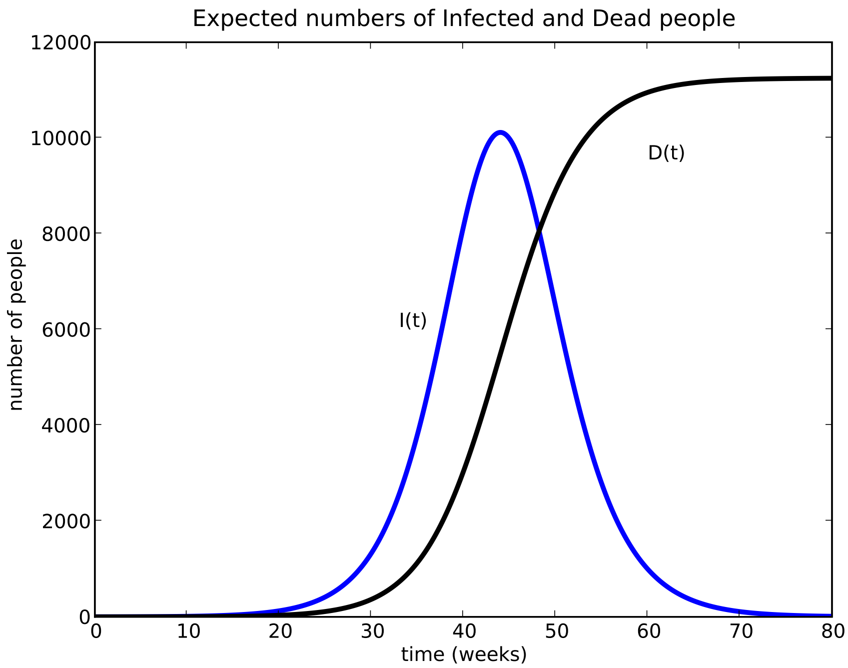
***Example** 17.2.10* When we studied the SIR model we saw that the fraction of the population that needs to be vaccinated to prevent an epidemic is $1 - b/a$. This new model includes the additional compartment "Dead", so the fraction of the population that should be vaccinated is

$$1 - \frac{b+c}{a} \approx 23\%.$$

To allow a safety margin, the aim could be to vaccinate about 30% of the population, or 300,000 people. The model verifies that in this case, almost nobody dies.

However, perhaps financial or time constraints mean it is not feasible to vaccinate that many people (and it is generally accepted that this would be the case in most countries).

If 100,000 people are vaccinated, the model shows that the death rate drops by about half, the peak number of infections at any time drops by about two thirds, and the outbreak lasts longer.

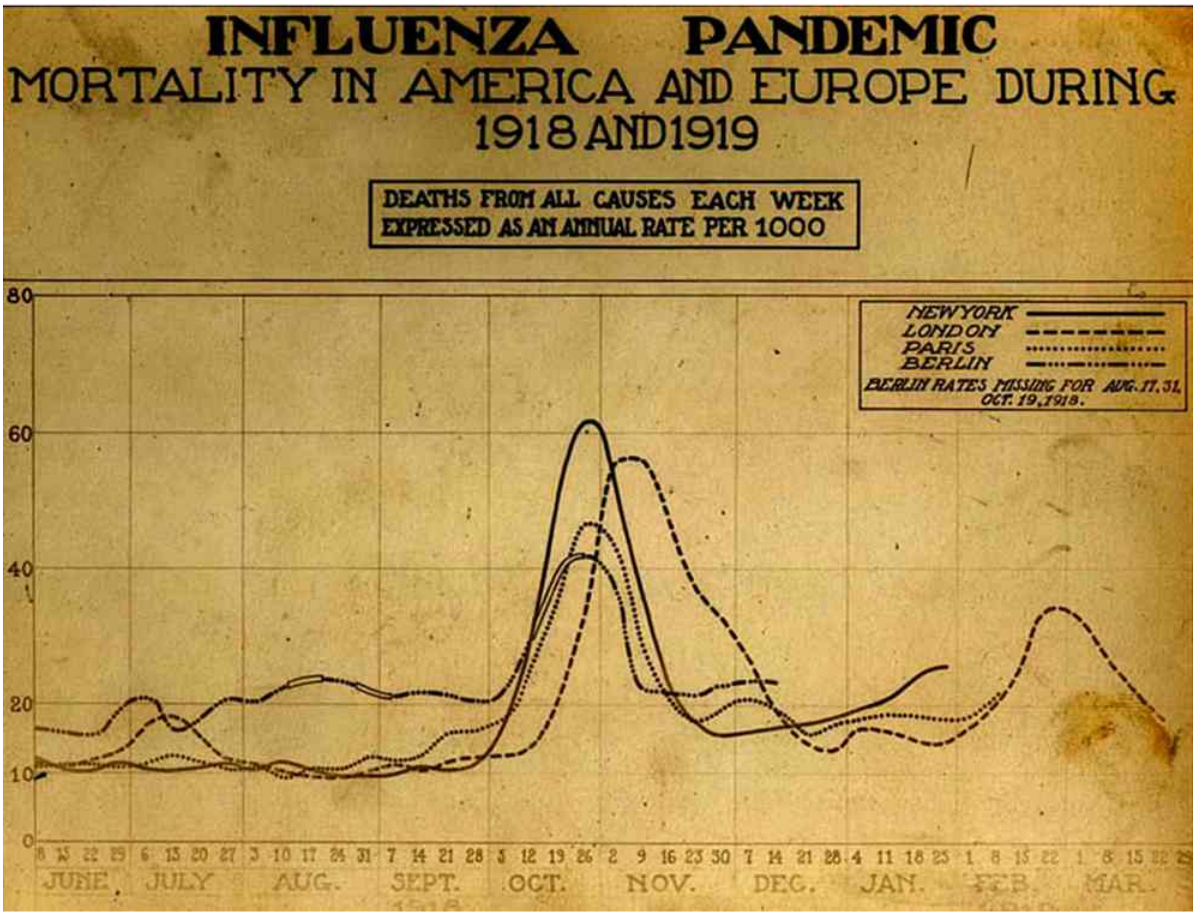


Question *17.2.11* The capital city of Malaysia is Kuala Lumpur. The city population is about 1.8 million, located within a regional population of more than 7 million. Malaysia is a densely populated, rapidly modernising, third-world country. How would your model change if the Malaysian government asked you to apply it to a possible outbreak of avian influenza in Kuala Lumpur? Explain your answer.

Avian influenza *(continued)*

***Example** 17.2.12* Of course, our catastrophe model for avian influenza is purely speculative. Is it realistic?

For comparison, the following graph shows the mortality rate (per thousand population) for the Spanish flu in several cities in 1918−1919. The impact of the Spanish flu is very clear, and the graphs are of similar shape to those in our catastrophe model.



- Our catastrophe model predicts an overall infection rate of 45% and a mortality rate of 4.2% of infected people.
- For the Spanish flu, infection rates reached around 50%, with mortality rates ranging from 2% to 5%.
- Comparison of both scenarios shows that the catastrophe model that we have presented is (at least) plausible. (Perhaps we all should be very afraid, or least stop missing poultry!)

End of Case Study 35.

17.3 Space for additional notes