Computational Mathematics II (MATH2731)

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Introduction

Welcome to Computational Mathematics II!

This course aims to help you build skills and knowledge in using modern computational methods to do and apply mathematics. It will involve a blend of hands-on computing work and mathematical theory—this theory will include aspects of numerical analysis, computational algebra, and other topics within scientific computing. These areas consist of studying the mathematical properties of the computational representations of mathematical objects (numerical values as well as symbolic manipulations). The computing skills developed in this module will be valuable in all subsequent courses in your degree at Durham and well beyond. We will also introduce you to the use (and abuse) of various computational tools invaluable for doing mathematics, such as AI and searchable websites. While we will encourage you throughout to use all the tools at your disposal, it is **imperative that you understand the details and scope of what you are doing!** You will also develop your communication, presentation, and group-work skills through the various assessments involved in the course – more on that below!

This module has **no final exam**. In fact, there are no exams of any kind. Instead, the summative assessment and associated final grade are entirely based on coursework undertaken during the term. This means that you should expect to spend more time on this course during the term relative to your other modules. We believe this workload distribution is a better way to train the skills we are trying to develop, and as a bonus, you will not need to worry about this course any further once the term ends!

Content

The module's content is divided into six chapters of roughly equal length; some will focus slightly more on theory, while others have a more practical and hands-on nature.

- **Chapter 1: Introduction to Computational Mathematics**
  - Programming basics (including GitHub, and numerical versus symbolic computation)
  - LaTeX, Overleaf, and presenting lab reports
  - Finite-precision arithmetic, rounding error, symbolic representations

- **Chapter 2: Continuous Functions**
  - Interpolation using polynomials – fitting curves to data (Lagrange polynomials, error estimates, convergence, and Chebyshev nodes)
  - Solving nonlinear equations (bisection, fixed-point iteration, Newton's method)
- **Chapter 3: Linear Algebra**
  - Solving linear systems numerically (LU decomposition, Gaussian elimination, conditioning) and symbolically
  - Applications: PageRank, computer graphics
- **Chapter 4: Calculus**
  - Numerical differentiation (finite differences)
  - Numerical integration (quadrature rules, Newton-Cotes formulae)
- **Chapter 5: Ordinary Differential Equations (ODEs)**
  - Numerically approximating solutions of ODEs
  - Timestepping: explicit and implicit methods
  - Stability and convergence order
- **Chapter 6: Selected Further Topics**
  - Intro. to random numbers and stochastic processes
  - Intro. to partial differential equations

Weekly workflow and summative assessment

The final grade for this module is determined as follows:

- **Weekly lab reports (weeks 1-6)** – 20%
- **Weekly e-assessments (weeks 1-6)** – 30%
- **Project (weeks 7-10)** – 50%

Lab reports

Each week for the first six weeks of the course, we will release a short set of exercises based on the lectures from the previous week. Students will be expected to submit a brief report (1-2 pages A4, including figures) with their solutions to the set of exercises – the report will consist of written answers and figures/plots. The reports will be evaluated for correctness and quality of the presentation and communication (quality of figures, clarity of argumentation, etc.).

The lab report for a given week will be due at noon on Monday of the following week (e.g., week one's lab report is due on Monday of week two and so on). Solutions and generalised feedback will be provided to the class on common mistakes and issues arising in each report. Students can also seek detailed feedback on their submission from the lecturers during drop-in sessions and office hours. There will be six lab reports in total, and **your mark is based on your four highest-scoring submissions.**

E-assessments

Each week for the first six weeks of the course, we will release an e-assessment based on the lectures from the previous week. These exercises are designed to complement the lab reports by focusing exclusively on coding skills. The e-assessments will involve submitting code auto-marked by an online grading tool, and hence give immediate feedback. As with the lab reports, **the e-assessment for a given week will be due at noon on Monday of the following week**. There will be six e-assessments in total, and **your mark is based on your four highest-scoring submissions.**

Project

The single largest component of the assessment for this module is the project. **Weeks 7-10 of this course focus exclusively on project work with lectures ending in Week 6.** We will be releasing more detailed instructions on the project submission format and assessment criteria separately, but briefly, the main aspects of the project are as follows:

- There will be approximately eight different project options to choose from across different areas of mathematics (e.g., pure, applied, probability, mathematical physics, etc.); each project has a distinct member of the Maths Department as supervisor.
- Students will submit their preferred project options (ranked choice preferences) in Week 4 of the term and be allocated to projects by the end of Week 6 (there are maximum subscription numbers for each option to ensure equity of supervision).
- Each project consists of two parts: a **guided component** that is completed as part of a small group and an **extension component** that is open-ended and completed as an individual. Group allocations will be done by the lecturers.
- Each group will jointly submit a five-page report for the guided component of the project, and this is worth 60% of the project grade.
- Each student will also submit a three-page report and a six-minute video presentation on their extension component. This submission is worth 40% of the project grade.

In Weeks 7-10 of the term, lectures will be replaced by project workshop sessions during which students can discuss their project with the designated supervisor. This will be an opportunity to discuss progress, ask questions, and seek clarification. Each student only needs to attend the one project drop-in weekly session relevant to their project. Computing drop-in sessions will

continue as scheduled in the first six weeks to provide additional support for coding pertinent tasks for the projects – there will be two timetabled computing drop-ins per week and students are encouraged to attend at least one of them.

Lectures, computing drop-ins & project workshops

Lectures will primarily present, explain, and discuss new material (especially theory), but will also feature computer demonstrations of the algorithms and numerical methods. As such, students are encouraged to bring their laptops to lectures to run the examples themselves. Students must bring a laptop or device capable of running code to the computer drop-ins to work on the e-assessments and lab reports.

	Activities	Content
Week 1	Introductory lecture, 2 lectures	Chapter 1
Week 2	3 lectures, 1 computing drop-in	Chapter 2
Week 3	3 lectures, 1 computing drop-in	Chapter 3
Week 4	3 lectures, 1 computing drop-in	Chapter 4
Week 5	3 lectures, 1 computing drop-in	Chapter 5
Week 6	3 lectures, 1 computing drop-in	Chapter 5/6
Week 7	0 lectures, 1 project workshop	Project
Week 8	0 lectures, 1 project workshop	Project
Week 9	0 lectures, 1 project workshop	Project
Week 10	0 lectures, 1 project workshop	Project

Contact details and Reading Materials

If you have questions or need clarification on any of the above, please speak to us during lectures, drop-in sessions, or office hours. Alternatively, email one or both of us at denis.d.patterson@durham.ac.uk or andrew.krause@durham.ac.uk.

The lecture notes are designed to be sufficient and self-contained. Hence, students do not need to purchase a textbook to complete the course successfully. References for additional reading will also be given at the end of each chapter.

The following texts may be useful supplementary references for students wishing to read further into topics from the course:

- Burden, R. L., & Faires, J. D. (1997). *Numerical Analysis* (6th ed.). Pacific Grove, CA: Brooks/Cole Publishing Company.
- Süli, E., & Mayers, D. F. (2003). *An Introduction to Numerical Analysis*. Cambridge: Cambridge University Press.

Acknowledgements

We are indebted to Prof. Anthony Yeates (Durham) whose numerical analysis notes formed the basis of several chapters of the coures notes.

1 Floating Point Arithmetic

The goal of this chapter is to explore and begin to answer the following question:

> *How do we represent numbers on a computer?*

Integers can be represented exactly, up to some maximum size.

If 1 bit (binary digit) is used to store the sign $\pm$, the largest possible number is

$$1 \times 2^{62} + 1 \times 2^{61} + \ldots + 1 \times 2^1 + 1 \times 2^0 = 2^{63} - 1.$$

In contrast to the integers, only a subset of real numbers within any given interval can be represented exactly.

> **Note**
>
> Some modern languages (such as Python) automatically promote large integers to arbitrary precision ("long"), but most statically-typed languages (C, Java, Matlab, etc.) do not; an **overflow** will occur and the type remains fixed.

> **Note**
>
> A statically typed language is one in which the type of every variable is determined before the program runs.

1.1 Fixed-point numbers

In everyday life, we tend to use a **fixed point** representation

$$x = \pm(d_1 d_2 \cdots d_{k-1}.d_k \cdots d_n)_\beta, \quad \text{where} \quad d_1, \ldots, d_n \in \{0, 1, \ldots, \beta - 1\}.$$

Here β is the base (e.g. 10 for decimal arithmetic or 2 for binary).

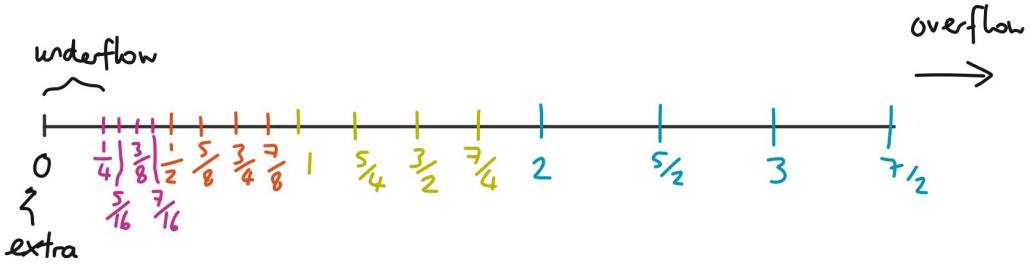
If we require that $d_1 \neq 0$ unless $k = 2$, then every number has a unique representation of this form, except for infinite trailing sequences of digits $\beta - 1$.

1.2 Floating-point numbers

Computers use a **floating-point** representation. Only numbers in a **floating-point number system** $F \subset \mathbb{R}$ can be represented exactly, where

$$F = \{ \pm (0.d_1 d_2 \cdots d_m)_\beta \beta^e \mid \beta, d_i, e \in \mathbb{Z},\ 0 \le d_i \le \beta - 1,\ e_{\min} \le e \le e_{\max} \}.$$

Here $(0.d_1 d_2 \cdots d_m)_\beta$ is called the **fraction** (or **significand** or **mantissa**), β is the base, and e is the **exponent**. This can represent a much larger range of numbers than a fixed-point system of the same size, although at the cost that the numbers are not equally spaced. If $d_1 \neq 0$ then each number in F has a unique representation and F is called **normalised**.



> **Note**
>
> Notice that the spacing between numbers jumps by a factor β at each power of β. The largest possible number is $(0.111)_2 2^2 = (\frac{1}{2} + \frac{1}{4} + \frac{1}{8})(4) = \frac{7}{2}$. The smallest non-zero number is $(0.100)_2 2^{-1} = \frac{1}{2}(\frac{1}{2}) = \frac{1}{4}$.

Here $\beta = 2$, and there are 52 bits for the fraction, 11 for the exponent, and 1 for the sign. The actual format used is

$$\pm(1.d_1 \cdots d_{52})_2 2^{e-1023} = \pm(0.1 d_1 \cdots d_{52})_2 2^{e-1022}, \quad e = (e_1 e_2 \cdots e_{11})_2.$$

When $\beta = 2$, the first digit of a normalized number is always 1, so doesn't need to be stored in memory. The **exponent bias** of 1022 means that the actual exponents are in the range -1022 to 1025, since $e \in [0, 2047]$. Actually the exponents -1022 and 1025 are used to store ± 0 and $\pm\infty$ respectively.

The smallest non-zero number in this system is $(0.1)_2 2^{-1021} \approx 2.225 \times 10^{-308}$, and the largest number is $(0.1 \cdots 1)_2 2^{1024} \approx 1.798 \times 10^{308}$.

> **Note**
>
> IEEE stands for Institute of Electrical and Electronics Engineers. Matlab uses the IEEE 754 standard for floating point arithmetic. The automatic 1 is sometimes called the "hidden bit". The exponent bias avoids the need to store the sign of the exponent.

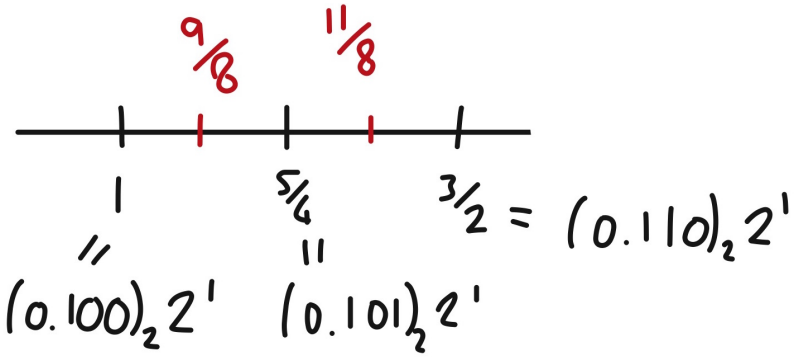
Numbers outside the finite set F cannot be represented exactly. If a calculation falls below the lower non-zero limit (in absolute value), it is called **underflow**, and usually set to 0. If it falls above the upper limit, it is called **overflow**, and usually results in a floating-point exception.

> **Note**
>
> **Ariane 5 rocket failure (1996):** The maiden flight ended in failure. Only 40 seconds after initiation, at altitude 3700m, the launcher veered off course and exploded. The cause was a software exception during data conversion from a 64-bit float to a 16-bit integer. The converted number was too large to be represented, causing an exception.

> **Note**
>
> In IEEE arithmetic, some numbers in the "zero gap" can be represented using $e = 0$, since only two possible fraction values are needed for ± 0. The other fraction values may be used with first (hidden) bit 0 to store a set of so-called **subnormal** numbers.

The mapping from $\mathbb{R}$ to F is called **rounding** and denoted $\mathrm{fl}(x)$. Usually it is simply the nearest number in F to x. If x lies exactly midway between two numbers in F, a method of breaking ties is required. The IEEE standard specifies *round to nearest even*—i.e., take the neighbour with last digit 0 in the fraction.

> **Note**
>
> This avoids statistical bias or prolonged drift.



$\frac{9}{8} = (1.001)_2$ has neighbours $1 = (0.100)_2 2^1$ and $\frac{5}{4} = (0.101)_2 2^1$, so is rounded down to 1.
$\frac{11}{8} = (1.011)_2$ has neighbours $\frac{5}{4} = (0.101)_2 2^1$ and $\frac{3}{2} = (0.110)_2 2^1$, so is rounded up to $\frac{3}{2}$.

> **Note**
>
> **Vancouver stock exchange index:** In 1982, the index was established at 1000. By November 1983, it had fallen to 520, even though the exchange seemed to be doing well. Explanation: the index was rounded *down* to 3 digits at every recomputation. Since the errors were always in the same direction, they added up to a large error over time. Upon recalculation, the index doubled!

1.3 Significant figures

When doing calculations without a computer, we often use the terminology of **significant figures**. To count the number of significant figures in a number x, start with the first non-zero digit from the left, and count all the digits thereafter, including final zeros if they are after the decimal point.

To round x to n s.f., replace x by the nearest number with n s.f. An approximation $\hat{x}$ of x is "correct to n s.f." if both $\hat{x}$ and x round to the same number to n s.f.

1.4 Rounding error

If $|x|$ lies between the smallest non-zero number in F and the largest number in F, then

$$\mathrm{fl}(x) = x(1+\delta),$$

where the relative error incurred by rounding is

$$|\delta| = \frac{|\mathrm{fl}(x) - x|}{|x|}.$$

> **Note**
>
> Relative errors are often more useful because they are scale invariant. E.g., an error of 1 hour is irrelevant in estimating the age of this lecture theatre, but catastrophic in timing your arrival at the lecture.

Now x may be written as $x = (0.d_1 d_2 \cdots)_\beta \beta^e$ for some $e \in [e_{\min}, e_{\max}]$, but the fraction will not terminate after m digits if $x \notin F$. However, this fraction will differ from that of $\mathrm{fl}(x)$ by at most $\frac{1}{2}\beta^{-m}$, so

$$|\mathrm{fl}(x) - x| \leq \tfrac{1}{2}\beta^{-m}\beta^e \quad \Longrightarrow \quad |\delta| \leq \tfrac{1}{2}\beta^{1-m}.$$

Here we used that the fractional part of $|x|$ is at least $(0.1)_\beta \equiv \beta^{-1}$. The number $\epsilon_{\mathrm{M}} = \frac{1}{2}\beta^{1-m}$ is called the **machine epsilon** (or **unit roundoff**), and is independent of x. So the relative rounding error satisfies

$$|\delta| \leq \epsilon_{\mathrm{M}}.$$

> **Note**
>
> To check the machine epsilon value in Matlab you can just type 'eps' in the command line, which will return the value 2.2204e-16.

> **Note**
>
> The name "unit roundoff" arises because β^{1-m} is the distance between 1 and the next number in the system.

When adding/subtracting/multiplying/dividing two numbers in F, the result will not be in F in general, so must be rounded.

Let us multiply $x = \frac{5}{8}$ and $y = \frac{7}{8}$. We have

$$xy = \tfrac{35}{64} = \tfrac{1}{2} + \tfrac{1}{32} + \tfrac{1}{64} = (0.100011)_2.$$

This has too many significant digits to represent in our system, so the best we can do is round the result to $\mathrm{fl}(xy) = (0.100)_2 = \frac{1}{2}$.

> **Note**
>
> Typically additional digits are used during the computation itself, as in our example.

For $\circ = +, -, \times, \div$, IEEE standard arithmetic requires rounded exact operations, so that

$$\mathrm{fl}(x \circ y) = (x \circ y)(1+\delta), \quad |\delta| \leq \epsilon_{\mathrm{M}}.$$

1.5 Loss of significance

You might think that the above guarantees the accuracy of calculations to within ϵ_{M}, but this is true only if x and y are themselves exact. In reality, we are probably starting from $\bar{x} = x(1+\delta_1)$ and $\bar{y} = y(1+\delta_2)$, with $|\delta_1|, |\delta_2| \leq \epsilon_{\mathrm{M}}$. In that case, there is an error even before we round the result, since

$$\begin{aligned} \bar{x} \pm \bar{y} &= x(1+\delta_1) \pm y(1+\delta_2) \\ &= (x \pm y)\left(1 + \frac{x\delta_1 \pm y\delta_2}{x \pm y}\right). \end{aligned}$$

If the correct answer $x \pm y$ is very small, then there can be an arbitrarily large relative error in the result, compared to the errors in the initial $\bar{x}$ and $\bar{y}$. In particular, this relative error can be much larger than ϵ_{M}. This is called **loss of significance**, and is a major cause of errors in floating-point calculations.

To 4 s.f., the roots are

$$x_1 = 28 + \sqrt{783} = 55.98, \quad x_2 = 28 - \sqrt{783} = 0.01786.$$

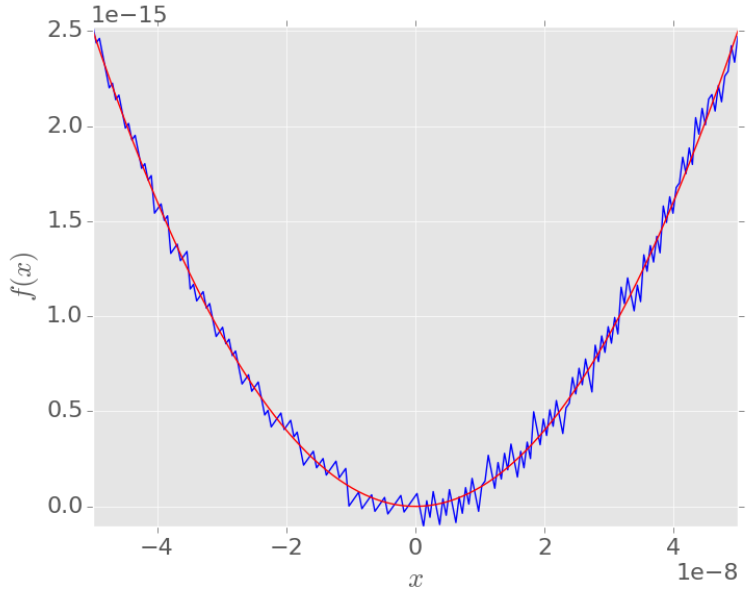
However, working to 4 s.f. we would compute $\sqrt{783} = 27.98$, which would lead to the results

$$\bar{x}_1 = 55.98, \quad \bar{x}_2 = 0.02000.$$

The smaller root is not correct to 4 s.f., because of cancellation error. One way around this is to note that $x^2 - 56x + 1 = (x - x_1)(x - x_2)$, and compute x_2 from $x_2 = 1/x_1$, which gives the correct answer.

> **Note**
>
> Note that the error crept in when we rounded $\sqrt{783}$ to 27.98, because this removed digits that would otherwise have been significant after the subtraction.

Let us plot this function in the range $-5 \times 10^{-8} \leq x \leq 5 \times 10^{-8}$ – even in IEEE double precision arithmetic we find significant errors, as shown by the blue curve:



The red curve shows the correct result approximated using the Taylor series

$$\begin{aligned} f(x) &= \left(1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \dots\right) - \left(1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \dots\right) - x \\ &\approx x^2 + \frac{x^3}{6}. \end{aligned}$$

This avoids subtraction of nearly equal numbers.

> **Note**
>
> We will look in more detail at polynomial approximations in the next section.

Note that floating-point arithmetic violates many of the usual rules of real arithmetic, such as $(a + b) + c = a + (b + c)$.

$$\begin{aligned} \text{fl}\big[(5.9 + 5.5) + 0.4\big] &= \text{fl}\big[\text{fl}(11.4) + 0.4\big] = \text{fl}(11.0 + 0.4) = 11.0, \\ \text{fl}\big[5.9 + (5.5 + 0.4)\big] &= \text{fl}\big[5.9 + 5.9\big] = \text{fl}(11.8) = 12.0. \end{aligned}$$

In $\mathbb{R}$, the average of two numbers always lies between the numbers. But if we work to 3 decimal digits,

$$\text{fl}\left(\frac{5.01 + 5.02}{2}\right) = \frac{\text{fl}(10.03)}{2} = \frac{10.0}{2} = 5.0.$$

The moral of the story is that sometimes care is needed to ensure that we carry out a calculation accurately and as intended!

Knowledge checklist

Key topics:

1. Integer and floating point representations of real numbers on computers.
2. Overflow, underflow and loss of significance.

Key skills:

- Understanding and distinguishing integer, fixed-point, and floating-point representations.
- Analyzing the effects of rounding and machine epsilon in calculations.
- Diagnosing and managing rounding errors, overflow, and underflow.

2 Continuous Functions

The goal of this chapter is to explore and begin to answer the following question:

How do we represent and manipulate continuous functions on a computer?

2.1 Interpolation

2.1.1 Polynomial Interpolation: Motivation

The main idea of this section is to find a polynomial that approximates a general function f. But why polynomials? Polynomials have many nice mathematical properties but from the perspective of function approximation, the key one is the following: Any continuous function on a compact interval can be approximated to arbitrary accuracy using a polynomial (provided you are willing to go high enough degree).

Theorem 2.1: Weierstrass Approximation Theorem (1885)

For any $f \in C([0,1])$ and any $\epsilon > 0$, there exists a polynomial $p(x)$ such that

$$\max_{0 \leq x \leq 1} |f(x) - p(x)| \leq \epsilon.$$

Note

This may be proved using an explicit sequence of polynomials, called Bernstein polynomials.

If f is a polynomial of degree n,

$$f(x) = p_n(x) = a_0 + a_1 x + \ldots + a_n x^n,$$

then we only need to store the $n+1$ coefficients $a_0, \ldots, a_n$. Operations such as taking the derivative or integrating f are also convenient. If f is not continuous, then something other than a polynomial is required, since polynomials can't handle asymptotic behaviour.

> **Note**
>
> To approximate functions like $1/x$, there is a well-developed theory of rational function interpolation, which is beyond the scope of this course.

In this chapter, we look for a suitable polynomial p_n by **interpolation**—that is, requiring $p_n(x_i) = f(x_i)$ at a finite set of points x_i, usually called **nodes**. Sometimes we will also require the derivative(s) of p_n to match those of f. This type of function approximation where we want to match values of the function that we know at particular points is very natural in many applications. For example, weather forecasts involve numerically solving huge systems of partial differential equations (PDEs), which means actually solving them on a discrete grid of points. If we want weather predictions between grid points, we must **interpolate**. Figure Figure 2.1 shows the spatial resolutions of a range of current and past weather models produced by the UK Met Office.

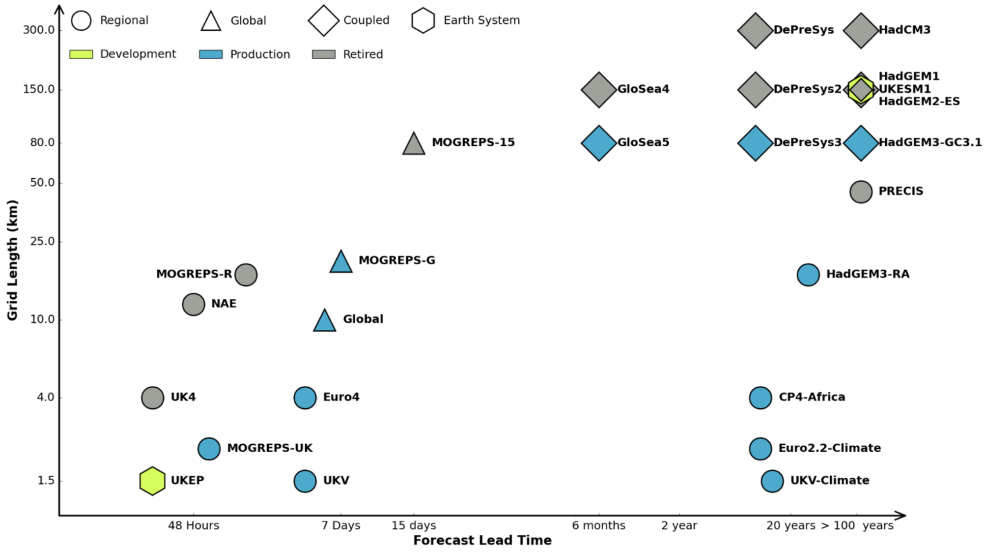


Figure 2.1: Chart showing a range of weather models produce by the UK Met Office. Even the highest spatial resolution models have more than 1.5km between grid point due to computational constraints.

2.1.2 Taylor series

A truncated Taylor series is (in some sense) the simplest interpolating polynomial since it uses only a single node x_0, although it does require p_n to match both f and some of its derivatives.

We can approximate this using a Taylor series about the point $x_0 = 0$, which is

$$\sin(x) = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \dots.$$

This comes from writing

$$f(x) = a_0 + a_1(x - x_0) + a_2(x - x_0)^2 + \dots,$$

then differentiating term-by-term and matching values at x_0:

$$\begin{aligned}
f(x_0) &= a_0, \\
f'(x_0) &= a_1, \\
f''(x_0) &= 2a_2, \\
f'''(x_0) &= 3(2)a_3, \\
&\vdots \\
\implies f(x) &= f(x_0) + f'(x_0)(x - x_0) + \frac{f''(x_0)}{2!}(x - x_0)^2 + \frac{f'''(x_0)}{3!}(x - x_0)^3 + \dots.
\end{aligned}$$

So

$$\begin{aligned}
\text{1 term} &\implies f(0.1) \approx 0.1, \\
\text{2 terms} &\implies f(0.1) \approx 0.1 - \frac{0.1^3}{6} = 0.099833\dots, \\
\text{3 terms} &\implies f(0.1) \approx 0.1 - \frac{0.1^3}{6} + \frac{0.1^5}{120} = 0.09983341\dots.
\end{aligned}$$

The next term will be $-0.1^7/7! \approx -10^{-7}/10^3 = -10^{-10}$, which won't change the answer to 6 s.f.

> **Note**
>
> The exact answer is $\sin(0.1) = 0.09983341$.

Mathematically, we can write the remainder as follows.

Theorem 2.2: Taylor's Theorem

Let f be $n+1$ times differentiable on (a, b), and let $f^{(n)}$ be continuous on $[a, b]$. If $x, x_0 \in [a, b]$ then there exists $\xi \in (a, b)$ such that

$$f(x) = \sum_{k=0}^{n} \frac{f^{(k)}(x_0)}{k!}(x - x_0)^k + \frac{f^{(n+1)}(\xi)}{(n+1)!}(x - x_0)^{n+1}.$$

The sum is called the **Taylor polynomial** of degree n, and the last term is called the **Lagrange form** of the remainder. Note that the unknown number ξ depends on x.

For $f(x) = \sin(x)$, we found the Taylor polynomial $p_6(x) = x - x^3/3! + x^5/5!$, and $f^{(7)}(x) = -\sin(x)$. So we have

$$|f(x) - p_6(x)| = \left| \frac{f^{(7)}(\xi)}{7!}(x - x_0)^7 \right|$$

for some ξ between x_0 and x. For $x = 0.1$, we have

$$|f(0.1) - p_6(0.1)| = \frac{1}{5040}(0.1)^7 |f^{(7)}(\xi)| \quad \text{for some } \xi \in [0, 0.1].$$

Since $|f^{(7)}(\xi)| = |\sin(\xi)| \leq 1$, we can say, before calculating, that the error satisfies

$$|f(0.1) - p_6(0.1)| \leq 1.984 \times 10^{-11}.$$

Note

The actual error is 1.983×10^{-11}, so this is a tight estimate.

Since this error arises from approximating f with a truncated series, rather than due to rounding, it is known as **truncation error**. Note that it tends to be lower if you use more terms (larger n), or if the function oscillates less (smaller $f^{(n+1)}$ on the interval (x_0, x)).

Error estimates like the Lagrange remainder play an important role in numerical analysis and computation, so it is important to understand where it comes from. The number ξ will ultimately come from Rolle's theorem, which is a special case of the mean value theorem from first-year calculus:

Theorem 2.3: Rolle's Theorem

If f is continuous on $[a, b]$ and differentiable on (a, b), with $f(a) = f(b) = 0$, then there exists $\xi \in (a, b)$ with $f'(\xi) = 0$.

Note

Note that Rolle's Theorem does not tell us what the value of ξ might actually be, so in practice we must take some kind of worst case estimate to get an error bound, e.g. calculate the max value of $f'(\xi)$ over the range of possible ξ values.

2.1.3 Polynomial Interpolation

The classical problem of **polynomial interpolation** is to find a polynomial

$$p_n(x) = a_0 + a_1 x + \ldots + a_n x^n = \sum_{k=0}^{n} a_k x^k$$

that interpolates our function f at a finite set of nodes $\{x_0, x_1, \ldots, x_m\}$. In other words, $p_n(x_i) = f(x_i)$ at each of the nodes x_i. Since the polynomial has $n+1$ unknown coefficients, we expect to need $n+1$ distinct nodes, so let us assume that $m = n$.

Here we have two nodes x_0, x_1, and seek a polynomial $p_1(x) = a_0 + a_1 x$. Then the interpolation conditions require that

$$\begin{cases} p_1(x_0) = a_0 + a_1 x_0 = f(x_0) \\ p_1(x_1) = a_0 + a_1 x_1 = f(x_1) \end{cases} \quad \Longrightarrow \quad p_1(x) = \frac{x_1 f(x_0) - x_0 f(x_1)}{x_1 - x_0} + \frac{f(x_1) - f(x_0)}{x_1 - x_0} x.$$

For general n, the interpolation conditions require

$$\begin{array}{ccccccc} a_0 & +a_1 x_0 & +a_2 x_0^2 & +\ldots & +a_n x_0^n & = f(x_0), \\ a_0 & +a_1 x_1 & +a_2 x_1^2 & +\ldots & +a_n x_1^n & = f(x_1), \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ a_0 & +a_1 x_n & +a_2 x_n^2 & +\ldots & +a_n x_n^n & = f(x_n), \end{array}$$

so we have to solve

$$\begin{pmatrix} 1 & x_0 & x_0^2 & \cdots & x_0^n \\ 1 & x_1 & x_1^2 & \cdots & x_1^n \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & x_n & x_n^2 & \cdots & x_n^n \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_n \end{pmatrix} = \begin{pmatrix} f(x_0) \\ f(x_1) \\ \vdots \\ f(x_n) \end{pmatrix}.$$

This is called a **Vandermonde matrix**. The determinant of this matrix is

$$\det(A) = \prod_{0 \le i < j \le n} (x_j - x_i),$$

which is non-zero provided the nodes are all distinct. This establishes an important result, where $\mathcal{P}_n$ denotes the space of all real polynomials of degree $\le n$.

Theorem 2.4: Existence/uniqueness

Given $n+1$ distinct nodes $x_0, x_1, \ldots, x_n$, there is a unique polynomial $p_n \in \mathcal{P}_n$ that interpolates $f(x)$ at these nodes.

We may also prove uniqueness by the following elegant argument.

Proof (Uniqueness part of Existence/Uniqueness Theorem):
Suppose that in addition to p_n there is another interpolating polynomial $q_n \in \mathcal{P}_n$. Then the difference $r_n := p_n - q_n$ is also a polynomial with degree $\leq n$. But we have

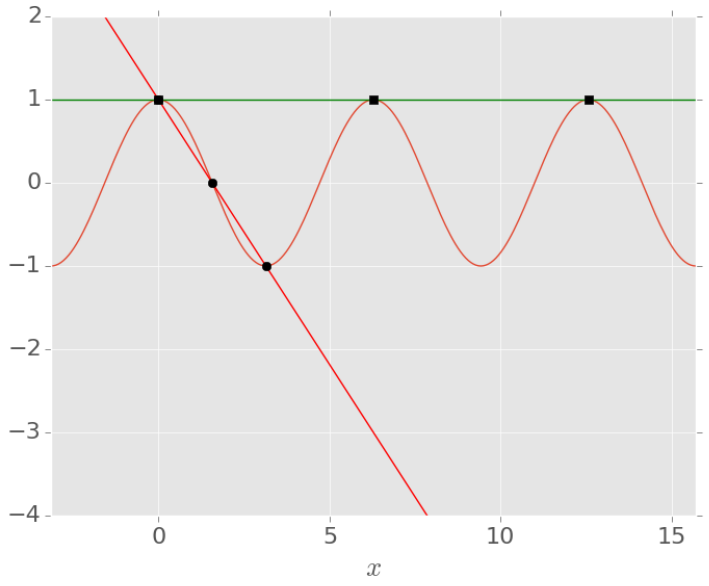
$$r_n(x_i) = p_n(x_i) - q_n(x_i) = f(x_i) - f(x_i) = 0 \quad \text{for } i = 0, \ldots, n,$$

so $r_n(x)$ has $n+1$ roots. From the Fundamental Theorem of Algebra, this is possible only if $r_n(x) \equiv 0$, which implies that $q_n = p_n$.

> **Note**
>
> Note that the unique polynomial through $n+1$ points may have degree $< n$. This happens when $a_0 = 0$ in the solution to the Vandermonde system above.

We have $x_0 = 0$, $x_1 = \frac{\pi}{2}$, $x_2 = \pi$, so $f(x_0) = 1$, $f(x_1) = 0$, $f(x_2) = -1$. Clearly the unique interpolant is a straight line $p_2(x) = 1 - \frac{2}{\pi}x$.

If we took the nodes $\{0, 2\pi, 4\pi\}$, we would get a constant function $p_2(x) = 1$.



One way to compute the interpolating polynomial would be to solve the Vandermonde system above, e.g. by Gaussian elimination. However, this is not recommended. In practice, we choose a different basis for p_n; there are two common and effective choices due to Lagrange and Newton.

> **Note**
>
> The Vandermonde matrix arises when we write p_n in the **natural basis** $\{1, x, x^2, \ldots\}$, but we could also choose to work in some other basis...

2.1.4 Lagrange Polynomials

This uses a special basis of polynomials $\{\ell_k\}$ in which the interpolation equations reduce to the identity matrix. In other words, the coefficients in this basis are just the function values,

$$p_n(x) = \sum_{k=0}^{n} f(x_k)\ell_k(x).$$

Example 2.1: Linear interpolation again.

We can re-write our linear interpolant to separate out the function values:

$$p_1(x) = \underbrace{\frac{x - x_1}{x_0 - x_1}}_{\ell_0(x)} f(x_0) + \underbrace{\frac{x - x_0}{x_1 - x_0}}_{\ell_1(x)} f(x_1).$$

Then ℓ_0 and ℓ_1 form the necessary basis. In particular, they have the property that

$$\ell_0(x_i) = \begin{cases} 1 & \text{if } i = 0, \\ 0 & \text{if } i = 1, \end{cases} \qquad \ell_1(x_i) = \begin{cases} 0 & \text{if } i = 0, \\ 1 & \text{if } i = 1, \end{cases}$$

For general n, the $n + 1$ **Lagrange polynomials** are defined as a product

$$\ell_k(x) = \prod_{\substack{j=0 \\ j \neq k}}^{n} \frac{x - x_j}{x_k - x_j}.$$

By construction, they have the property that

$$\ell_k(x_i) = \begin{cases} 1 & \text{if } i = k, \\ 0 & \text{otherwise.} \end{cases}$$

From this, it follows that the interpolating polynomial may be written as above.

Note

By the Existence/Uniqueness Theorem, the Lagrange polynomials are the *unique* polynomials with this property.

Example 2.2: Compute the quadratic interpolating polynomial to $f(x) = \cos(x)$ with nodes $\{-\frac{\pi}{4}, 0, \frac{\pi}{4}\}$ using Lagrange polynomials.

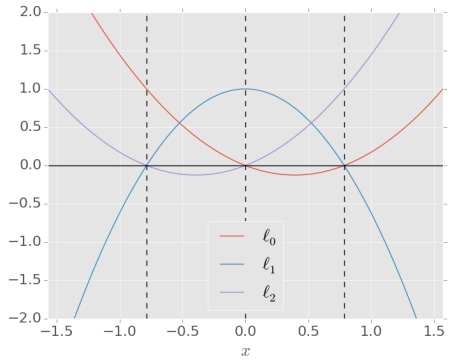
The Lagrange polynomials of degree 2 for these nodes are

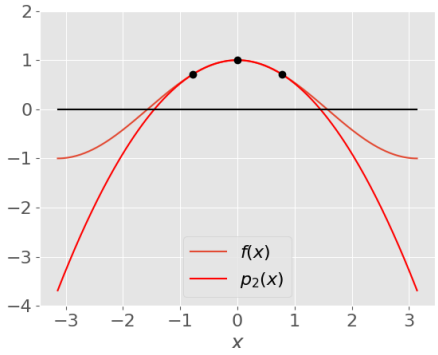
$$\begin{aligned}
\ell_0(x) &= \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} = \frac{x(x-\frac{\pi}{4})}{\frac{\pi}{4}\cdot\frac{\pi}{2}}, \\
\ell_1(x) &= \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} = \frac{(x+\frac{\pi}{4})(x-\frac{\pi}{4})}{-\frac{\pi}{4}\cdot\frac{\pi}{4}}, \\
\ell_2(x) &= \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} \\
&= \frac{x(x+\frac{\pi}{4})}{\frac{\pi}{2}\cdot\frac{\pi}{4}}.
\end{aligned}$$

So the interpolating polynomial is

$$\begin{aligned}
p_2(x) &= f(x_0)\ell_0(x) + f(x_1)\ell_1(x) + f(x_2)\ell_2(x) \\
&= \tfrac{1}{\sqrt{2}}\tfrac{8}{\pi^2}x(x-\tfrac{\pi}{4}) - \tfrac{16}{\pi^2}(x+\tfrac{\pi}{4})(x-\tfrac{\pi}{4}) + \tfrac{1}{\sqrt{2}}\tfrac{8}{\pi^2}x(x+\tfrac{\pi}{4}) = \tfrac{16}{\pi^2}(\tfrac{1}{\sqrt{2}}-1)x^2 + 1.
\end{aligned}$$

The Lagrange polynomials and the resulting interpolant are shown below:





Note

Lagrange polynomials were actually discovered by Edward Waring in 1776 and rediscovered by Euler in 1783, before they were published by Lagrange himself in 1795; a classic example

of Stigler's law of eponymy!

The Lagrange form of the interpolating polynomial is easy to write down, but expensive to evaluate since all of the ℓ_k must be computed. Moreover, changing any of the nodes means that the ℓ_k must all be recomputed from scratch, and similarly for adding a new node (moving to higher degree).

2.1.5 Newton/Divided-Difference Polynomials

It would be easy to increase the degree of p_n if

$$p_{n+1}(x) = p_n(x) + g_{n+1}(x), \quad \text{where } g_{n+1} \in \mathcal{P}_{n+1}.$$

From the interpolation conditions, we know that

$$g_{n+1}(x_i) = p_{n+1}(x_i) - p_n(x_i) = f(x_i) - f(x_i) = 0 \quad \text{for } i = 0, \ldots, n,$$

so

$$g_{n+1}(x) = a_{n+1}(x - x_0) \cdots (x - x_n).$$

The coefficient a_{n+1} is determined by the remaining interpolation condition at x_{n+1}, so

$$p_n(x_{n+1}) + g_{n+1}(x_{n+1}) = f(x_{n+1}) \quad \Longrightarrow \quad a_{n+1} = \frac{f(x_{n+1}) - p_n(x_{n+1})}{(x_{n+1} - x_0) \cdots (x_{n+1} - x_n)}.$$

The polynomial $(x - x_0)(x - x_1) \cdots (x - x_n)$ is called a **Newton polynomial**. These form a new basis

$$n_0(x) = 1, \qquad n_k(x) = \prod_{j=0}^{k-1} (x - x_j) \quad \text{for } k > 0.$$

The **Newton form** of the interpolating polynomial is then

$$p_n(x) = \sum_{k=0}^{n} a_k n_k(x), \qquad a_0 = f(x_0), \qquad a_k = \frac{f(x_k) - p_{k-1}(x_k)}{(x_k - x_0) \cdots (x_k - x_{k-1})} \text{ for } k > 0.$$

Notice that a_k depends only on $x_0, \ldots x_k$, so we can construct first a_0, then a_1, etc.

It turns out that the a_k are easy to compute, but it will take a little work to derive the method. We define the **divided difference** $f[x_0, x_1, \ldots, x_k]$ to be the coefficient of x^k in the polynomial interpolating f at nodes $x_0, \ldots, x_k$. It follows that

$$f[x_0, x_1, \ldots, x_k] = a_k,$$

where a_k is the coefficient in the Newton form above.

Example 2.3: Compute the Newton interpolating polynomial at two nodes.

$$f[x_0] = a_0 = f(x_0),$$
$$f[x_0, x_1] = a_1 = \frac{f(x_1) - p_0(x_1)}{x_1 - x_0} = \frac{f(x_1) - a_0}{x_1 - x_0} = \frac{f[x_1] - f[x_0]}{x_1 - x_0}.$$

So the **first-order** divided difference $f[x_0, x_1]$ is obtained from the **zeroth-order** differences $f[x_0]$, $f[x_1]$ by subtracting and dividing, hence the name "divided difference".

Example 2.4: Compute the Newton interpolating polynomial at three nodes.

Continuing from the previous example, we find

$$\begin{aligned} f[x_0, x_1, x_2] = a_2 &= \frac{f(x_2) - p_1(x_2)}{(x_2 - x_0)(x_2 - x_1)} = \frac{f(x_2) - a_0 - a_1(x_2 - x_0)}{(x_2 - x_0)(x_2 - x_1)} \\ &= \ldots = \frac{1}{x_2 - x_0}\left(\frac{f[x_2] - f[x_1]}{x_2 - x_1} - \frac{f[x_1] - f[x_0]}{x_1 - x_0}\right) \\ &= \frac{f[x_1, x_2] - f[x_0, x_1]}{x_2 - x_0}. \end{aligned}$$

So again, we subtract and divide.

In general, we have the following.

Theorem 2.5

For $k > 0$, the divided differences satisfy

$$f[x_i, x_{i+1}, \ldots, x_{i+k}] = \frac{f[x_{i+1}, \ldots, x_{i+k}] - f[x_i, \ldots, x_{i+k-1}]}{x_{i+k} - x_i}.$$

Proof:
Without loss of generality, we relabel the nodes so that $i = 0$. So we want to prove that

$$f[x_0, x_1, \ldots, x_k] = \frac{f[x_1, \ldots, x_k] - f[x_0, \ldots, x_{k-1}]}{x_k - x_0}.$$

The trick is to write the interpolant with nodes $x_0, \ldots, x_k$ in the form

$$p_k(x) = \frac{(x_k - x)q_{k-1}(x) + (x - x_0)\tilde{q}_{k-1}(x)}{x_k - x_0},$$

where $q_{k-1} \in \mathcal{P}_{k-1}$ interpolates f at the subset of nodes $x_0, x_1, \ldots, x_{k-1}$ and $\tilde{q}_{k-1} \in \mathcal{P}_{k-1}$ interpolates f at the subset $x_1, x_2, \ldots, x_k$. If this holds, then matching the coefficient of x^k on each side will give the divided difference formula, since, e.g., the leading coefficient of q_{k-1} is

$f[x_0, \ldots, x_{k-1}]$. To see that p_k may really be written this way, note that

$$\begin{aligned} p_k(x_0) &= q_{k-1}(x_0) = f(x_0), \\ p_k(x_k) &= \tilde{q}_{k-1}(x_k) = f(x_k), \\ p_k(x_i) &= \frac{(x_k - x_i)q_{k-1}(x_i) + (x_i - x_0)\tilde{q}_{k-1}(x_i)}{x_k - x_0} = f(x_i) \quad \text{for } i = 1, \ldots, k-1. \end{aligned}$$

Since p_k agrees with f at the $k+1$ nodes, it is the unique interpolant in $\mathcal{P}_k$.

Theorem above gives us our convenient method, which is to construct a **divided-difference table**.

Example 2.5: Construct the Newton polynomial at the nodes $\{-1, 0, 1, 2\}$ and with corresponding function values $\{5, 1, 1, 11\}$

We construct a divided-difference table as follows.

$$\begin{array}{llllll} x_0 = -1 & f[x_0] = 5 & & & & \\ & & f[x_0, x_1] = -4 & & & \\ x_1 = 0 & f[x_1] = 1 & & f[x_0, x_1, x_2] = 2 & & \\ & & f[x_1, x_2] = 0 & & f[x_0, x_1, x_2, x_3] = 1 & \\ x_2 = 1 & f[x_2] = 1 & & f[x_1, x_2, x_3] = 5 & & \\ & & f[x_2, x_3] = 10 & & & \\ x_3 = 2 & f[x_3] = 11 & & & & \end{array}$$

The coefficients of the p_3 lie at the top of each column, so

$$\begin{aligned} p_3(x) &= f[x_0] + f[x_0, x_1](x - x_0) + f[x_0, x_1, x_2](x - x_0)(x - x_1) \\ &\quad + f[x_0, x_1, x_2, x_3](x - x_0)(x - x_1)(x - x_2) \\ &= 5 - 4(x + 1) + 2x(x + 1) + x(x + 1)(x - 1). \end{aligned}$$

Now suppose we add the extra nodes $\{-2, 3\}$ with data $\{5, 35\}$. All we need to do to compute p_5 is add two rows to the bottom of the table — there is no need to recalculate the rest. This gives

$$\begin{array}{llllll} -1 & 5 & & & & \\ & & -4 & & & \\ 0 & 1 & & 2 & & \\ & & 0 & & 1 & \\ 1 & 1 & & 5 & & -\frac{1}{12} \\ & & 10 & & \frac{13}{12} & \\ 2 & 11 & & \frac{17}{6} & & -\frac{1}{12} \\ & & \frac{3}{2} & & \frac{5}{6} & \\ -2 & 5 & & \frac{9}{2} & & \\ & & 6 & & & \\ 3 & 35 & & & & \end{array} \qquad 0$$

The new interpolating polynomial is

$$p_5(x) = p_3(x) - \tfrac{1}{12}x(x+1)(x-1)(x-2).$$

Note

Notice that the x^5 coefficient vanishes for these particular data, meaning that they are consistent with $f \in \mathcal{P}_4$.

Note

Note that the value of $f[x_0, x_1, \ldots, x_k]$ is independent of the order of the nodes in the table. This follows from the uniqueness of p_k.

Divided differences are actually approximations for *derivatives* of f. In the limit that the nodes all coincide, the Newton form of $p_n(x)$ becomes the Taylor polynomial.

2.1.6 Interpolation Error

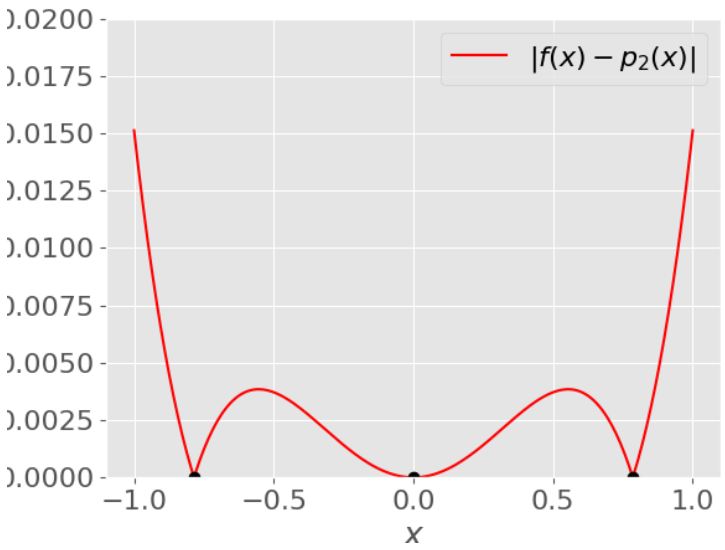
The goal here is to estimate the error $|f(x) - p_n(x)|$ when we approximate a function f by a polynomial interpolant p_n. Clearly this will depend on x.

Example 2.6: Quadratic interpolant for $f(x) = \cos(x)$ with $\{-\frac{\pi}{4}, 0, \frac{\pi}{4}\}$.

From Section 2.1.4, we have $p_2(x) = \frac{16}{\pi^2}\left(\frac{1}{\sqrt{2}} - 1\right)x^2 + 1$, so the error is

$$|f(x) - p_2(x)| = \left|\cos(x) - \tfrac{16}{\pi^2}\left(\tfrac{1}{\sqrt{2}} - 1\right)x^2 - 1\right|.$$

This is shown below:



Clearly the error vanishes at the nodes themselves, but note that it generally does better near the middle of the set of nodes — this is quite typical behaviour.

We can adapt the proof of Taylor's theorem to get a quantitative error estimate.

Theorem 2.6: Cauchy's Interpolation Error Theorem

Let $p_n \in \mathcal{P}_n$ be the unique polynomial interpolating $f(x)$ at the $n+1$ distinct nodes $x_0, x_1, \ldots, x_n \in [a,b]$, and let f be continuous on $[a,b]$ with $n+1$ continuous derivatives on (a,b). Then for each $x \in [a,b]$ there exists $\xi \in (a,b)$ such that

$$f(x) - p_n(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!}(x - x_0)(x - x_1)\cdots(x - x_n).$$

This looks similar to the error formula for Taylor polynomials (see Taylor's Theorem). But now the error vanishes at multiple nodes rather than just at x_0.

From the formula, you can see that the error will be larger for a more "wiggly" function, where the derivative $f^{(n+1)}$ is larger. It might also appear that the error will go down as the number of nodes n increases; we will see in Section 2.1.7 that this is not always true.

Note

As in Taylor's theorem, note the appearance of an undetermined point ξ. This will prevent us knowing the error exactly, but we can make an estimate as before.

Example 2.7: Quadratic interpolant for $f(x) = \cos(x)$ with $\{-\frac{\pi}{4}, 0, \frac{\pi}{4}\}$.

For $n = 2$, Cauchy's Interpolation Error Theorem says that

$$f(x) - p_2(x) = \frac{f^{(3)}(\xi)}{6} x(x + \tfrac{\pi}{4})(x - \tfrac{\pi}{4}) = \tfrac{1}{6} \sin(\xi) x(x + \tfrac{\pi}{4})(x - \tfrac{\pi}{4}),$$

for some $\xi \in [-\frac{\pi}{4}, \frac{\pi}{4}]$.
For an upper bound on the error at a particular x, we can just use $|\sin(\xi)| \leq 1$ and plug in x.
To bound the maximum error within the interval $[-1, 1]$, let us maximise the polynomial $w(x) = x(x + \frac{\pi}{4})(x - \frac{\pi}{4})$. We have $w'(x) = 3x^2 - \frac{\pi^2}{16}$ so turning points are at $x = \pm\frac{\pi}{4\sqrt{3}}$. We have

$$w(-\tfrac{\pi}{4\sqrt{3}}) = 0.186\ldots, \quad w(\tfrac{\pi}{4\sqrt{3}}) = -0.186\ldots, \quad w(-1) = -0.383\ldots, \quad w(1) = 0.383\ldots.$$

So our error estimate for $x \in [-1, 1]$ is

$$|f(x) - p_2(x)| \leq \tfrac{1}{6}(0.383) = 0.0638\ldots$$

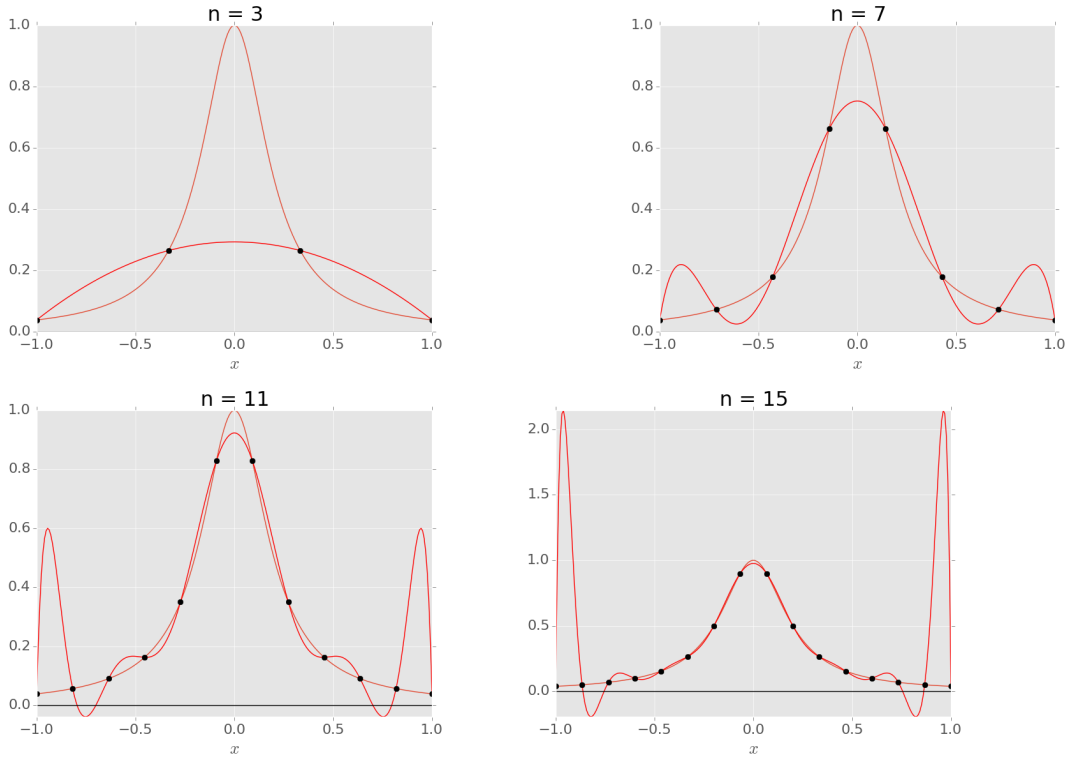
From the plot earlier, we see that this bound is satisfied (as it has to be), although not tight.

2.1.7 Node Placement: Chebyshev nodes

You might expect polynomial interpolation to *converge* as $n \to \infty$. Surprisingly, this is not the case if you take **equally-spaced** nodes x_i. This was shown by Runge in a famous 1901 paper.

Example 2.8: The Runge function $f(x) = 1/(1 + 25x^2)$ on $[-1, 1]$.

Here are illustrations of p_n for increasing n:



Notice that p_n is converging to f in the middle, but diverging more and more near the ends, even within the interval $[x_0, x_n]$. This is called the **Runge phenomenon**.

Note

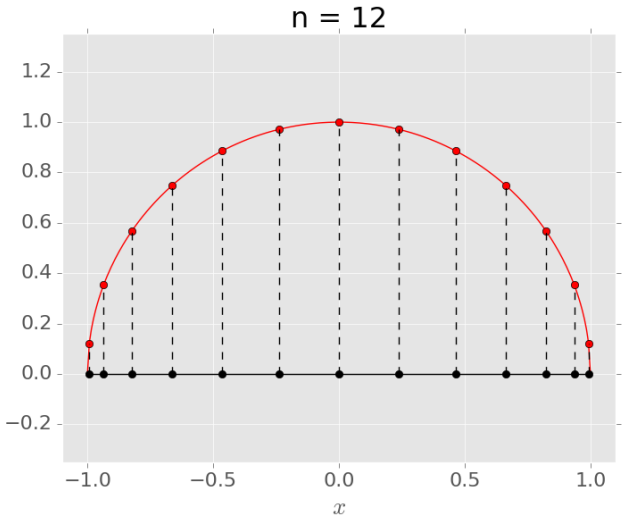
A full mathematical explanation for this divergence usually uses complex analysis — see Chapter 13 of *Approximation Theory and Approximation Practice* by L.N. Trefethen (SIAM, 2013). For a more elementary proof, see this StackExchange post.

The problem is (largely) coming from the interpolating polynomial

$$w(x) = \prod_{i=0}^{n} (x - x_i).$$

We can avoid the Runge phenomenon by choosing different nodes x_i that are **not uniformly spaced**.

Since the problems are occurring near the ends of the interval, it would be logical to put more nodes there. A good choice is given by taking equally-spaced points on the unit circle $|z| = 1$, and projecting to the real line:



The points around the circle are

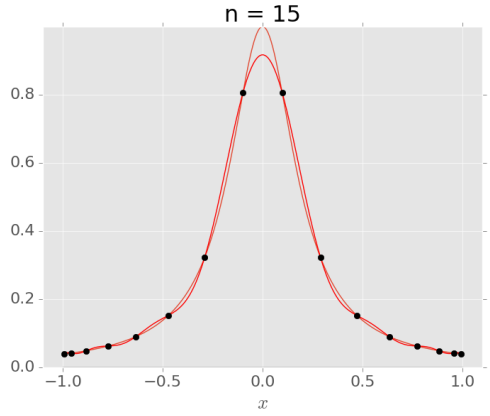
$$\phi_j = \frac{(2j+1)\pi}{2(n+1)}, \quad j = 0, \ldots, n,$$

so the corresponding **Chebyshev nodes** are

$$x_j = \cos\left[\frac{(2j+1)\pi}{2(n+1)}\right], \quad j = 0, \ldots, n.$$

Example 2.9: The Runge function $f(x) = 1/(1+25x^2)$ on $[-1,1]$ using the Chebyshev nodes.

For $n = 3$, the nodes are $x_0 = \cos(\frac{\pi}{8})$, $x_1 = \cos(\frac{3\pi}{8})$, $x_2 = \cos(\frac{5\pi}{8})$, $x_3 = \cos(\frac{7\pi}{8})$. Below we illustrate the resulting interpolant for $n = 15$:



Compare this to the example with equally spaced nodes.

In fact, the Chebyshev nodes are, in one sense, an optimal choice. To see this, we first note that they are zeroes of a particular polynomial.

The Chebyshev points $x_j = \cos\left[\frac{(2j+1)\pi}{2(n+1)}\right]$ for $j = 0, \ldots, n$ are zeroes of the Chebyshev polynomial

$$T_{n+1}(t) := \cos\left[(n+1)\arccos(t)\right]$$

> **Note**
>
> The Chebyshev polynomials are denoted T_n rather than C_n because the name is transliterated from Russian as "Tchebychef" in French, for example.

In choosing the Chebyshev nodes, we are choosing the error polynomial $w(x) := \prod_{i=0}^{n}(x - x_i)$ to be $T_{n+1}(x)/2^n$. (This normalisation makes the leading coefficient 1) This is a good choice because of the following result.

Theorem 2.7: Chebyshev interpolation

Let $x_0, x_1, \ldots, x_n \in [-1, 1]$ be distinct. Then $\max_{[-1,1]} |w(x)|$ is minimized if

$$w(x) = \frac{1}{2^n} T_{n+1}(x),$$

where $T_{n+1}(x)$ is the **Chebyshev polynomial** $T_{n+1}(x) = \cos\Big((n+1)\arccos(x)\Big)$.

Having established that the Chebyshev polynomial minimises the maximum error, we can see convergence as $n \to \infty$ from the fact that

$$|f(x) - p_n(x)| = \frac{|f^{(n+1)}(\xi)|}{(n+1)!}|w(x)| = \frac{|f^{(n+1)}(\xi)|}{2^n(n+1)!}|T_{n+1}(x)| \leq \frac{|f^{(n+1)}(\xi)|}{2^n(n+1)!}.$$

If the function is well-behaved enough that $|f^{(n+1)}(x)| < M$ for some constant whenever $x \in [-1, 1]$, then the error will tend to zero as $n \to \infty$.

2.2 Nonlinear Equations

How do we find roots of nonlinear equations?

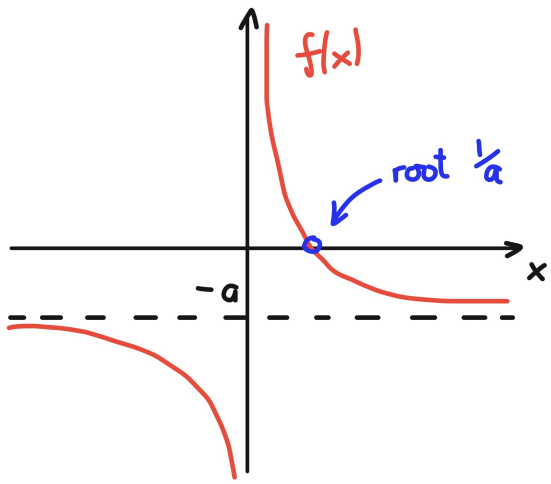
Given a general equation

$$f(x) = 0,$$

there will usually be no explicit formula for the root(s) x_*, so we must use an iterative method.

Rootfinding is a delicate business, and it is essential to begin by plotting a graph of $f(x)$, so that you can tell whether the answer you get from your numerical method is correct.

Example 2.10: $f(x) = \frac{1}{x} - a$, for $a > 0$.



Clearly we know the root is exactly $x_* = \frac{1}{a}$, but this will serve as a running example to test some of our methods

2.2.1 Interval Bisection

If f is continuous and we can find an interval where it changes sign, then it must have a root in this interval. Formally, this is based on:

Theorem 2.8: Intermediate Value Theorem

If f is continuous on $[a, b]$ and c lies between $f(a)$ and $f(b)$, then there is at least one point $x \in [a, b]$ such that $f(x) = c$.

If $f(a)f(b) < 0$, then f changes sign at least once in $[a, b]$, so by the Intermediate Value Theorem there must be a point $x_* \in [a, b]$ where $f(x_*) = 0$.

We can turn this into the following iterative algorithm:

Algorithm 2.1: Interval bisection

Let f be continuous on $[a_0, b_0]$, with $f(a_0)f(b_0) < 0$.

- At each step, set $m_k = (a_k + b_k)/2$.
- If $f(a_k)f(m_k) \geq 0$ then set $a_{k+1} = m_k$, $b_{k+1} = b_k$, otherwise set $a_{k+1} = a_k$, $b_{k+1} = m_k$.

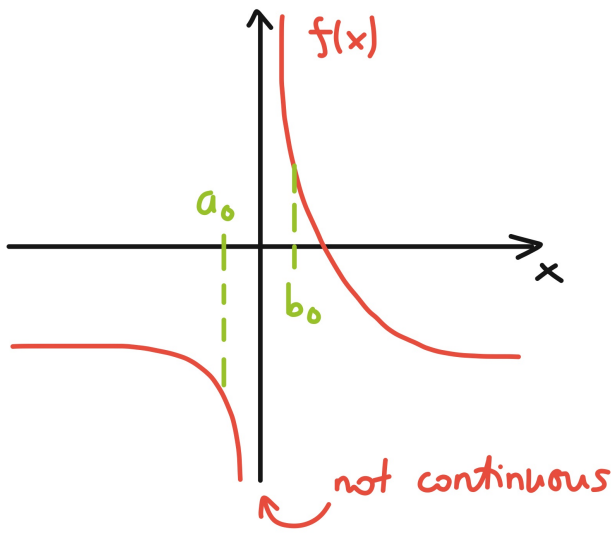
Example 2.11: $f(x) = \frac{1}{x} - 0.5$.

1. Try $a_0 = 1$, $b_0 = 3$ so that $f(a_0)f(b_0) = 0.5(-0.1666) < 0$.
   Now the midpoint is $m_0 = (1 + 3)/2 = 2$, with $f(m_0) = 0$.
   We are lucky and have already stumbled on the root $x_* = m_0 = 2$!

2. Suppose we had tried $a_0 = 1.5$, $b_0 = 3$, so $f(a_0) = 0.1666$ and $f(b_0) = -0.1666$, and again $f(a_0)f(b_0) < 0$.
   Now $m_0 = 2.25$, $f(m_0) = -0.0555$. We have $f(a_0)f(m_0) < 0$, so we set $a_1 = a_0 = 1.5$ and $b_1 = m_0 = 2.25$. The root must lie in $[1.5, 2.25]$.
   Now $m_1 = 1.875$, $f(m_1) = 0.0333$, and $f(a_1)f(m_1) > 0$, so we take $a_2 = m_1 = 1.875$, $b_2 = b_1 = 2.25$. The root must lie in $[1.875, 2.25]$.
   We can continue this algorithm, halving the length of the interval each time.

Since the interval halves in size at each iteration, and always contains a root, we are guaranteed to converge to a root provided that f is continuous. Stopping at step k, we get the minimum possible error by choosing m_k as our approximation.

Example 2.12: Same example with initial interval $[-0.5, 0.5]$.



In this case $f(a_0)f(b_0) < 0$, but there is no root in the interval.

The rate of convergence is steady, so we can pre-determine how many iterations will be needed to converge to a given accuracy. After k iterations, the interval has length

$$|b_k - a_k| = \frac{|b_0 - a_0|}{2^k},$$

so the error in the mid-point satisfies

$$|m_k - x_*| \leq \frac{|b_0 - a_0|}{2^{k+1}}.$$

In order for $|m_k - x_*| \leq \delta$, we need n iterations, where

$$\frac{|b_0 - a_0|}{2^{n+1}} \leq \delta \quad \Longrightarrow \log|b_0 - a_0| - (n+1)\log(2) \leq \log(\delta) \quad \Longrightarrow \quad n \geq \frac{\log|b_0 - a_0| - \log(\delta)}{\log(2)} - 1.$$

Example 2.13: Previous example continued

With $a_0 = 1.5$, $b_0 = 3$, as in the above example, then for $\delta = \epsilon_{\mathrm{M}} = 1.1 \times 10^{-16}$ we would need

$$n \geq \frac{\log(1.5) - \log(1.1 \times 10^{-16})}{\log(2)} - 1 \quad \Longrightarrow \quad n \geq 53 \text{ iterations.}$$

Note

This convergence is pretty slow, but the method has the advantage of being very robust (i.e., use it if all else fails...). It has the more serious disadvantage of *only working in one dimension.*

2.2.2 Fixed point iteration

This is a very common type of rootfinding method. The idea is to transform $f(x) = 0$ into the form $g(x) = x$, so that a root x_* of f is a **fixed point** of g, meaning $g(x_*) = x_*$. To find x_*, we start from some initial guess x_0 and iterate

$$x_{k+1} = g(x_k)$$

until $|x_{k+1} - x_k|$ is sufficiently small. For a given equation $f(x) = 0$, there are many ways to transform it into the form $x = g(x)$. Only some will result in a convergent iteration.

Example 2.14: $f(x) = x^2 - 2x - 3$.

Note that the roots are -1 and 3. Consider some different rearrangements, with $x_0 = 0$.

1. $g(x) = \sqrt{2x + 3}$, gives $x_k \to 3$ [to machine accuracy after 33 iterations].
2. $g(x) = 3/(x - 2)$, gives $x_k \to -1$ [to machine accuracy after 33 iterations].
3. $g(x) = (x^2 - 3)/2$, gives $x_k \to -1$ [but very slowly!].
4. $g(x) = x^2 - x - 3$, gives $x_k \to \infty$.
5. $g(x) = (x^2 + 3)/(2x - 2)$, gives $x_k \to -1$ [to machine accuracy after 5 iterations].

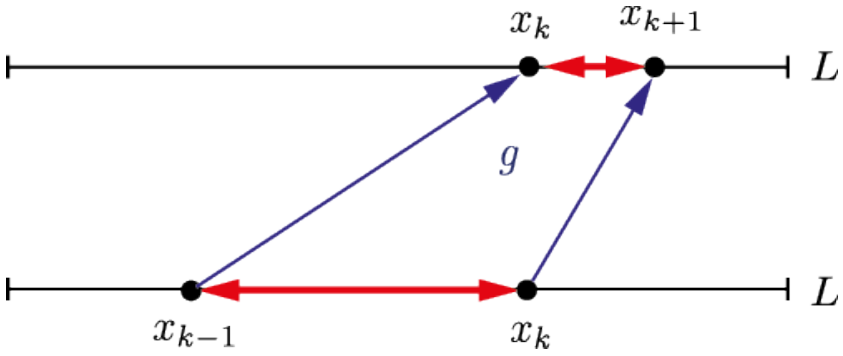
If instead we take $x_0 = 42$, then (1) and (2) still converge to the same roots, (3) now diverges, (4) still diverges, and (5) now converges to the other root $x_k \to 3$.

In this section, we will consider which iterations will converge, before addressing the *rate* of convergence in Section 2.2.3.

One way to ensure that the iteration will work is to find a **contraction mapping** g, which is a map $L \to L$ (for some closed interval L) satisfying

$$|g(x) - g(y)| \leq \lambda |x - y|$$

for some $\lambda < 1$ and for all $x, y \in L$. The sketch below shows the idea:



Theorem 2.9: Contraction Mapping Theorem

If g is a contraction mapping on $L = [a, b]$, then 1. There exists a unique fixed point $x_* \in L$ with $g(x_*) = x_*$. 2. For any $x_0 \in L$, the iteration $x_{k+1} = g(x_k)$ will converge to x_* as $k \to \infty$.

Proof:
To prove *existence*, consider $h(x) = g(x) - x$. Since $g : L \to L$ we have $h(a) = g(a) - a \geq 0$ and $h(b) = g(b) - b \leq 0$. Moreover, it follows from the contraction property above that g is continuous (think of "$\epsilon\delta$"), therefore so is h. So the Intermediate Value Theorem guarantees the existence of at least one point $x_* \in L$ such that $h(x_*) = 0$, i.e. $g(x_*) = x_*$.

For *uniqueness*, suppose x_* and y_* are both fixed points of g in L. Then

$$|x_* - y_*| = |g(x_*) - g(y_*)| \leq \lambda |x_* - y_*| < |x_* - y_*|,$$

which is a contradiction.

Finally, to show *convergence*, consider

$$|x_* - x_{k+1}| = |g(x_*) - g(x_k)| \leq \lambda |x_* - x_k| \leq \ldots \leq \lambda^{k+1} |x_* - x_0|.$$

Since $\lambda < 1$, we see that $x_k \to x_*$ as $k \to \infty$.

i Note

The Contraction Mapping Theorem is also known as the **Banach fixed point theorem**, and was proved by Stefan Banach in his 1920 PhD thesis.

To apply this result in practice, we need to know whether a given function g is a contraction mapping on some interval.

If g is differentiable, then Taylor's theorem says that there exists $\xi \in (x, y)$ with

$$g(x) = g(y) + g'(\xi)(x - y) \implies |g(x) - g(y)| \leq \left(\max_{\xi \in L} |g'(\xi)| \right) |x - y|.$$

So if (a) $g : L \to L$ and (b) $|g'(x)| \leq M$ for all $x \in L$ with $M < 1$, then g is a contraction mapping on L.

Example 2.15: Iteration (a) from previous example, $g(x) = \sqrt{2x+3}$.

Here $g' = (2x+3)^{-1/2}$, so we see that $|g'(x)| < 1$ for all $x > -1$.
For g to be a contraction mapping on an interval L, we also need that g maps L into itself. Since our particular g is continuous and monotonic increasing (for $x > -\frac{3}{2}$), it will map an interval $[a, b]$ to another interval whose end-points are $g(a)$ and $g(b)$.
For example, $g(-\frac{1}{2}) = \sqrt{2}$ and $g(4) = \sqrt{11}$, so the interval $L = [-\frac{1}{2}, 4]$ is mapped into itself. It follows by the Contraction Mapping Theorem that (1) there is a unique fixed point $x_* \in [-\frac{1}{2}, 4]$ (which we know is $x_* = 3$), and (2) the iteration will converge to x_* for any x_0 in this interval (as we saw for $x_0 = 0$).

In practice, it is not always easy to find a suitable interval L. But knowing that $|g'(x_*)| < 1$ is enough to guarantee that the iteration will converge if x_0 is close enough to x_*.

Theorem 2.10: Local Convergence Theorem

Let g and g' be continuous in the neighbourhood of an isolated fixed point $x_* = g(x_*)$. If $|g'(x_*)| < 1$ then there is an interval $L = [x_* - \delta, x_* + \delta]$ such that $x_{k+1} = g(x_k)$ converges to x_* whenever $x_0 \in L$.

Proof:
By continuity of g', there exists some interval $L = [x_* - \delta, x_* + \delta]$ with $\delta > 0$ such that $|g'(x)| \leq M$ for some $M < 1$, for all $x \in L$. Now let $x \in L$. It follows that

$$|x_* - g(x)| = |g(x_*) - g(x)| \leq M|x_* - x| < |x_* - x| \leq \delta,$$

so $g(x) \in L$. Hence g is a contraction mapping on L and the Contraction Mapping Theorem shows that $x_k \to x_*$.

Example 2.16: Iteration (a) again, $g(x) = \sqrt{2x+3}$.

Here we know that $x_* = 3$, and $|g'(3)| = \frac{1}{3} < 1$, so the Local Convergence Theorem tells us that the iteration will converge to 3 if x_0 is close enough to 3.

Example 2.17: Iteration (e) again, $g(x) = (x^2+3)/(2x-2)$.

Here we have

$$g'(x) = \frac{x^2 - 2x - 3}{2(x-1)^2},$$

so we see that $g'(-1) = g'(3) = 0 < 1$. So the Local Convergence Theorem tells us that

the iteration will converge to either root if we start close enough.

Note

As we will see, the fact that $g'(x_*) = 0$ is related to the fast convergence of iteration (e).

2.2.3 Orders of convergence

To measure the speed of convergence, we compare the error $|x_* - x_{k+1}|$ to the error at the previous step, $|x_* - x_k|$.

Example 2.18: Interval bisection.

Here we had $|x_* - m_{k+1}| \leq \frac{1}{2}|x_* - m_k|$. This is called **linear convergence**, meaning that we have $|x_* - x_{k+1}| \leq \lambda |x_* - x_k|$ for some constant $\lambda < 1$.

We can compare a few different iteration schemes that should converge to the same answer to get a sense for how our choice of scheme can impact the convergence order.

Example 2.19: Iteration (a) again, $g(x) = \sqrt{2x+3}$.

Look at the sequence of errors in this case:

x_k	$\lvert 3 - x_k \rvert$	$\lvert 3 - x_k \rvert / \lvert 3 - x_{k-1} \rvert$
0.0000000000	3.0000000000	-
1.7320508076	1.2679491924	0.4226497308
2.5424597568	0.4575402432	0.3608506129
2.8433992885	0.1566007115	0.3422665304
2.9473375404	0.0526624596	0.3362849319
2.9823941860	0.0176058140	0.3343143126
2.9941256440	0.0058743560	0.3336600063

We see that the ratio $|x_* - x_k|/|x_* - x_{k-1}|$ is indeed less than 1, and seems to be converging to $\lambda \approx \frac{1}{3}$. So this is a linearly convergent iteration.

Example 2.20: Iteration (e) again, $g(x) = (x^2 + 3)/(2x - 2)$.

Now the sequence is:

x_k	$\lvert(-1) - x_k\rvert$	$\lvert(-1) - x_k\rvert / \lvert(-1) - x_{k-1}\rvert$
0.0000000000	1.0000000000	-
-1.5000000000	0.5000000000	0.5000000000
-1.0500000000	0.0500000000	0.1000000000
-1.0006097561	0.0006097561	0.0121951220
-1.0000000929	0.0000000929	0.0001523926

Again the ratio $|x_* - x_k|/|x_* - x_{k-1}|$ is certainly less than 1, but this time we seem to have $\lambda \to 0$ as $k \to \infty$. This is called **superlinear convergence**, meaning that the convergence is in some sense "accelerating".

In general, if $x_k \to x_*$ then we say that the sequence $\{x_k\}$ **converges linearly** if

$$\lim_{k\to\infty} \frac{|x_* - x_{k+1}|}{|x_* - x_k|} = \lambda \quad \text{with} \quad 0 < \lambda < 1.$$

If $\lambda = 0$ then the convergence is **superlinear**.

> **Note**
>
> The constant λ is called the **rate** or **ratio**.

The following result establishes conditions for linear and superlinear convergence.

Theorem 2.11

Let g' be continuous in the neighbourhood of a fixed point $x_* = g(x_*)$, and suppose that $x_{k+1} = g(x_k)$ converges to x_* as $k \to \infty$.

1. If $|g'(x_*)| \neq 0$ then the convergence will be linear with rate $\lambda = |g'(x_*)|$.
2. If $|g'(x_*)| = 0$ then the convergence will be superlinear.

Proof:
By Taylor's theorem, note that

$$x_* - x_{k+1} = g(x_*) - g(x_k) = g(x_*) - \Big[g(x_*) + g'(\xi_k)(x_k - x_*)\Big] = g'(\xi_k)(x_* - x_k)$$

for some ξ_k between x_* and x_k. Since $x_k \to x_*$, we have $\xi_k \to x_*$ as $k \to \infty$, so

$$\lim_{k\to\infty} \frac{|x_* - x_{k+1}|}{|x_* - x_k|} = \lim_{k\to\infty} |g'(\xi_k)| = |g'(x_*)|.$$

This proves the result.

Example 2.21: Iteration (a) again, $g(x) = \sqrt{2x+3}$.

We saw before that $g'(3) = \frac{1}{3}$, so the theorem above shows that convergence will be linear with $\lambda = |g'(3)| = \frac{1}{3}$ as we found numerically.

Example 2.22: Iteration (e) again, $g(x) = (x^2+3)/(2x-2)$.

We saw that $g'(-1) = 0$, so the theorem above shows that convergence will be superlinear, again consistent with our numerical findings.

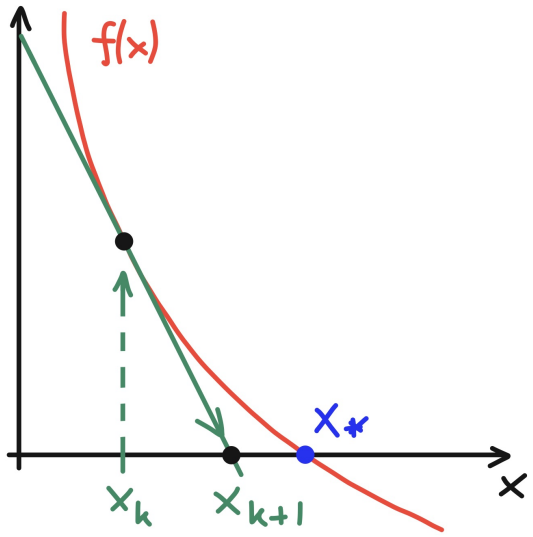
We can further classify superlinear convergence by the **order of convergence**, defined as

$$\alpha = \sup\left\{\beta \,:\, \lim_{k\to\infty} \frac{|x_* - x_{k+1}|}{|x_* - x_k|^\beta} < \infty\right\}.$$

For example, $\alpha = 2$ is called **quadratic** convergence and $\alpha = 3$ is called **cubic** convergence, although for a general sequence α need not be an integer (e.g. the secant method below).

2.2.4 Newton's method

This is a particular fixed point iteration that is very widely used because (as we will see) it usually converges superlinearly.



Graphically, the idea of **Newton's method** is simple: given x_k, draw the tangent line to f at $x = x_k$, and let x_{k+1} be the x-intercept of this tangent. So

$$\frac{0 - f(x_k)}{x_{k+1} - x_k} = f'(x_k) \qquad \Longrightarrow \qquad x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}.$$

> **Note**
>
> In fact, Newton only applied the method to polynomial equations, and without using calculus. The general form using derivatives ("fluxions") was first published by Thomas Simpson in 1740. [See "Historical Development of the Newton-Raphson Method" by T.J. Ypma, *SIAM Review* **37**, 531 (1995).]

Another way to derive this iteration is to approximate $f(x)$ by the linear part of its Taylor series centred at x_k:

$$0 \approx f(x_{k+1}) \approx f(x_k) + f'(x_k)(x_{k+1} - x_k).$$

The iteration function for Newton's method is

$$g(x) = x - \frac{f(x)}{f'(x)},$$

so using $f(x_*) = 0$ we see that $g(x_*) = x_*$. To assess the convergence, note that

$$g'(x) = 1 - \frac{f'(x)f'(x) - f(x)f''(x)}{[f'(x)]^2} = \frac{f(x)f''(x)}{[f'(x)]^2} \qquad \Longrightarrow\ g'(x_*) = 0 \quad \text{if } f'(x_*) \neq 0.$$

So if $f'(x_*) \neq 0$, the Local Convergence Theorem shows that the iteration will converge for x_0 close enough to x_*. Moreover, since $g'(x_*) = 0$, the order theorem shows that this convergence will be superlinear.

Example 2.23: Calculate a^{-1} using $f(x) = \frac{1}{x} - a$ for $a > 0$.

Newton's method gives the iterative formula

$$x_{k+1} = x_k - \frac{\frac{1}{x_k} - a}{-\frac{1}{x_k^2}} = 2x_k - ax_k^2.$$

From the graph of f, it is clear that the iteration will converge for any $x_0 \in (0, a^{-1})$, but will diverge if x_0 is too large. With $a = 0.5$ and $x_0 = 1$, Python gives

x_k	$\lvert 2 - x_k \rvert$	$\lvert 2 - x_k \rvert / \lvert 2 - x_{k-1} \rvert$	$\lvert 2 - x_k \rvert / \lvert 2 - x_{k-1} \rvert^2$
1.0	1.0	-	-

1.5	0.5	0.5	0.5
1.875	0.125	0.25	0.5
1.9921875	0.0078125	0.0625	0.5
1.999969482	3.05×10^{-5}	0.00390625	0.5
2.0	4.65×10^{-10}	1.53×10^{-5}	0.5
2.0	1.08×10^{-19}	2.33×10^{-10}	0.5

In 6 steps, the error is below ϵ_{M}: pretty rapid convergence! The third column shows that the convergence is superlinear. The fourth column shows that $|x_* - x_{k+1}|/|x_* - x_k|^2$ is constant, indicating that the convergence is quadratic (order $\alpha = 2$).

Note

Although the solution $\frac{1}{a}$ is known exactly, this method is so efficient that it is sometimes used in computer hardware to do division!

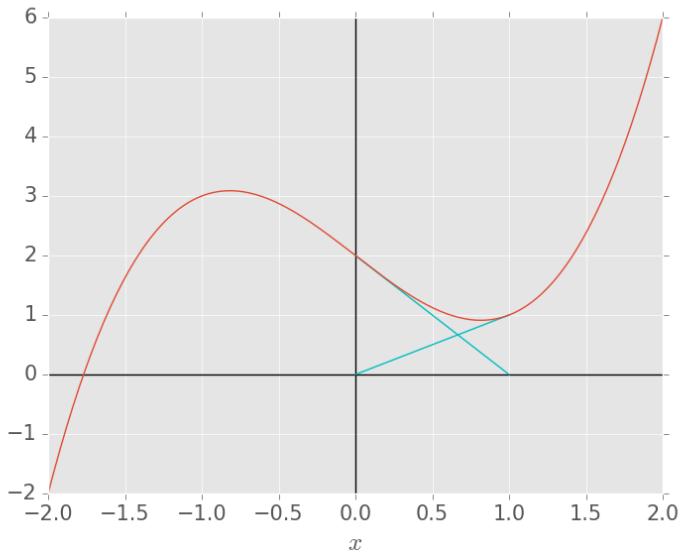
In practice, it is not usually possible to determine ahead of time whether a given starting value x_0 will converge.

A robust computer implementation should catch any attempt to take too large a step, and switch to a less sensitive (but slower) algorithm (e.g. bisection).

However, it always makes sense to avoid any points where $f'(x) = 0$.

Example 2.24: $f(x) = x^3 - 2x + 2$.

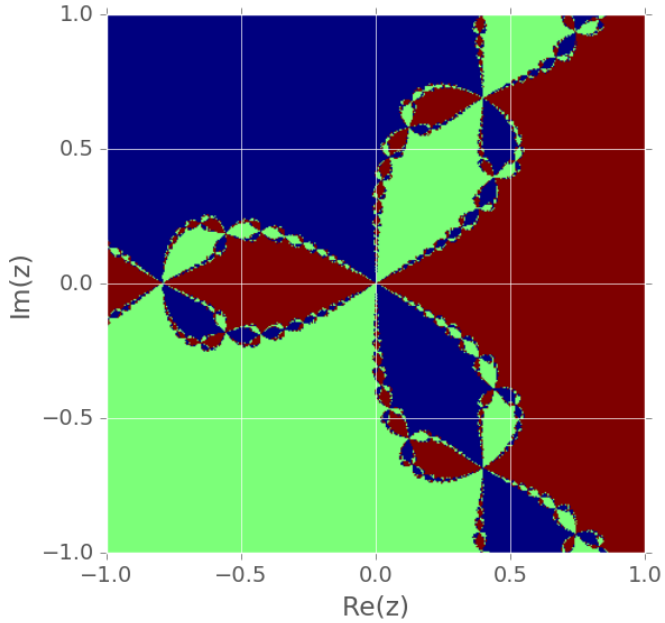
Here $f'(x) = 3x^2 - 2$ so there are turning points at $x = \pm\sqrt{\frac{2}{3}}$ where $f'(x) = 0$, as well as a single real root at $x_* \approx -1.769$. The presence of points where $f'(x) = 0$ means that care is needed in choosing a starting value x_0.
If we take $x_0 = 0$, then $x_1 = 0 - f(0)/f'(0) = 1$, but then $x_2 = 1 - f(1)/f'(1) = 0$, so the iteration gets stuck in an infinite loop:



Other starting values, e.g. $x_0 = -0.5$ can also be sucked into this infinite loop! The correct answer is obtained for $x_0 = -1.0$.

Note

The sensitivity of Newton's method to the choice of x_0 is beautifully illustrated by applying it to a **complex** function such as $f(z) = z^3 - 1$. The following plot colours points z_0 in the complex plane according to which root they converge to (1, $e^{2\pi i/3}$, or $e^{-2\pi i/3}$):



The boundaries of these **basins of attraction** are fractal.

2.2.5 Newton's method for systems

Newton's method generalizes to higher-dimensional problems where we want to find $\mathbf{x} \in \mathbb{R}^m$ that satisfies $\mathbf{f}(\mathbf{x}) = 0$ for some function $\mathbf{f} : \mathbb{R}^m \to \mathbb{R}^m$.

To see how it works, take $m = 2$ so that $\mathbf{x} = (x_1, x_2)^\top$ and $\mathbf{f} = [f_1(\mathbf{x}), f_2(\mathbf{x})]^\top$. Taking the linear terms in Taylor's theorem for two variables gives

$$0 \approx f_1(\mathbf{x}_{k+1}) \approx f_1(\mathbf{x}_k) + \left.\frac{\partial f_1}{\partial x_1}\right|_{\mathbf{x}_k} (x_{1,k+1} - x_{1,k}) + \left.\frac{\partial f_1}{\partial x_2}\right|_{\mathbf{x}_k} (x_{2,k+1} - x_{2,k}),$$
$$0 \approx f_2(\mathbf{x}_{k+1}) \approx f_2(\mathbf{x}_k) + \left.\frac{\partial f_2}{\partial x_1}\right|_{\mathbf{x}_k} (x_{1,k+1} - x_{1,k}) + \left.\frac{\partial f_2}{\partial x_2}\right|_{\mathbf{x}_k} (x_{2,k+1} - x_{2,k}).$$

In matrix form, we can write

$$\begin{pmatrix} 0 \\ 0 \end{pmatrix} = \begin{pmatrix} f_1(\mathbf{x}_k) \\ f_2(\mathbf{x}_k) \end{pmatrix} + \begin{pmatrix} \frac{\partial f_1}{\partial x_1}(\mathbf{x}_k) & \frac{\partial f_1}{\partial x_2}(\mathbf{x}_k) \\ \frac{\partial f_2}{\partial x_1}(\mathbf{x}_k) & \frac{\partial f_2}{\partial x_2}(\mathbf{x}_k) \end{pmatrix} \begin{pmatrix} x_{1,k+1} - x_{1,k} \\ x_{2,k+1} - x_{2,k} \end{pmatrix}.$$

The matrix of partial derivatives is called the **Jacobian matrix** $J(\mathbf{x}_k)$, so (for any m) we have

$$\mathbf{0} = \mathbf{f}(\mathbf{x}_k) + J(\mathbf{x}_k)(\mathbf{x}_{k+1} - \mathbf{x}_k).$$

To derive Newton's method, we rearrange this equation for $\mathbf{x}_{k+1}$,

$$J(\mathbf{x}_k)(\mathbf{x}_{k+1} - \mathbf{x}_k) = -\mathbf{f}(\mathbf{x}_k) \quad \Longrightarrow \quad \mathbf{x}_{k+1} = \mathbf{x}_k - J^{-1}(\mathbf{x}_k)\mathbf{f}(\mathbf{x}_k).$$

So to apply the method, we need the inverse of J.

> **Note**
>
> If $m = 1$, then $J(x_k) = \frac{\partial f}{\partial x}(x_k)$, and $J^{-1} = 1/J$, so this reduces to the scalar Newton's method.

Example 2.25: Apply Newton's method to the simultaneous equations $xy - y^3 - 1 = 0$ and $x^2y + y - 5 = 0$, with starting values $x_0 = 2$, $y_0 = 3$.

The Jacobian matrix is

$$J(x, y) = \begin{pmatrix} y & x - 3y^2 \\ 2xy & x^2 + 1 \end{pmatrix},$$

and hence its inverse is given by

$$J^{-1}(x, y) = \frac{1}{y(x^2 + 1) - 2xy(x - 3y^2)} \begin{pmatrix} x^2 + 1 & 3y^2 - x \\ -2xy & y \end{pmatrix}.$$

The first iteration of Newton's method gives

$$\begin{pmatrix} x_1 \\ y_1 \end{pmatrix} = \begin{pmatrix} 2 \\ 3 \end{pmatrix} - \frac{1}{3(5) - 12(2 - 27)} \begin{pmatrix} 5 & 25 \\ -12 & 3 \end{pmatrix} \begin{pmatrix} -22 \\ 10 \end{pmatrix} = \begin{pmatrix} 1.55555556 \\ 2.06666667 \end{pmatrix}.$$

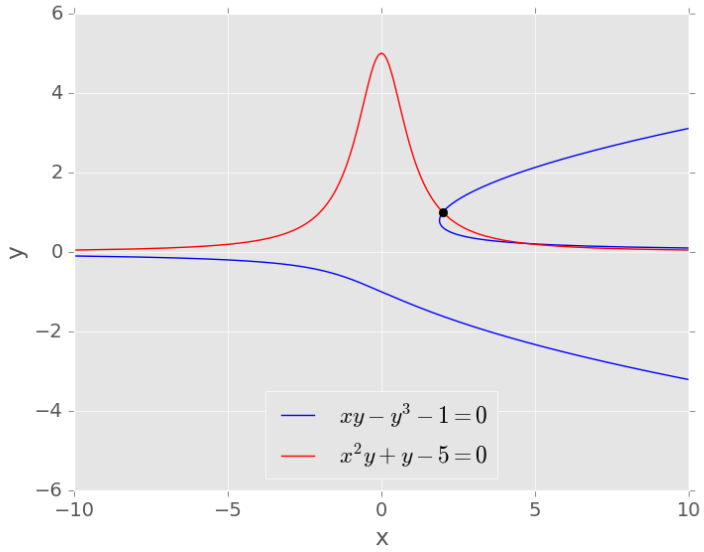
Subsequent iterations give

$$\begin{pmatrix} x_2 \\ y_2 \end{pmatrix} = \begin{pmatrix} 1.54720541 \\ 1.47779333 \end{pmatrix}, \begin{pmatrix} x_3 \\ y_3 \end{pmatrix} = \begin{pmatrix} 1.78053503 \\ 1.15886481 \end{pmatrix},$$

and

$$\begin{pmatrix} x_4 \\ y_4 \end{pmatrix} = \begin{pmatrix} 1.952843 \\ 1.02844269 \end{pmatrix}, \begin{pmatrix} x_5 \\ y_5 \end{pmatrix} = \begin{pmatrix} 1.99776297 \\ 1.00124041 \end{pmatrix},$$

so the method is converging accurately to the root $x_* = 2$, $y_* = 1$, shown in the following plot:



By generalising the scalar analysis (beyond the scope of this course), it can be shown that the convergence is quadratic for $\mathbf{x}_0$ sufficiently close to $\mathbf{x}_*$, provided that $J(\mathbf{x}_*)$ is non-singular (i.e., $\det[J(\mathbf{x}_*)] \neq 0$).

> **Note**
>
> In general, finding a good starting point in more than one dimension is difficult, particularly because interval bisection is not available. Algorithms that try to mimic bisection in higher dimensions are available, proceeding by a 'grid search' approach.

2.2.6 Quasi-Newton methods

A drawback of Newton's method is that the derivative $f'(x_k)$ must be computed at each iteration. This may be expensive to compute, or may not be available as a formula. For example, the function f might be the right-hand side of some complex partial differential equation, and hence both difficult to differentiate and very high dimensional!

Instead we can use a **quasi-Newton method**

$$x_{k+1} = x_k - \frac{f(x_k)}{g_k},$$

where g_k is some easily-computed approximation to $f'(x_k)$.

Example 2.26: Steffensen's method

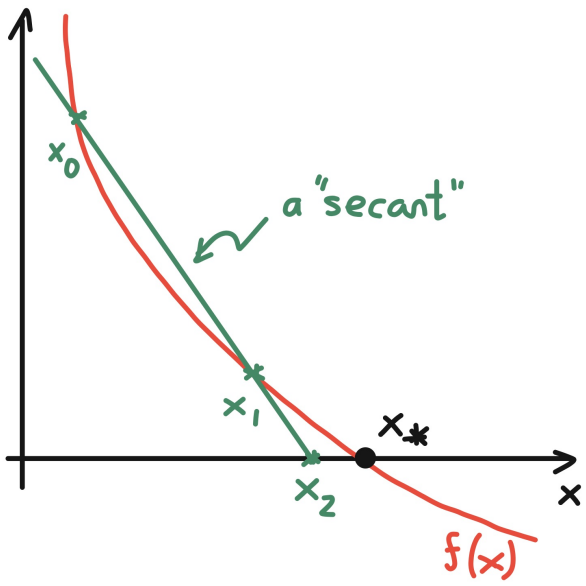
$$g_k = \frac{f(f(x_k) + x_k) - f(x_k)}{f(x_k)}.$$

This has the form $\frac{1}{h}(f(x_k + h) - f(x_k))$ with $h = f(x_k)$.

Steffensen's method requires two function evaluations per iteration. But once the iteration has started, we already have two nearby points x_{k-1}, x_k, so we could approximate $f'(x_k)$ by a backward difference

$$g_k = \frac{f(x_k) - f(x_{k-1})}{x_k - x_{k-1}} \quad \Longrightarrow \quad x_{k+1} = x_k - \frac{f(x_k)(x_k - x_{k-1})}{f(x_k) - f(x_{k-1})}.$$

This is called the **secant method**, and requires only one function evaluation per iteration (once underway). The name comes from its graphical interpretation:



Note

The secant method was introduced by Newton.

Example 2.27: $f(x) = \frac{1}{x} - 0.5$.

Now we need two starting values, so take $x_0 = 0.25$, $x_1 = 0.5$. The secant method gives:

k	x_k	$\lvert x_* - x_k\rvert / \lvert x_* - x_{k-1}\rvert$
2	0.6875	0.75
3	1.01562	0.75
4	1.354	0.65625
5	1.68205	0.492188
6	1.8973	0.322998
7	1.98367	0.158976
8	1.99916	0.0513488

Convergence to ϵ_{M} is achieved in 12 iterations. Notice that the error ratio is decreasing, so the convergence is superlinear.

The secant method is a **two-point method** since $x_{k+1} = g(x_{k-1}, x_k)$. So theorems about single-point fixed-point iterations do not apply.

In general, one can have **multipoint methods** based on higher-order interpolation.

Theorem 2.12

If $f'(x_*) \neq 0$ then the secant method converges for x_0, x_1 sufficiently close to x_*, and the order of convergence is $(1 + \sqrt{5})/2 = 1.618\ldots$.

Note

This illustrates that orders of convergence need not be integers, and is also an appearance of the **golden ratio**.

Proof:
To simplify the notation, denote the truncation error by

$$\varepsilon_k := x_* - x_k.$$

Expanding in Taylor series around x_*, and using $f(x_*) = 0$, gives

$$f(x_{k-1}) = -f'(x_*)\varepsilon_{k-1} + \frac{f''(x_*)}{2}\varepsilon_{k-1}^2 + \mathcal{O}(\varepsilon_{k-1}^3),$$
$$f(x_k) = -f'(x_*)\varepsilon_k + \frac{f''(x_*)}{2}\varepsilon_k^2 + \mathcal{O}(\varepsilon_k^3).$$

So using the secant formula above we get

$$\begin{aligned}
\varepsilon_{k+1} &= \varepsilon_k - (\varepsilon_k - \varepsilon_{k-1}) \frac{-f'(x_*)\varepsilon_k + \frac{f''(x_*)}{2}\varepsilon_k^2 + \mathcal{O}(\varepsilon_k^3)}{-f'(x_*)(\varepsilon_k - \varepsilon_{k-1}) + \frac{f''(x_*)}{2}(\varepsilon_k^2 - \varepsilon_{k-1}^2) + \mathcal{O}(\varepsilon_{k-1}^3)} \\
&= \varepsilon_k - \frac{-f'(x_*)\varepsilon_k + \frac{f''(x_*)}{2}\varepsilon_k^2 + \mathcal{O}(\varepsilon_k^3)}{-f'(x_*) + \frac{f''(x_*)}{2}(\varepsilon_k + \varepsilon_{k-1}) + \mathcal{O}(\varepsilon_{k-1}^2)} \\
&= \varepsilon_k + \frac{-\varepsilon_k + \frac{1}{2}\varepsilon_k^2 f''(x_*)/f'(x_*) + \mathcal{O}(\varepsilon_k^3)}{1 - \frac{1}{2}(\varepsilon_k + \varepsilon_{k-1})f''(x_*)/f'(x_*) + \mathcal{O}(\varepsilon_{k-1}^2)} \\
&= \varepsilon_k + \left(-\varepsilon_k + \frac{f''(x_*)}{2f'(x_*)}\varepsilon_k^2 + \mathcal{O}(\varepsilon_k^3)\right)\left(1 + (\varepsilon_k + \varepsilon_{k-1})\frac{f''(x_*)}{2f'(x_*)} + \mathcal{O}(\varepsilon_{k-1}^2)\right) \\
&= \varepsilon_k - \varepsilon_k + \frac{f''(x_*)}{2f'(x_*)}\varepsilon_k^2 - \frac{f''(x_*)}{2f'(x_*)}\varepsilon_k(\varepsilon_k + \varepsilon_{k-1}) + \mathcal{O}(\varepsilon_{k-1}^3) \\
&= -\frac{f''(x_*)}{2f'(x_*)}\varepsilon_k\varepsilon_{k-1} + \mathcal{O}(\varepsilon_{k-1}^3).
\end{aligned}$$

This is similar to the corresponding formula for Newton's method, where we have

$$\varepsilon_{k+1} = -\frac{f''(x_*)}{2f'(x_*)}\varepsilon_k^2 + \mathcal{O}(\varepsilon_k^3).$$

The above tells us that the error for the secant method tends to zero faster than linearly, but not quadratically (because $\varepsilon_{k-1} > \varepsilon_k$).

To find the order of convergence, note that $\varepsilon_{k+1} \sim \varepsilon_k\varepsilon_{k-1}$ suggests a power-law relation of the form

$$|\varepsilon_k| = |\varepsilon_{k-1}|^\alpha \left|\frac{f''(x_*)}{2f'(x_*)}\right|^\beta \quad \Longrightarrow \quad |\varepsilon_{k-1}| = |\varepsilon_k|^{1/\alpha} \left|\frac{f''(x_*)}{2f'(x_*)}\right|^{-\beta/\alpha}.$$

Putting this in both sides of the previous equation gives

$$|\varepsilon_k|^\alpha \left|\frac{f''(x_*)}{2f'(x_*)}\right|^\beta = |\varepsilon_k|^{(1+\alpha)/\alpha} \left|\frac{f''(x_*)}{2f'(x_*)}\right|^{(\alpha-\beta)/\alpha}.$$

Equating powers gives

$$\alpha = \frac{1+\alpha}{\alpha} \quad \Longrightarrow \alpha = \frac{1+\sqrt{5}}{2}, \quad \beta = \frac{\alpha-\beta}{\alpha} \quad \Longrightarrow \beta = \frac{\alpha}{\alpha+1} = \frac{1}{\alpha}.$$

It follows that

$$\lim_{k\to\infty} \frac{|x_* - x_{k+1}|}{|x_* - x_k|^\alpha} = \lim_{k\to\infty} \frac{|\varepsilon_{k+1}|}{|\varepsilon_k|^\alpha} = \left|\frac{f''(x_*)}{2f'(x_*)}\right|^{1/\alpha},$$

so the secant method has order of convergence α.

Knowledge checklist

Key topics:

1. Polynomial interpolation, including the Lagrange and Newton divided-difference forms of polynomial interpolation.
2. Interpolation error estimates, truncation error, and the significance of node placement (e.g. the Runge phenomenon).
3. Numerical rootfinding methods, including interval bisection and fixed point iteration, with discussion of existence, uniqueness, and orders of convergence (linear, superlinear).

Key skills:

- Constructing and analyzing polynomial interpolants for a given data set and function, using Taylor, Lagrange, and Newton methods.
- Estimating approximation errors and choosing optimal interpolation nodes to improve numerical stability and convergence.
- Implementing and evaluating iterative algorithms for solving nonlinear equations, including measuring and understanding convergence rates.

3 Linear Algebra

3.1 Systems of Linear Equations

The central goal of this chapter is to answer the following seemingly straightforward question:

How do we solve a linear system numerically?

Linear systems of the form

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + \ldots + a_{1n}x_n &= b_1, \\ a_{21}x_1 + a_{22}x_2 + \ldots + a_{2n}x_n &= b_2, \\ \vdots \quad \vdots \quad & \quad \vdots \\ a_{n1}x_1 + a_{n2}x_2 + \ldots + a_{nn}x_n &= b_n \end{aligned}$$

occur in many applications (often with very large n). It is convenient to express this in matrix form:

$$A\mathbf{x} = \mathbf{b},$$

where A is an $n \times n$ square matrix with elements a_{ij}, and $\mathbf{x}$, $\mathbf{b}$ are $n \times 1$ vectors.

We will need some basic facts from linear algebra:

1. $A^\top$ is the **transpose** of A, so $(a^\top)_{ij} = a_{ji}$.
2. A is **symmetric** if $A = A^\top$.
3. A is **non-singular** iff there exists a solution $\mathbf{x} \in \mathbb{R}^n$ for every $\mathbf{b} \in \mathbb{R}^n$.
4. A is non-singular iff $\det(A) \neq 0$.
5. A is non-singular iff there exists a unique **inverse** A^{-1} such that $AA^{-1} = A^{-1}A = I$.

It follows from fact 5 above that $A\mathbf{x} = \mathbf{b}$ has a unique solution iff A is non-singular, given by $\mathbf{x} = A^{-1}\mathbf{b}$.

In this chapter, we will see how to solve $A\mathbf{x} = \mathbf{b}$ both **efficiently** and **accurately**.

Although this seems like a conceptually easy problem (just use Gaussian elimination!), it is actually a hard one when n gets large. Nowadays, linear systems with $n = 1$ million arise

routinely in computational problems. And even for small n there are some potential pitfalls, as we will see.

> **Note**
>
> If A is instead rectangular $(m \times n)$, then there are different numbers of equations and unknowns, and we do not expect a unique solution. Nevertheless, we can still look for an approximate solution in this case and there are methods for this problem in the course reading list.

Many algorithms are based on the idea of rewriting $A\mathbf{x} = \mathbf{b}$ in a form where the matrix is easier to invert. Easiest to invert are diagonal matrices, followed by orthogonal matrices (where $A^{-1} = A^{\top}$). However, the most common method for solving $A\mathbf{x} = \mathbf{b}$ transforms the system to *triangular* form.

3.2 Triangular systems

If the matrix A is triangular, then $A\mathbf{x} = \mathbf{b}$ is straightforward to solve.

A matrix L is called **lower triangular** if all entries above the diagonal are zero:

$$L = \begin{pmatrix} l_{11} & 0 & \cdots & 0 \\ l_{21} & l_{22} & \ddots & \vdots \\ \vdots & & \ddots & 0 \\ l_{n1} & \cdots & \cdots & l_{nn} \end{pmatrix}.$$

The determinant is just

$$\det(L) = l_{11} l_{22} \cdots l_{nn},$$

so the matrix will be non-singular iff all of the diagonal elements are non-zero.

Example 3.1: Solve $L\mathbf{x} = \mathbf{b}$ for $n = 4$.

The system is

$$\begin{pmatrix} l_{11} & 0 & 0 & 0 \\ l_{21} & l_{22} & 0 & 0 \\ l_{31} & l_{32} & l_{33} & 0 \\ l_{41} & l_{42} & l_{43} & l_{44} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{pmatrix}$$

which is equivalent to

$$\begin{aligned} l_{11}x_1 &= b_1, \\ l_{21}x_1 + l_{22}x_2 &= b_2, \\ l_{31}x_1 + l_{32}x_2 + l_{33}x_3 &= b_3, \\ l_{41}x_1 + l_{42}x_2 + l_{43}x_3 + l_{44}x_4 &= b_4. \end{aligned}$$

We can just solve step-by-step:

$$x_1 = \frac{b_1}{l_{11}},\ x_2 = \frac{b_2 - l_{21}x_1}{l_{22}},$$

$$x_3 = \frac{b_3 - l_{31}x_1 - l_{32}x_2}{l_{33}},\ x_4 = \frac{b_4 - l_{41}x_1 - l_{42}x_2 - l_{43}x_3}{l_{44}}.$$

This is fine since we know that l_{11}, l_{22}, l_{33}, l_{44} are all non-zero when a solution exists.

In general, any lower triangular system $L\mathbf{x} = \mathbf{b}$ can be solved by **forward substitution**

$$x_j = \frac{b_j - \sum_{k=1}^{j-1} l_{jk}x_k}{l_{jj}}, \quad j = 1, \ldots, n.$$

Similarly, an **upper triangular** matrix U has the form

$$U = \begin{pmatrix} u_{11} & u_{12} & \cdots & u_{1n} \\ 0 & u_{22} & & \vdots \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & u_{nn} \end{pmatrix},$$

and an upper-triangular system $U\mathbf{x} = \mathbf{b}$ may be solved by **backward substitution**

$$x_j = \frac{b_j - \sum_{k=j+1}^{n} u_{jk}x_k}{u_{jj}}, \quad j = n, \ldots, 1.$$

To estimate the computational cost of forward substitution, we can count the number of floating-point operations ($+$, $-$, $\times$, $\div$).

Example 3.2: Number of operations required for forward substitution.

Consider each x_j. We have - $j = 1$: 1 division - $j = 2$: 1 division + [1 subtraction + 1 multiplication] - $j = 3$: 1 division + 2 $\times$[1 subtraction + 1 multiplication] - $\vdots$ - $j = n$: 1 division + $(n-1)$ $\times$[1 subtraction + 1 multiplication]

So the total number of operations required is

$$\sum_{j=1}^{n} \Big(1 + 2(j-1)\Big) = 2\sum_{j=1}^{n} j - \sum_{j=1}^{n} 1 = n(n+1) - n = n^2.$$

So solving a triangular system by forward (or backward) substitution takes n^2 operations. We may say that the **computational complexity** of the algorithm is n^2.

> **Note**
>
> In practice, this is only a rough estimate of the computational cost, because reading from and writing to the computer's memory also take time. This can be estimated given a "memory model", but this depends on the particular computer.

3.3 Gaussian elimination

If our matrix A is not triangular, we can try to transform it to triangular form. **Gaussian elimination** uses elementary row operations to transform the system to upper triangular form $U\mathbf{x} = \mathbf{y}$.

Elementary row operations include swapping rows and adding multiples of one row to another. They won't change the solution $\mathbf{x}$, but will change the matrix A and the right-hand side $\mathbf{b}$.

Example 3.3: Transform to upper triangular form the system

$$\begin{aligned} x_1 + 2x_2 + x_3 &= 0, \\ x_1 - 2x_2 + 2x_3 &= 4, \\ 2x_1 + 12x_2 - 2x_3 &= 4. \end{aligned}$$

$$A = \begin{pmatrix} 1 & 2 & 1 \\ 1 & -2 & 2 \\ 2 & 12 & -2 \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} 0 \\ 4 \\ 4 \end{pmatrix}.$$

Stage 1. Subtract 1 times equation 1 from equation 2, and 2 times equation 1 from equation 3, so as to eliminate x_1 from equations 2 and 3:

$$\begin{aligned} x_1 + 2x_2 + x_3 &= 0, \\ -4x_2 + x_3 &= 4, \\ 8x_2 - 4x_3 &= 4. \end{aligned}$$

$$A^{(2)} = \begin{pmatrix} 1 & 2 & 1 \\ 0 & -4 & 1 \\ 0 & 8 & -4 \end{pmatrix} \quad \mathbf{b}^{(2)} = \begin{pmatrix} 0 \\ 4 \\ 4 \end{pmatrix}, \quad m_{21} = 1, \quad m_{31} = 2.$$

Stage 2. Subtract -2 times equation 2 from equation 3, to eliminate x_2 from equation 3:

$$\begin{aligned} x_1 + 2x_2 + x_3 &= 0, \\ -4x_2 + x_3 &= 4, \\ -2x_3 &= 12. \end{aligned}$$

$$A^{(3)} = \begin{pmatrix} 1 & 2 & 1 \\ 0 & -4 & 1 \\ 0 & 0 & -2 \end{pmatrix} \quad \mathbf{b}^{(3)} = \begin{pmatrix} 0 \\ 4 \\ 12 \end{pmatrix}, \quad m_{32} = -2.$$

Now the system is upper triangular, and back substitution gives $x_1 = 11$, $x_2 = -\frac{5}{2}$, $x_3 = -6$.

We can write the general algorithm as follows.

Algorithm 3.1: Gaussian elimination

Let $A^{(1)} = A$ and $\mathbf{b}^{(1)} = \mathbf{b}$. Then for each k from 1 to $n-1$, compute a new matrix $A^{(k+1)}$ and right-hand side $\mathbf{b}^{(k+1)}$ by the following procedure:

1. Define the row multipliers

$$m_{ik} = \frac{a_{ik}^{(k)}}{a_{kk}^{(k)}}, \quad i = k+1, \ldots, n.$$

2. Use these to remove the unknown x_k from equations $k+1$ to n, leaving

$$a_{ij}^{(k+1)} = a_{ij}^{(k)} - m_{ik} a_{kj}^{(k)}, \quad b_i^{(k+1)} = b_i^{(k)} - m_{ik} b_k^{(k)}, \quad i, j = k+1, \ldots, n.$$

The final matrix $A^{(n)} = U$ will then be upper triangular.

This procedure will work providing $a_{kk}^{(k)} \neq 0$ for every k. (We will worry about this later.)

What about the computational cost of Gaussian elimination?

Example 3.4: Number of operations required to find U.

Computing $A^{(k+1)}$ requires: - $n-(k+1)+1 = n-k$ divisions to compute m_{ik}. - $(n-k)^2$ subtractions and the same number of multiplications to compute $a_{ij}^{(k+1)}$.
So in total $A^{(k+1)}$ requires $2(n-k)^2 + n - k$ operations. Overall, we need to compute $A^{(k+1)}$ for $k = 1, \ldots, n-1$, so the total number of operations is

$$\begin{aligned} N &= \sum_{k=1}^{n-1} \left(2n^2 + n - (4n+1)k + 2k^2\right) \\ &= n(2n+1)\sum_{k=1}^{n-1} 1 - (4n+1)\sum_{k=1}^{n-1} k + 2\sum_{k=1}^{n-1} k^2. \end{aligned}$$

Recalling that

$$\sum_{k=1}^{n} k = \tfrac{1}{2}n(n+1), \ \sum_{k=1}^{n} k^2 = \tfrac{1}{6}n(n+1)(2n+1),$$

we find

$$\begin{aligned} N &= n(2n+1)(n-1) - \tfrac{1}{2}(4n+1)(n-1)n + \tfrac{1}{3}(n-1)n(2n-1) \\ &= \tfrac{2}{3}n^3 - \tfrac{1}{2}n^2 - \tfrac{1}{6}n. \end{aligned}$$

So the number of operations required to find U is $\mathcal{O}(n^3)$.

It is known that $\mathcal{O}(n^3)$ is not optimal, and the best theoretical algorithm known for inverting a matrix takes $\mathcal{O}(n^{2.3728639})$ operations. However, algorithms achieving this bound are highly impractical for most real-world uses due to massive constant factors and implementation overhead. It remains an open conjecture that there exists an $\mathcal{O}(n^{2+\epsilon})$ algorithm, for ϵ arbitrarily small.

3.4 LU decomposition

In Gaussian elimination, both the final matrix U and the sequence of row operations are determined solely by A, and do not depend on $\mathbf{b}$. We will see that the sequence of row operations that transforms A to U is equivalent to left-multiplying by a matrix F, so that

$$FA = U, \qquad U\mathbf{x} = F\mathbf{b}.$$

To see this, note that step k of Gaussian elimination can be written in the form

$$A^{(k+1)} = F^{(k)}A^{(k)}, \quad \mathbf{b}^{(k+1)} = F^{(k)}\mathbf{b}^{(k)},$$

where

$$F^{(k)} := \begin{pmatrix} 1 & 0 & \cdots & \cdots & \cdots & 0 \\ 0 & \ddots & \ddots & & & \vdots \\ \vdots & \ddots & 1 & \ddots & & \vdots \\ \vdots & & -m_{k+1,k} & \ddots & \ddots & \vdots \\ \vdots & & \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & -m_{n,k} & \cdots & 0 & 1 \end{pmatrix}.$$

Multiplying by $F^{(k)}$ has the effect of subtracting m_{ik} times row k from row i, for $i = k+1, \ldots, n$.

> **Note**
>
> A matrix with this structure (the identity except for a single column below the diagonal) is called a **Frobenius matrix**.

Example 3.5

You can check in the earlier example that

$$F^{(1)}A = \begin{pmatrix} 1 & 0 & 0 \\ -1 & 1 & 0 \\ -2 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 2 & 1 \\ 1 & -2 & 2 \\ 2 & 12 & -2 \end{pmatrix} = \begin{pmatrix} 1 & 2 & 1 \\ 0 & -4 & 1 \\ 0 & 8 & -4 \end{pmatrix} = A^{(2)},$$

and

$$F^{(2)}A^{(2)} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 2 & 1 \end{pmatrix} \begin{pmatrix} 1 & 2 & 1 \\ 0 & -4 & 1 \\ 0 & 8 & -4 \end{pmatrix} = \begin{pmatrix} 1 & 2 & 1 \\ 0 & -4 & 1 \\ 0 & 0 & -2 \end{pmatrix} = A^{(3)} = U.$$

It follows that

$$U = A^{(n)} = F^{(n-1)}F^{(n-2)} \cdots F^{(1)}A.$$

Now the $F^{(k)}$ are invertible, and the inverse is just given by adding rows instead of subtracting:

$$(F^{(k)})^{-1} = \begin{pmatrix} 1 & 0 & \cdots & \cdots & \cdots & 0 \\ 0 & \ddots & \ddots & & & \vdots \\ \vdots & \ddots & 1 & \ddots & & \vdots \\ \vdots & & m_{k+1,k} & \ddots & \ddots & \vdots \\ \vdots & & \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & m_{n,k} & \cdots & 0 & 1 \end{pmatrix}.$$

So we could write

$$A = (F^{(1)})^{-1}(F^{(2)})^{-1} \cdots (F^{(n-1)})^{-1}U.$$

Since the successive operations don't "interfere" with each other, we can write

$$(F^{(1)})^{-1}(F^{(2)})^{-1}\cdots(F^{(n-1)})^{-1} = \begin{pmatrix} 1 & 0 & \cdots & \cdots & \cdots & 0 \\ m_{2,1} & 1 & \ddots & & & \vdots \\ m_{3,1} & m_{3,2} & 1 & \ddots & & \vdots \\ m_{4,1} & m_{4,2} & m_{4,3} & \ddots & \ddots & \vdots \\ \vdots & \vdots & \vdots & & 1 & 0 \\ m_{n,1} & m_{n,2} & m_{n,3} & \cdots & m_{n,n-1} & 1 \end{pmatrix} := L.$$

Thus we have established the following result.

Theorem 3.1: LU decomposition

Let U be the upper triangular matrix from Gaussian elimination of A (without pivoting), and let L be the unit lower triangular matrix above. Then

$$A = LU.$$

Note

Unit lower triangular means that there are all 1's on the diagonal.

The theorem above says that Gaussian elimination is equivalent to factorising A as the product of a lower triangular and an upper triangular matrix. This is not at all obvious from the algorithm! The decomposition is unique up to a scaling LD, $D^{-1}U$ for some diagonal matrix D.

The system $A\mathbf{x} = \mathbf{b}$ becomes $LU\mathbf{x} = \mathbf{b}$, which we can readily solve by setting $U\mathbf{x} = \mathbf{y}$. We first solve $L\mathbf{y} = \mathbf{b}$ for $\mathbf{y}$, then $U\mathbf{x} = \mathbf{y}$ for $\mathbf{x}$. Both are triangular systems.

Moreover, if we want to solve several systems $A\mathbf{x} = \mathbf{b}$ with different $\mathbf{b}$ but the same matrix, we just need to compute L and U once. This saves time because, although the initial LU factorisation takes $\mathcal{O}(n^3)$ operations, the evaluation takes only $\mathcal{O}(n^2)$.

Note

This matrix factorisation viewpoint dates only from the 1940s, and LU decomposition was introduced by Alan Turing in a 1948 paper (*Q. J. Mechanics Appl. Mat.* **1**, 287). Other common factorisations used in numerical linear algebra are **QR** (which we will see later) and *Cholesky*.

Example 3.6

Solve our earlier example by LU decomposition.

$$\begin{pmatrix} 1 & 2 & 1 \\ 1 & -2 & 2 \\ 2 & 12 & -2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 4 \\ 4 \end{pmatrix}.$$

We apply Gaussian elimination as before, but ignore $\mathbf{b}$ (for now), leading to

$$U = \begin{pmatrix} 1 & 2 & 1 \\ 0 & -4 & 1 \\ 0 & 0 & -2 \end{pmatrix}.$$

As we apply the elimination, we record the multipliers so as to construct the matrix

$$L = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 2 & -2 & 1 \end{pmatrix}.$$

Thus we have the factorisation/decomposition

$$\begin{pmatrix} 1 & 2 & 1 \\ 1 & -2 & 2 \\ 2 & 12 & -2 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 2 & -2 & 1 \end{pmatrix} \begin{pmatrix} 1 & 2 & 1 \\ 0 & -4 & 1 \\ 0 & 0 & -2 \end{pmatrix}.$$

With the matrices L and U, we can readily solve for any right-hand side $\mathbf{b}$. We illustrate for our particular $\mathbf{b}$. Firstly, solve $L\mathbf{y} = \mathbf{b}$:

$$\begin{pmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 2 & -2 & 1 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 4 \\ 4 \end{pmatrix}$$

$$\implies y_1 = 0,\ y_2 = 4 - y_1 = 4,\ y_3 = 4 - 2y_1 + 2y_2 = 12.$$

Notice that $\mathbf{y}$ is the right-hand side $\mathbf{b}^{(3)}$ constructed earlier. Then, solve $U\mathbf{x} = \mathbf{y}$:

$$\begin{pmatrix} 1 & 2 & 1 \\ 0 & -4 & 1 \\ 0 & 0 & -2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 4 \\ 12 \end{pmatrix}$$

$$\implies x_3 = -6,\ x_2 = -\tfrac{1}{4}(4 - x_3) = -\tfrac{5}{2},\ x_1 = -2x_2 - x_3 = 11.$$

3.5 Vector norms

To measure the error when the solution is a vector, as opposed to a scalar, we usually summarize the error in a single number called a **norm**. A **norm** effectively gives us a way to define a notion of distance in higher dimensions.

A **vector norm** on $\mathbb{R}^n$ is a real-valued function that satisfies: 1. $\|\mathbf{x}+\mathbf{y}\| \leq \|\mathbf{x}\| + \|\mathbf{y}\|$ for every $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$ (**triangle inequality**). 2. $\|\alpha\mathbf{x}\| = |\alpha| \, \|\mathbf{x}\|$ for every $\mathbf{x} \in \mathbb{R}^n$ and every $\alpha \in \mathbb{R}$. 3. $\|\mathbf{x}\| \geq 0$ for every $\mathbf{x} \in \mathbb{R}^n$, and $\|\mathbf{x}\| = 0$ implies $\mathbf{x} = 0$.

Example 3.7: There are three common examples:

1. The ℓ_2**-norm**

$$\|\mathbf{x}\|_2 := \sqrt{\sum_{k=1}^{n} x_k^2} = \sqrt{\mathbf{x}^\top \mathbf{x}}.$$

   This is just the usual Euclidean length of $\mathbf{x}$.

2. The ℓ_1**-norm**

$$\|\mathbf{x}\|_1 := \sum_{k=1}^{n} |x_k|.$$

   This is sometimes known as the **taxicab** or **Manhattan** norm, because it corresponds to the distance that a taxi has to drive on a rectangular grid of streets to get to $\mathbf{x} \in \mathbb{R}^2$.

3. The ℓ_∞**-norm**

$$\|\mathbf{x}\|_\infty := \max_{k=1,\ldots,n} |x_k|.$$

   This is sometimes known as the **maximum** norm.

The norms in the example above are all special cases of the ℓ_p-norm,

$$\|\mathbf{x}\|_p = \left(\sum_{k=1}^{n} |x_k|^p \right)^{1/p},$$

which is a norm for any real number $p \geq 1$. Increasing p means that more and more emphasis is given to the maximum element $|x_k|$.

Example 3.8: Consider the vectors $\mathbf{a} = (1, -2, 3)^\top$, $\mathbf{b} = (2, 0, -1)^\top$, and $\mathbf{c} = (0, 1, 4)^\top$.

The ℓ_1-, ℓ_2-, and ℓ_∞-norms are:

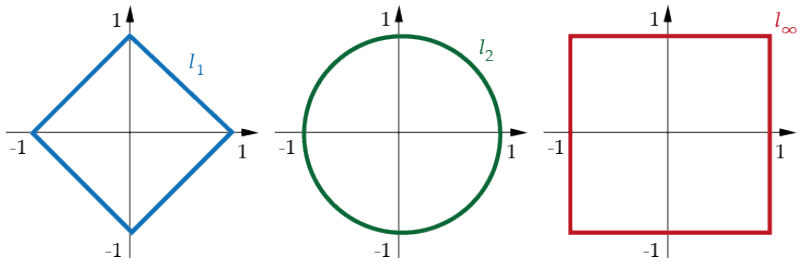
$$\begin{aligned} \|\mathbf{a}\|_1 &= 1 + 2 + 3 = 6 \\ \|\mathbf{b}\|_1 &= 2 + 0 + 1 = 3 \\ \|\mathbf{c}\|_1 &= 0 + 1 + 4 = 5 \end{aligned}$$

$$\begin{aligned} \|\mathbf{a}\|_2 &= \sqrt{1 + 4 + 9} \approx 3.74 \\ \|\mathbf{b}\|_2 &= \sqrt{4 + 0 + 1} \approx 2.24 \\ \|\mathbf{c}\|_2 &= \sqrt{0 + 1 + 16} \approx 4.12 \end{aligned}$$

$$\begin{aligned} \|\mathbf{a}\|_\infty &= \max\{1, 2, 3\} = 3 \\ \|\mathbf{b}\|_\infty &= \max\{2, 0, 1\} = 2 \\ \|\mathbf{c}\|_\infty &= \max\{0, 1, 4\} = 4 \end{aligned}$$

Notice that, for a single vector $\mathbf{x}$, the norms satisfy the ordering $\|\mathbf{x}\|_1 \geq \|\mathbf{x}\|_2 \geq \|\mathbf{x}\|_\infty$, but that vectors may be ordered differently by different norms.

Example 3.9: Sketch the 'unit circles' $\{\mathbf{x} \in \mathbb{R}^2 : \|\mathbf{x}\|_p = 1\}$ for $p = 1, 2, \infty$.



3.6 Matrix norms

We also use norms to measure the "size" of matrices. Since the set $\mathbb{R}^{n\times n}$ of $n \times n$ matrices with real entries is a vector space, we could just use a vector norm on this space. But usually we add an additional axiom.

A **matrix norm** is a real-valued function $\|\cdot\|$ on $\mathbb{R}^{n\times n}$ that satisfies:

1. $\|A + B\| \leq \|A\| + \|B\|$ for every $A, B \in \mathbb{R}^{n\times n}$.

2. $\|\alpha A\| = |\alpha| \, \|A\|$ for every $A \in \mathbb{R}^{n \times n}$ and every $\alpha \in \mathbb{R}$.
3. $\|A\| \geq 0$ for every $A \in \mathbb{R}^{n \times n}$ and $\|A\| = 0$ implies $A = 0$.
4. $\|AB\| \leq \|A\| \|B\|$ for every $A, B \in \mathbb{R}^{n \times n}$ (**consistency**).

> **i** Note
>
> We usually want this additional axiom because matrices are more than just vectors. Some books call this a **submultiplicative norm** and define a "matrix norm" to satisfy just the first three properties, perhaps because (4) only works for square matrices.

Example 3.10: Frobenius norm

If we treat a matrix as a big vector with n^2 components, then the ℓ_2-norm is called the **Frobenius norm** of the matrix:

$$\|A\|_F = \sqrt{\sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij}^2}.$$

This norm is rarely used in numerical analysis because it is not induced by any vector norm (as we are about to define).

The most important matrix norms are so-called **induced** or **operator** norms. Remember that A is a linear map on $\mathbb{R}^n$, meaning that it maps every vector to another vector. So we can measure the size of A by how much it can stretch vectors with respect to a given vector norm. Specifically, if $\|\cdot\|_p$ is a vector norm, then the **induced** norm is defined as

$$\|A\|_p := \sup_{\mathbf{x} \neq \mathbf{0}} \frac{\|A\mathbf{x}\|_p}{\|\mathbf{x}\|_p} = \max_{\|\mathbf{x}\|_p = 1} \|A\mathbf{x}\|_p.$$

To see that the two definitions here are equivalent, use the fact that $\|\cdot\|_p$ is a vector norm. So by property (2) we have

$$\sup_{\mathbf{x} \neq \mathbf{0}} \frac{\|A\mathbf{x}\|_p}{\|\mathbf{x}\|_p} = \sup_{\mathbf{x} \neq \mathbf{0}} \left\| A \frac{\mathbf{x}}{\|\mathbf{x}\|_p} \right\|_p = \sup_{\|\mathbf{y}\|_p = 1} \|A\mathbf{y}\|_p = \max_{\|\mathbf{y}\|_p = 1} \|A\mathbf{y}\|_p.$$

> **i** Note
>
> Usually we use the same notation for the induced matrix norm as for the original vector norm. The meaning should be clear from the context.

Example 3.11

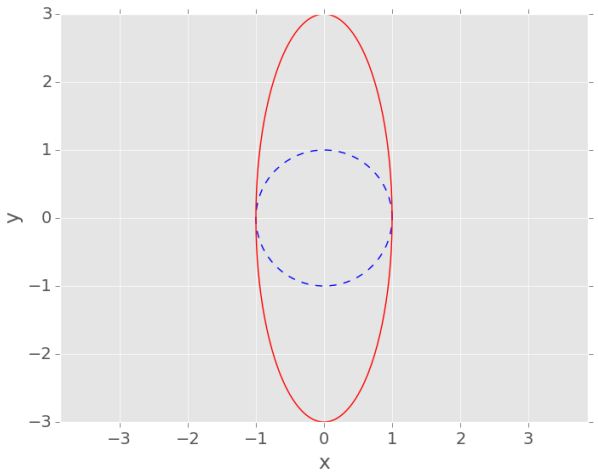
Let

$$A = \begin{pmatrix} 0 & 1 \\ 3 & 0 \end{pmatrix}.$$

In the ℓ_2-norm, a unit vector in $\mathbb{R}^2$ has the form $\mathbf{x} = (\cos\theta, \sin\theta)^\top$, so the image of the unit circle is

$$A\mathbf{x} = \begin{pmatrix} \sin\theta \\ 3\cos\theta \end{pmatrix}.$$

This is illustrated below:



The induced matrix norm is the maximum stretching of this unit circle, which is

$$\|A\|_2 = \max_{\|\mathbf{x}\|_2=1} \|A\mathbf{x}\|_2 = \max_\theta \left(\sin^2\theta + 9\cos^2\theta\right)^{1/2} = \max_\theta \left(1 + 8\cos^2\theta\right)^{1/2} = 3.$$

Theorem 3.2: Induced norms are matrix norms

The induced norm corresponding to any vector norm is a matrix norm, and the two norms satisfy $\|A\mathbf{x}\| \leq \|A\|\|\mathbf{x}\|$ for any matrix $A \in \mathbb{R}^{n\times n}$ and any vector $\mathbf{x} \in \mathbb{R}^n$.

Proof:
Properties (1)-(3) follow from the fact that the vector norm satisfies the corresponding properties. To show (4), note that, by the definition above, we have for any vector $\mathbf{y} \in \mathbb{R}^n$ that

$$\|A\| \geq \frac{\|A\mathbf{y}\|}{\|\mathbf{y}\|} \quad \Longrightarrow \quad \|A\mathbf{y}\| \leq \|A\|\|\mathbf{y}\|.$$

Taking $\mathbf{y} = B\mathbf{x}$ for some $\mathbf{x}$ with $\|\mathbf{x}\| = 1$, we get

$$\|AB\mathbf{x}\| \leq \|A\|\|B\mathbf{x}\| \leq \|A\|\|B\|.$$

This holds in particular for the vector $\mathbf{x}$ that maximises $\|AB\mathbf{x}\|$, so

$$\|AB\| = \max_{\|\mathbf{x}\|=1} \|AB\mathbf{x}\| \leq \|A\|\|B\|.$$

It is cumbersome to compute the induced norms from their definition, but fortunately there are some very useful alternative formulae.

Theorem 3.3: Matrix norms induced by ℓ_1 and ℓ_∞

The matrix norms induced by the ℓ_1-norm and ℓ_∞-norm satisfy

$$\|A\|_1 = \max_{j=1,\ldots,n} \sum_{i=1}^{n} |a_{ij}|, \quad \text{(maximum column sum)}$$

$$\|A\|_\infty = \max_{i=1,\ldots,n} \sum_{j=1}^{n} |a_{ij}|. \quad \text{(maximum row sum)}$$

Proof:
We will prove the result for the ℓ_1-norm as an illustration of the method:

$$\|A\mathbf{x}\|_1 = \sum_{i=1}^{n} \left| \sum_{j=1}^{n} a_{ij}x_j \right| \leq \sum_{i=1}^{n} \sum_{j=1}^{n} |a_{ij}|\,|x_j| = \sum_{j=1}^{n} |x_j| \sum_{i=1}^{n} |a_{ij}|.$$

If we let

$$c = \max_{j=1,\ldots,n} \sum_{i=1}^{n} |a_{ij}|,$$

then

$$\|A\mathbf{x}\|_1 \leq c\|\mathbf{x}\|_1 \quad \Longrightarrow \quad \|A\|_1 \leq c.$$

Now let m be the column where the maximum sum is attained. If we choose $\mathbf{y}$ to be the vector with components $y_k = \delta_{km}$, then we have $\|A\mathbf{y}\|_1 = c$. Since $\|\mathbf{y}\|_1 = 1$, we must have that

$$\max_{\|\mathbf{x}\|_1=1} \|A\mathbf{x}\|_1 \geq \|A\mathbf{y}\|_1 = c \quad \Longrightarrow \quad \|A\|_1 \geq c.$$

The only way to satisfy both inequalities is if $\|A\|_1 = c$.

Example 3.12

For the matrix

$$A = \begin{pmatrix} -7 & 3 & -1 \\ 2 & 4 & 5 \\ -4 & 6 & 0 \end{pmatrix}$$

we have

$$\|A\|_1 = \max\{13, 13, 6\} = 13, \qquad \|A\|_\infty = \max\{11, 11, 10\} = 11.$$

What about the matrix norm induced by the ℓ_2-norm? This turns out to be related to the eigenvalues of A. Recall that $\lambda \in \mathbb{C}$ is an **eigenvalue** of A with associated **eigenvector u** if

$$A\mathbf{u} = \lambda\mathbf{u}.$$

We define the **spectral radius** $\rho(A)$ of A to be the maximum $|\lambda|$ over all eigenvalues λ of A.

Theorem 3.4: Spectral norm

The matrix norm induced by the ℓ_2-norm satisfies

$$\|A\|_2 = \sqrt{\rho(A^\top A)}.$$

As a result of the theorem above, this norm is sometimes known as the **spectral norm**.

Example 3.13

For our matrix

$$A = \begin{pmatrix} 0 & 1 \\ 3 & 0 \end{pmatrix},$$

we have

$$A^\top A = \begin{pmatrix} 0 & 3 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 3 & 0 \end{pmatrix} = \begin{pmatrix} 9 & 0 \\ 0 & 1 \end{pmatrix}.$$

We see that the eigenvalues of $A^\top A$ are $\lambda = 1, 9$, so $\|A\|_2 = \sqrt{9} = 3$ (as we calculated earlier).

Proof:
We want to show that

$$\max_{\|\mathbf{x}\|_2=1} \|A\mathbf{x}\|_2 = \max\{\sqrt{|\lambda|} \,:\, \lambda \text{ eigenvalue of } A^\top A\}.$$

For A real, $A^\top A$ is symmetric, so has real eigenvalues $\lambda_1 \le \lambda_2 \le \ldots \le \lambda_n$ with corresponding orthonormal eigenvectors $\mathbf{u}_1, \ldots, \mathbf{u}_n$ in $\mathbb{R}^n$. (Orthonormal means that $\mathbf{u}_j^\top \mathbf{u}_k = \delta_{jk}$.) Note also

that all of the eigenvalues are non-negative, since

$$A^\top A\mathbf{u}_1 = \lambda_1 \mathbf{u}_1 \quad \implies \lambda_1 = \frac{\mathbf{u}_1^\top A^\top A\mathbf{u}_1}{\mathbf{u}_1^\top \mathbf{u}_1} = \frac{\|A\mathbf{u}_1\|_2^2}{\|\mathbf{u}_1\|_2^2} \geq 0.$$

So we want to show that $\|A\|_2 = \sqrt{\lambda_n}$. The eigenvectors form a basis, so every vector $\mathbf{x} \in \mathbb{R}^n$ can be expressed as a linear combination $\mathbf{x} = \sum_{k=1}^n \alpha_k \mathbf{u}_k$. Therefore

$$\|A\mathbf{x}\|_2^2 = \mathbf{x}^\top A^\top A\mathbf{x} = \mathbf{x}^\top \sum_{k=1}^n \alpha_k \lambda_k \mathbf{u}_k = \sum_{j=1}^n \alpha_j \mathbf{u}_j^\top \sum_{k=1}^n \alpha_k \lambda_k \mathbf{u}_k = \sum_{k=1}^n \alpha_k^2 \lambda_k,$$

where the last step uses orthonormality of the $\mathbf{u}_k$. It follows that

$$\|A\mathbf{x}\|_2^2 \leq \lambda_n \sum_{k=1}^n \alpha_k^2.$$

But if $\|\mathbf{x}\|_2 = 1$, then $\|\mathbf{x}\|_2^2 = \sum_{k=1}^n \alpha_k^2 = 1$, so $\|A\mathbf{x}\|_2^2 \leq \lambda_n$. To show that the maximum of $\|A\mathbf{x}\|_2^2$ is equal to λ_n, we can choose $\mathbf{x}$ to be the corresponding eigenvector $\mathbf{x} = \mathbf{u}_n$. In that case, $\alpha_1 = \ldots = \alpha_{n-1} = 0$ and $\alpha_n = 1$, so $\|A\mathbf{x}\|_2^2 = \lambda_n$.

3.7 Conditioning

Some linear systems are inherently more difficult to solve than others, because the solution is sensitive to small perturbations in the input. We will examine how to quantify this sensitivity and how to adjust our methods to control for it.

Example 3.14

Consider the linear system

$$\begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \implies \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

If we add a small rounding error $0 < \delta \ll 1$ to the data b_1 then

$$\begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 1+\delta \\ 1 \end{pmatrix} \implies \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} \delta \\ 1 \end{pmatrix}.$$

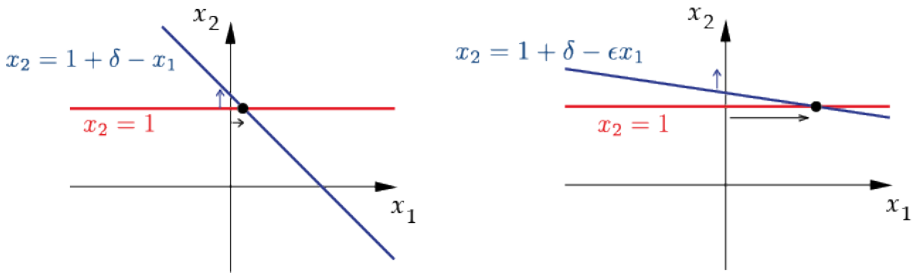
The solution is within rounding error of the true solution, so the system is called **well conditioned**.

Example 3.15

Now let $\epsilon \ll 1$ be a fixed positive number, and consider the linear system

$$\begin{pmatrix} \epsilon & 1 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 1+\delta \\ 1 \end{pmatrix} \implies \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} \delta/\epsilon \\ 1 \end{pmatrix}.$$

The true solution is still $(0,1)^\top$, but if the error δ is as big as the matrix entry ϵ, then the solution for x_1 will be completely wrong. This system is much more sensitive to errors in $\mathbf{b}$, so is called **ill-conditioned**.
Graphically, this system (right) is more sensitive to δ than the first system (left) because the two lines are closer to parallel:



To measure the **conditioning** of a linear system, consider the following estimate of the ratio of the relative errors in the output (x) versus the input (b):

$$\begin{aligned} \frac{|\text{relative error in } \mathbf{x}|}{|\text{relative error in } \mathbf{b}|} &= \frac{\|\delta\mathbf{x}\|/\|\mathbf{x}\|}{\|\delta\mathbf{b}\|/\|\mathbf{b}\|} = \left(\frac{\|\delta\mathbf{x}\|}{\|\mathbf{x}\|}\right)\left(\frac{\|\mathbf{b}\|}{\|\delta\mathbf{b}\|}\right) \\ &= \left(\frac{\|A^{-1}\delta\mathbf{b}\|}{\|\mathbf{x}\|}\right)\left(\frac{\|\mathbf{b}\|}{\|\delta\mathbf{b}\|}\right) \\ &\leq \frac{\|A^{-1}\|\|\delta\mathbf{b}\|}{\|\mathbf{x}\|}\left(\frac{\|\mathbf{b}\|}{\|\delta\mathbf{b}\|}\right) \\ &= \frac{\|A^{-1}\|\|\mathbf{b}\|}{\|\mathbf{x}\|} = \frac{\|A^{-1}\|\|A\mathbf{x}\|}{\|\mathbf{x}\|} \\ &\leq \|A^{-1}\|\|A\|. \end{aligned}$$

We define the **condition number** of a matrix A in some induced norm $\|\cdot\|_*$ to be

$$\kappa_*(A) = \|A^{-1}\|_*\|A\|_*.$$

If $\kappa_*(A)$ is large, then the solution will be sensitive to errors in $\mathbf{b}$, at least for some $\mathbf{b}$. A large condition number means that the matrix is close to being non-invertible (i.e. two rows are close to being linearly dependent).

Note

This is a "worst case" amplification of the error by a given matrix. The actual result will depend on $\delta\mathbf{b}$ (which we usually don't know if it arises from previous rounding error).

Note that $\det(A)$ will tell you whether a matrix is singular or not, but not whether it is ill-conditioned. Since $\det(\alpha A) = \alpha^n \det(A)$, the determinant can be made arbitrarily large or small by scaling (which does not change the condition number). For instance, the matrix

$$\begin{pmatrix} 10^{-50} & 0 \\ 0 & 10^{-50} \end{pmatrix}$$

has tiny determinant but is well-conditioned.

Example 3.16

Return to our earlier examples and consider the condition numbers in the 1-norm. We have (assuming $0 < \epsilon \ll 1$) that

$$A = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} \implies A^{-1} = \begin{pmatrix} 1 & -1 \\ 0 & 1 \end{pmatrix} \implies \|A\|_1 = \|A^{-1}\|_1 = 2 \implies \kappa_1(A) = 4,$$

$$B = \begin{pmatrix} \epsilon & 1 \\ 0 & 1 \end{pmatrix} \implies B^{-1} = \frac{1}{\epsilon}\begin{pmatrix} 1 & -1 \\ 0 & \epsilon \end{pmatrix}$$

$$\implies \|B\|_1 = 2,\ \|B^{-1}\|_1 = \frac{1+\epsilon}{\epsilon} \implies \kappa_1(B) = \frac{2(1+\epsilon)}{\epsilon}.$$

For matrix B, $\kappa_1(B) \to \infty$ as $\epsilon \to 0$, showing that the matrix B is ill-conditioned.

Example 3.17

The **Hilbert matrix** H_n is the $n \times n$ symmetric matrix with entries

$$(h_n)_{ij} = \frac{1}{i+j-1}.$$

These matrices are notoriously ill-conditioned. For example, $\kappa_2(H_5) \approx 4.8 \times 10^5$, and $\kappa_2(H_{20}) \approx 2.5 \times 10^{28}$. Solving an associated linear system in floating-point arithmetic would be hopeless.

A practical limitation of the condition number is that you have to know A^{-1} before you can calculate it. We can always estimate $\|A^{-1}\|$ by taking some arbitrary vectors $\mathbf{x}$ and using

$$\|A^{-1}\| \geq \frac{\|\mathbf{x}\|}{\|\mathbf{b}\|}.$$

3.8 Iterative methods

For large systems, the $\mathcal{O}(n^3)$ cost of Gaussian elimination is prohibitive. Fortunately, many such systems that arise in practice are **sparse**, meaning that most of the entries of the matrix A are zero. In this case, we can often use iterative algorithms to do better than $\mathcal{O}(n^3)$.

In this course, we will only study algorithms for symmetric positive definite matrices. A matrix A is called **symmetric positive definite** (or **SPD**) if $\mathbf{x}^\top A\mathbf{x} > 0$ for every vector $\mathbf{x} \neq 0$.

> **Note**
>
> Recall that a symmetric matrix has real eigenvalues. It is positive definite iff all of its eigenvalues are positive.

Example 3.18

Show that the following matrix is SPD:

$$A = \begin{pmatrix} 3 & 1 & -1 \\ 1 & 4 & 2 \\ -1 & 2 & 5 \end{pmatrix}.$$

With $\mathbf{x} = (x_1, x_2, x_3)^\top$, we have

$$\begin{aligned} \mathbf{x}^\top A\mathbf{x} &= 3x_1^2 + 4x_2^2 + 5x_3^2 + 2x_1x_2 + 4x_2x_3 - 2x_1x_3 \\ &= x_1^2 + x_2^2 + 2x_3^2 + (x_1 + x_2)^2 + (x_1 - x_3)^2 + 2(x_2 + x_3)^2. \end{aligned}$$

This is positive for any non-zero vector $\mathbf{x} \in \mathbb{R}^3$, so A is SPD (eigenvalues 1.29, 4.14 and 6.57).

If A is SPD, then solving $A\mathbf{x} = \mathbf{b}$ is equivalent to minimizing the quadratic functional

$$f : \mathbb{R}^n \to \mathbb{R}, \qquad f(\mathbf{x}) = \tfrac{1}{2}\mathbf{x}^\top A\mathbf{x} - \mathbf{b}^\top \mathbf{x}.$$

When A is SPD, this functional behaves like a U-shaped parabola, and has a unique finite global minimizer $\mathbf{x}_*$ such that $f(\mathbf{x}_*) < f(\mathbf{x})$ for all $\mathbf{x} \in \mathbb{R}^n$, $\mathbf{x} \neq \mathbf{x}_*$.

To find $\mathbf{x}_*$, we need to set $\nabla f = \mathbf{0}$. We have

$$f(\mathbf{x}) = \tfrac{1}{2}\sum_{i=1}^{n} x_i \left(\sum_{j=1}^{n} a_{ij}x_j \right) - \sum_{j=1}^{n} b_j x_j$$

so

$$\begin{aligned}\frac{\partial f}{\partial x_k} &= \tfrac{1}{2}\left(\sum_{i=1}^{n} x_i a_{ik} + \sum_{j=1}^{n} a_{kj} x_j\right) - b_k \\ &= \tfrac{1}{2}\left(\sum_{i=1}^{n} a_{ki} x_i + \sum_{j=1}^{n} a_{kj} x_j\right) - b_k = \sum_{j=1}^{n} a_{kj} x_j - b_k.\end{aligned}$$

In the penultimate step we used the symmetry of A to write $a_{ik} = a_{ki}$. It follows that

$$\nabla f = A\mathbf{x} - \mathbf{b},$$

so locating the minimum of $f(\mathbf{x})$ is indeed equivalent to solving $A\mathbf{x} = \mathbf{b}$.

> **Note**
>
> Minimizing functions is a vast sub-field of numerical analysis known as **optimization**. We will only cover this specific case.

A popular class of methods for optimization are **line search** methods, where at each iteration the search is restricted to a single **search direction** $\mathbf{d}_k$. The iteration takes the form

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \mathbf{d}_k.$$

The **step size** α_k is chosen by minimizing $f(\mathbf{x})$ along the line $\mathbf{x} = \mathbf{x}_k + \alpha \mathbf{d}_k$. For our functional above, we have

$$f(\mathbf{x}_k + \alpha \mathbf{d}_k) = (\tfrac{1}{2}\mathbf{d}_k^\top A \mathbf{d}_k)\alpha^2 + \mathbf{d}_k^\top (A\mathbf{x}_k - \mathbf{b})\alpha + \tfrac{1}{2}\mathbf{x}_k^\top A \mathbf{x}_k - \mathbf{b}^\top \mathbf{x}_k.$$

This is a quadratic in α, and the coefficient of α^2 is positive because A is positive definite. It is therefore a U-shaped parabola and achieves its minimum when

$$\frac{\partial f}{\partial \alpha} = \mathbf{d}_k^\top A \mathbf{d}_k \alpha + \mathbf{d}_k^\top (A\mathbf{x}_k - \mathbf{b}) = 0.$$

Defining the **residual** $\mathbf{r}_k := A\mathbf{x}_k - \mathbf{b}$, we see that the desired choice of step size is

$$\alpha_k = -\frac{\mathbf{d}_k^\top \mathbf{r}_k}{\mathbf{d}_k^\top A \mathbf{d}_k}.$$

Different line search methods differ in how the search direction $\mathbf{d}_k$ is chosen at each iteration. For example, the **method of steepest descent** sets

$$\mathbf{d}_k = -\nabla f(\mathbf{x}_k) = -\mathbf{r}_k,$$

where we have remembered the gradient formula above.

Example 3.19

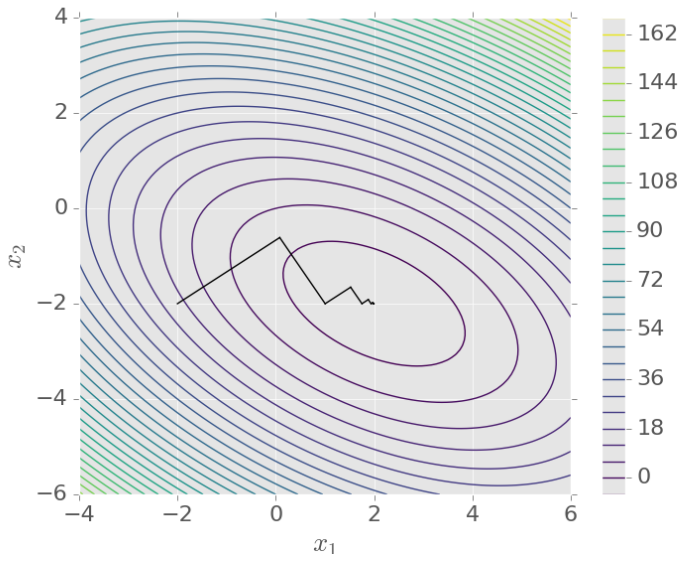
Use the method of steepest descent to solve the system

$$\begin{pmatrix} 3 & 2 \\ 2 & 6 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 2 \\ -8 \end{pmatrix}.$$

Starting from $\mathbf{x}_0 = (-2, -2)^\top$, we get

$$\mathbf{d}_0 = \mathbf{b} - A\mathbf{x}_0 = \begin{pmatrix} 12 \\ 8 \end{pmatrix} \implies \alpha_0 = \frac{\mathbf{d}_0^\top \mathbf{d}_0}{\mathbf{d}_0^\top A \mathbf{d}_0} = \frac{208}{1200}$$
$$\implies \mathbf{x}_1 = \mathbf{x}_0 + \alpha_0 \mathbf{d}_0 \approx \begin{pmatrix} 0.08 \\ -0.613 \end{pmatrix}.$$

Continuing the iteration, $\mathbf{x}_k$ proceeds towards the solution $(2, -2)^\top$ as illustrated below. The coloured contours show the value of $f(x_1, x_2)$.



Unfortunately, the method of steepest descent can be slow to converge. In the **conjugate gradient method**, we still take $\mathbf{d}_0 = -\mathbf{r}_0$, but subsequent search directions $\mathbf{d}_k$ are chosen to be A**-conjugate**, meaning that

$$\mathbf{d}_{k+1}^\top A \mathbf{d}_k = 0.$$

This means that minimization in one direction does not undo the previous minimizations.

In particular, we construct $\mathbf{d}_{k+1}$ by writing

$$\mathbf{d}_{k+1} = -\mathbf{r}_{k+1} + \beta_k \mathbf{d}_k,$$

then choosing the scalar β_k such that $\mathbf{d}_{k+1}^\top A\mathbf{d}_k = 0$. This gives

$$0 = (-\mathbf{r}_{k+1} + \beta_k \mathbf{d}_k)^\top A\mathbf{d}_k = -\mathbf{r}_{k+1}^\top A\mathbf{d}_k + \beta_k \mathbf{d}_k^\top A\mathbf{d}_k$$

and hence

$$\beta_k = \frac{\mathbf{r}_{k+1}^\top A\mathbf{d}_k}{\mathbf{d}_k^\top A\mathbf{d}_k}.$$

Thus we get the basic conjugate gradient algorithm.

Algorithm 3.2: Conjugate gradient method

Start with an initial guess $\mathbf{x}_0$ and initial search direction $\mathbf{d}_0 = -\mathbf{r}_0 = \mathbf{b} - A\mathbf{x}_0$. For each $k = 0, 1, \ldots$, do the following:

1. Compute step size
$$\alpha_k = -\frac{\mathbf{d}_k^\top \mathbf{r}_k}{\mathbf{d}_k^\top A\mathbf{d}_k}.$$
2. Compute $\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \mathbf{d}_k$.
3. Compute residual $\mathbf{r}_{k+1} = A\mathbf{x}_{k+1} - \mathbf{b}$.
4. If $\|\mathbf{r}_{k+1}\| <$ tolerance, output $\mathbf{x}_{k+1}$ and stop.
5. Determine new search direction
$$\mathbf{d}_{k+1} = -\mathbf{r}_{k+1} + \beta_k \mathbf{d}_k \quad \text{where} \quad \beta_k = \frac{\mathbf{r}_{k+1}^\top A\mathbf{d}_k}{\mathbf{d}_k^\top A\mathbf{d}_k}.$$

Example 3.20

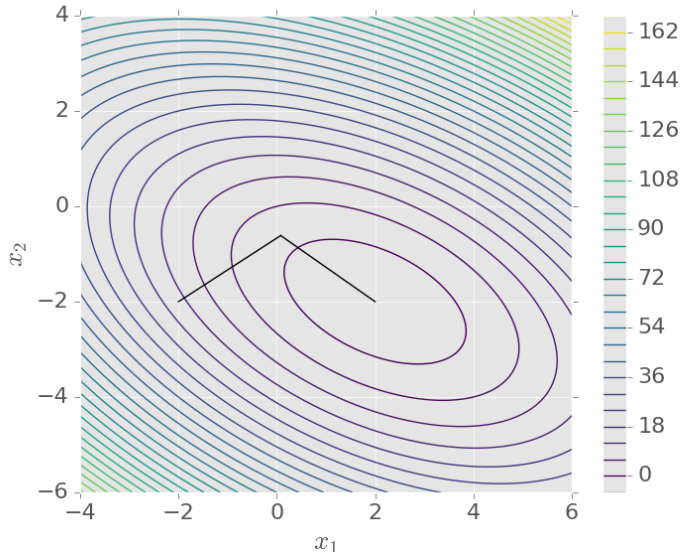
Solve our previous example with the conjugate gradient method.
Starting with $\mathbf{x}_0 = (-2, -2)^\top$, the first step is the same as in steepest descent, giving $\mathbf{x}_1 = (0.08, -0.613)^\top$. But then we take

$$\mathbf{r}_1 = A\mathbf{x}_1 - \mathbf{b} = \begin{pmatrix} -2.99 \\ 4.48 \end{pmatrix}, \quad \beta_0 = \frac{\mathbf{r}_1^\top A\mathbf{d}_0}{\mathbf{d}_0^\top A\mathbf{d}_0} = 0.139, \quad \mathbf{d}_1 = -\mathbf{r}_1 + \beta_0 \mathbf{d}_0 = \begin{pmatrix} 4.66 \\ -3.36 \end{pmatrix}.$$

The second iteration then gives

$$\alpha_1 = -\frac{\mathbf{d}_1^\top \mathbf{r}_1}{\mathbf{d}_1^\top A\mathbf{d}_1} = 0.412 \implies \mathbf{x}_2 = \mathbf{x}_1 + \alpha_1 \mathbf{d}_1 = \begin{pmatrix} 2 \\ -2 \end{pmatrix}.$$

This time there is no zig-zagging and the solution is reached in just two iterations:



In exact arithmetic, the conjugate gradient method will always give the exact answer in n iterations – one way to see this is to use the following.

Theorem 3.5

The residuals $\mathbf{r}_k := A\mathbf{x}_k - \mathbf{b}$ at each stage of the conjugate gradient method are mutually orthogonal, meaning $\mathbf{r}_j^\top \mathbf{r}_k = 0$ for $j = 0, \ldots, k-1$.

After n iterations, the only residual vector that can be orthogonal to all of the previous ones is $\mathbf{r}_n = \mathbf{0}$, so $\mathbf{x}_n$ must be the exact solution.

In practice, conjugate gradients is not competitive as a direct method. It is computationally intensive, and rounding errors can destroy the orthogonality, meaning that more than n iterations may be required. Instead, its main use is for large sparse systems. For suitable matrices (perhaps after **preconditioning**), it can converge very rapidly.

We can save computation by using the alternative formulae

$$\mathbf{r}_{k+1} = \mathbf{r}_k + \alpha_k A\mathbf{d}_k, \quad \alpha_k = \frac{\mathbf{r}_k^\top \mathbf{r}_k}{\mathbf{d}_k^\top A\mathbf{d}_k}, \quad \beta_k = \frac{\mathbf{r}_{k+1}^\top \mathbf{r}_{k+1}}{\mathbf{r}_k^\top \mathbf{r}_k}.$$

With these formulae, each iteration requires only one matrix-vector product, two vector-vector products, and three vector additions. Compare this to the basic algorithm above which requires two matrix-vector products, four vector-vector products and three vector additions.

Knowledge checklist

Key topics:

1. Integer and floating point representations of real numbers on computers.
2. Overflow, underflow and loss of significance.

Key skills:

- Understanding and distinguishing integer, fixed-point, and floating-point representations.
- Analyzing the effects of rounding and machine epsilon in calculations.
- Diagnosing and managing rounding errors, overflow, and underflow.