Computational Mathematics
Lecture 0: Introduction to Algorithms

Patrick E. Farrell

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For some mathematical problems, we can just write down the solution:

$$\text{For } a_0, a_1 \in \mathbb{R}, a_1 \neq 0, \text{ find } x \in \mathbb{R} \text{ such that } a_1 x + a_0 = 0.$$

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For most problems, we can't just write down the solution:

$$\text{For } a_0, \ldots, a_5 \in \mathbb{R}, \text{ find } x \in \mathbb{C} \text{ such that } a_5 x^5 + a_4 x^4 + \cdots + a_0 = 0.$$

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Theorem (Abel, 1824)

There are polynomials of degree 5 and higher that cannot be solved by radicals (addition, subtraction, multiplication, division, and nth root extraction).

Niels Henrik Abel, 1802–1829

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Response A: prove things *about* the solutions.

We could prove that if x is a root of a polynomial with real coefficients, so is $\bar{x}$. Or we could study Vieta's formulae, that (for example) the product of the roots of an n-th degree polynomial is $(-1)^n a_0/a_n$.

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Response B: devise *algorithms* for computing the solutions.

Develop a computational procedure that approximates to arbitrary accuracy the roots of our polynomial: *compute* a sequence that converges to the roots.

The central topic of computational mathematics is algorithms.

Definition (Algorithm, informal)

An algorithm is a finite set of instructions for solving a mathematical problem. It associates to each input a sequence of elementary computational steps to calculate some desired output.

The formalisation of this definition is studied in computer science, e.g. with *Turing machines*.

Muḥammad ibn Mūsā al-Khwārizmī, c. 780–850

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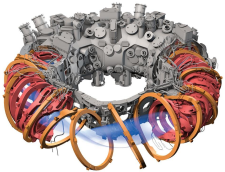
You will see another example in Part A Differential Equations: you will prove that under certain conditions a unique solution exists to the problem

$$\text{find } y(t) \text{ such that } \frac{\mathrm{d}y}{\mathrm{d}t} = f(y,t), \quad y(0) = y_0,$$

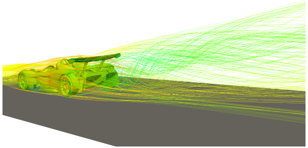
by constructing a sequence of approximations y_n that converges $y_n \to y$.

In applied mathematics, algorithms are used to solve problems arising in science and engineering.

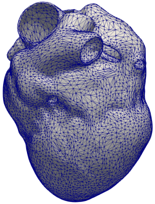
climate



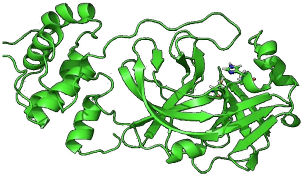
energy



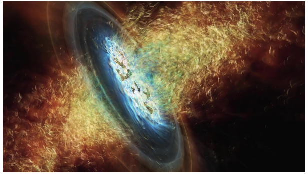
aerodynamics



physiology



covid



galaxies

Questions we ask:

Does our algorithm terminate?

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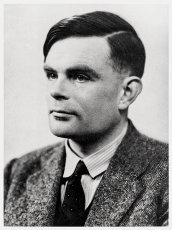
Theorem (Halting problem, 1936)

No algorithm exists that always correctly decides if another algorithm terminates on a given input.



Alan Turing, 1912–1954

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Does our algorithm give the correct answer, and if so, when?

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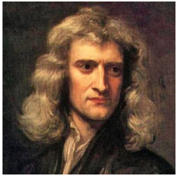
In later lectures we will see Newton's method for finding a solution x of a general rootfinding problem $f(x) = 0$.

This converges if we start the iteration close to x, but diverges if we start far away.



Isaac Newton, 1643–1727

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Consider two formulae for π:

$$\pi = 4\sum_{k=0}^{\infty} \frac{(-1)^k}{2k+1}, \quad \pi^{-1} = \frac{2\sqrt{2}}{99^2}\sum_{k=0}^{\infty} \frac{(4k)!}{k!^4}\frac{26390k+1103}{396^{4k}}.$$

If we approximate the series by its partial sums, how many terms do we require for accuracy to ten digits?

Gottfried Leibniz, 1646–1716

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About 5 billion, vs 2!

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There are many algorithms for sorting a list of n numbers.

The number of comparisons required by a naïve algorithm called *bubble* sort scales like n^2, while the *merge* sort of von Neumann in 1945 scales like $n \log n$. This is much, much faster for large n.

John von Neumann, 1903–1957

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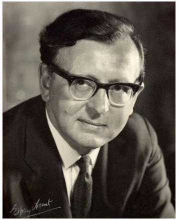
Consider $p(x) = (x-1)(x-2)\cdots(x-20)$. Expanding in monomials, we have

$$p(x) = x^{20} - 210x^{19} + 20615x^{18} + \cdots + 20!.$$



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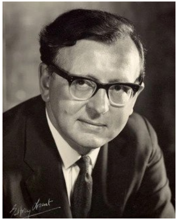
If we perturb -210 to -210.0000001192, then the roots become (to 5 digits)

1.00000 2.00000 3.00000 4.00000 5.00000



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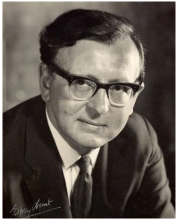

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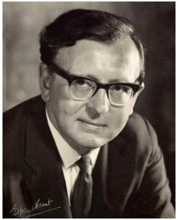

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Computational Mathematics
Week 1: Euclid's algorithm

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$$\mathbb{N} = \{0, 1, 2, 3, \dots\},$$

and consider dividing one natural number t by another $b \neq 0$:

$$t = qb + r, \quad 0 \leq r < b.$$

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Take $t = 80, b = 7$:

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The game ends when $r = 0$. We're interested in the last remainder before hitting 0. This is the greatest common divisor of the two inputs!

Here is the *algorithm*. It computes the *greatest common divisor* (also called *highest common factor*) of two numbers.

---

function gcd(t, b)
    $r \leftarrow t \bmod b$
    while $r \neq 0$ **do**
        $t \leftarrow b$
        $b \leftarrow r$
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    return b
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Note that this algorithm calls another one (the division algorithm).

Theorem (Elements, book VII, c. 300 BCE)

Given any $t, b \in \mathbb{N}$, $0 < b < t$, Euclid's algorithm computes the greatest common divisor of t and b.

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For convenience, let's label each intermediate value:

$$
\begin{aligned}
t &= q_0 b + r_0 \\
b &= q_1 r_0 + r_1 \\
r_0 &= q_2 r_1 + r_2 \\
&\vdots \\
r_j &= q_{j+2} r_{j+1} + r_{j+2} \\
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Also for convenience, denote

$$r_{-2} \coloneqq t, \quad r_{-1} \coloneqq b.$$

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Claim: the algorithm terminates.

Since division yields $r < b$, the sequence of remainders $(r_{-2}, r_{-1}, r_0, \dots)$ is a strictly decreasing sequence of natural numbers. The sequence must therefore eventually reach zero. The algorithm therefore always terminates.

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Let i be the index such that $r_i = 0$.

Claim: r_{i-1} divides r_j, $j < i - 1$ (common divisor).

Since $r_i = 0$, r_{i-1} divides r_{i-2}, i.e.

$$r_{i-2} = q_i r_{i-1}.$$

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Plugging this into the previous iteration tells us that r_{i-1} also divides r_{i-3}:

$$\begin{aligned} r_{i-3} &= q_{i-1} r_{i-2} + r_{i-1} \\ &= (\cdots) \times r_{i-1} \end{aligned}$$

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Proceeding by induction shows that r_{i-1} divides all remainders in the sequence. In particular, r_{i-1} is a common divisor of the original t and b.

Claim: r_{i-1} is the greatest common divisor.

Assume $d \in \mathbb{N}$ also divides t and b, so there exist $\alpha, \beta \in \mathbb{N}$ such that

$$t = \alpha d, \quad b = \beta d.$$

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The next equation is $b = q_1 r_0 + r_1$, but since d divides both b and r_0, it must also divide r_1. Proceeding by induction, d must divide *all* remainders, including r_{i-1}.

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Thus $d \leq r_{i-1}$, and r_{i-1} is the greatest common divisor of t and b.

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But it is possible to prove a tighter bound!

Theorem

Let $t > b > 0$. The smallest values of t and b for which Euclid's algorithm requires N iterations are the Fibonacci numbers $t = F_{N+2}$ and $b = F_{N+1}$.

Theorem (Complexity of Euclid's algorithm, 1844)

The number of steps taken in Euclid's algorithm can never be more than five times the number of decimal digits of b.

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This result shows that the cost grows *logarithmically* in the size of the input b.


PELOUZE
CARNOT
LAME

Section 2

Diophantine equations

A *Diophantine* equation is an algebraic equation for which solutions are sought in the integers $\mathbb{Z} = \{\ldots, -2, -1, 0, 1, 2, \ldots\}$. They are named after Diophantus of Alexandria (c. 200–290).

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Diophantus' work was collected in his magnum opus, *Arithmetica*. In 1637, Pierre de Fermat wrote in the margin of his copy of *Arithmetica*,

> *It is impossible …for any number which is a power greater than the second to be written as the sum of two like powers. I have a truly marvelous demonstration of this proposition which this margin is too narrow to contain.*

Pierre de Fermat, 1607–1665

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LDEs with $\gcd(a, b) = 1 = c$ are of particular interest. If we can solve

$$ax + by = 1$$

then we have solved the problem: find $x \in \mathbb{Z}$ such that

$$ax \equiv 1 \pmod{b},$$

the problem of finding modular multiplicative inverses.

A linear Diophantine equation (LDE) in two variables is of the form: given $a, b, c \in \mathbb{Z}$, find $x, y \in \mathbb{Z}$ such that

$$ax + by = c.$$

LDEs with $\gcd(a, b) = 1 = c$ are of particular interest. If we can solve

$$ax + by = 1$$

then we have solved the problem: find $x \in \mathbb{Z}$ such that

$$ax \equiv 1 \pmod{b},$$

the problem of finding modular multiplicative inverses.

In particular, this is a crucial step in RSA key generation: the private key d satisfies

$$de \equiv 1 \pmod{\lambda(n)},$$

where n, e are the public key, and $\lambda(n)$ is easy to compute if you know the prime factorisation of n and difficult otherwise.

Lemma (Bézout's Lemma)

If $\gcd(a, b) = d$, *then the LDE* $ax + by = d$ *always has an integer solution.*

Étienne Bézout, 1730–1783

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Many other results in number theory follow from Bézout's Lemma, such as Euclid's Lemma and Sunzi's Remainder Theorem.

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which is the solution $(x, y) = (-8, -11)$ that we saw earlier.

How do we prove Bézout's Lemma? We run Euclid's method.

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Proof.

Since $\gcd(a, b) = d$, we know that iterated divisions of the form

$$\begin{aligned} a &= q_0 b + r_0 \\ b &= q_1 r_0 + r_1 \\ r_0 &= q_2 r_1 + r_2 \\ &\vdots \end{aligned}$$

will eventually reach $r_{i-3} = q_{i-1} r_{i-2} + d$.

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We know that $r_{i-4} = q_{i-2} r_{i-3} + r_{i-2}$, so using this to eliminate r_{i-2} we have

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Proceeding by induction, we can write d as a combination of r_{i-5} and r_{i-4}, then r_{i-6} and r_{i-5}, and so on until we write

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This uses an *algorithm* to prove an existence result.

We saw in our previous calculations that $48x - 35y = 1$ had a solution $(x, y) = (-8, -11)$. However, there are other solutions, such as $(x, y) = (-43, -59)$. How do we find them *all*? What is the general solution?

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Suppose we have a *particular solution* (x_p, y_p) satisfying $ax_p + by_p = 1$. If we had $(\tilde{x}, \tilde{y})$ such that $a\tilde{x} + b\tilde{y} = 0$, then

$$a(x_p + \tilde{x}) + b(y_p + \tilde{y}) = ax_p + by_p = 1$$

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The general solution to $ax + by = c$ is thus

$$\{c(x_p, y_p) + n(-b, a) : n \in \mathbb{Z}\}.$$

Here is the whole algorithm for solving an LDE $ax + by = c$.

Step 1 Calculate $d = \gcd(a, b)$. If d does not divide c, stop; there are no solutions.

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$$\left\{\hat{c}(x_p, y_p) + n(-\hat{b}, \hat{a}) : n \in \mathbb{Z}\right\}.$$

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Step 4 The general solution is thus

$$\begin{aligned} &\{3(-8, -11) + n(35, 48) : n \in \mathbb{Z}\} \\ =&\{(-24, -33) + n(35, 48) : n \in \mathbb{Z}\}. \end{aligned}$$

Section 3

The extended Euclidean algorithm

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This appears to have first been explained by Āryabhaṭa (476–550).

Recall that Euclid's algorithm constructs a sequence

$$r_{-2}, r_{-1}, r_0, r_1, \ldots, r_{i-1},$$

where $r_{i-1} = \gcd(a, b)$ and again we denote $r_{-2} = a$, $r_{-1} = b$.

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We introduce two new sequences

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and we will enforce the property that

$$ax_j + by_j = r_j, \quad j = -2, \ldots, i-1.$$

If we can enforce this, then we will have

$$ax_{i-1} + by_{i-1} = r_{i-1} = \gcd(a, b).$$

How do we enforce

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so that our property is enforced at the start.

Consider some step of Euclid's method,

$$r_j = q_{j+2} r_{j+1} + r_{j+2}.$$

If we know the expansions of r_j and r_{j+1} in terms of our 'basis' a and b, then we can work out the expansion of r_{j+2} too:

$$x_{j+2} = x_j - q_{j+2} x_{j+1},$$
$$y_{j+2} = y_j - q_{j+2} y_{j+1}.$$

Section 4

Euclid for polynomials

So far we've applied Euclid's method only to integers. It applies to other types of algebraic objects, too.

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A *polynomial* p in $\mathbb{R}[x]$ of degree $d \in \mathbb{N}$ is an expression of the form

$$p(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_d x^d,$$

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A root of p is a number $x \in \mathbb{C}$ satisfying $p(x) = 0$.

Recall: dividing $p(x)$ by $q(x)$ writes

$$p(x) = c(x)q(x) + r(x)$$

with quotient $c(x)$ and remainder $r(x)$, with $\deg(r) < \deg(q)$.

The polynomials $\mathbb{R}[x]$ form a *Euclidean domain*.

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This is an algebraic structure R that can be equipped with a *Euclidean function*

$$f : R \setminus \{0\} \to \mathbb{N}$$

which is something that strictly decreases on division: given $a, b \in R$, there exist $q, r \in R$, such that

$$a = qb + r,$$

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We can generalise Euclid's method, greatest common divisors, Bézout's Lemma, and many other results to such domains.

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For now, we focus on computing *common* roots of two polynomials p and q, of possibly different degrees. The common roots are $x \in \mathbb{C}$ such that $p(x) = q(x) = 0$.

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A number a is a root of p iff $(x - a)$ divides p, which gives the link between common roots and common divisors.

Let's see an example of applying Euclid's method. Take

$$p(x) = x^4 + x^3 - 6x^2 + 5x - 1, \quad q(x) = x^3 + x^2 + 3x - 5.$$

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$$x^4 + x^3 - 6x^2 + 5x - 1 = (x)(x^3 + x^2 + 3x - 5) + (-9x^2 + 10x - 1)$$

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$$x^3 + x^2 + 3x - 5 = \left(-\frac{1}{9}x - \frac{19}{81}\right)\left(-9x^2 + 10x - 1\right) + \frac{424}{81}\left(x - 1\right)$$

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$$\begin{aligned} x^4 + x^3 - 6x^2 + 5x - 1 &= (x)(x^3 + x^2 + 3x - 5) + (-9x^2 + 10x - 1) \\ x^3 + x^2 + 3x - 5 &= \left(-\frac{1}{9}x - \frac{19}{81}\right)\left(-9x^2 + 10x - 1\right) + \frac{424}{81}(x - 1) \\ -9x^2 + 10x - 1 &= -\frac{81}{424}(9x - 1)\frac{424}{81}(x - 1) + 0. \end{aligned}$$

So $(x - 1)$ is the gcd, so $x = 1$ is their only common root:

$$p(1) = 0 = q(1)$$

.

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2. The sequence of remainders yielded by Euclid's method applied to p and p' can be used to compute its *Sturm sequence*. The number of times the Sturm sequence changes sign can be used to calculate how many real roots p has in any given interval (including $(-\infty, \infty)$).

Jacques Charles François Sturm, 1803–1855

Many interesting polynomials are defined via recurrence relations. Euclid's method can be used to deduce facts about these without calculating them.

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Consider a family of polynomials $p_k(x)$ for $k \in \mathbb{N}$ given by

$$p_0(x) = 1, \quad p_1(x) = x,$$

and

$$p_k(x) = \alpha_k(x) \times p_{k-1}(x) + \beta_k \times p_{k-2}(x),$$

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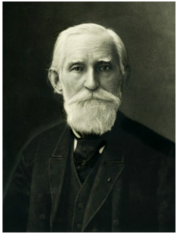
Without specifying α_k or β_k, we can show that p_k and p_{k+1} have no common roots for $k \geq 1$.

Chebyshev polynomials

The main well-conditioned basis for polynomials used in practical computations:

$$T_0(x) = 1, \quad T_1(x) = x,$$
$$T_k(x) = 2xT_{k-1}(x) - T_{k-2}(x).$$



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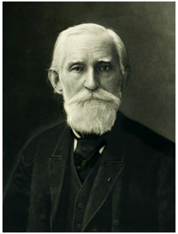

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Laguerre polynomials

These describe the radial part of the solution of the Schrödinger equation for a one-electron atom:

$$L_0(x) = 1, \quad L_1(x) = -x + 1,$$
$$L_k(x) = \frac{2k+1-x}{k+1} L_{k-1}(x) - \frac{k}{k+1} L_{k-2}(x).$$

Edmond Laguerre, 1834–1886

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Similarly, p_{k-2} is the remainder on division of p_k by p_{k-1}. Euclid's algorithm thus iterates until it terminates with

$$p_2(x) = \alpha_2(x) \times p_1(x) + \beta_2 p_0(x) = \alpha_2(x) \times x + \beta_2 \times 1,$$

so $\gcd(p_k, p_{k+1})$ is a nonzero constant (no roots). □

Computational Mathematics
Week 2: Rootfinding and fixed points

Patrick E. Farrell

University of Oxford

In the previous lecture we saw that we could use Euclid's method to compute the common roots of two polynomials p and q.

This, however, is very limited. We will want to find roots of general (not necessarily polynomial) functions $f : \mathbb{R} \to \mathbb{R}$.

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This, however, is very limited. We will want to find roots of general (not necessarily polynomial) functions $f : \mathbb{R} \to \mathbb{R}$.

For this, we turn to *rootfinding* algorithms. There are many different ones, differing in efficiency, robustness, and applicability.

Rootfinding problem

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Another use: if you want to calculate the decimal expansion of a number (like $\sqrt{2}$), set up a suitable equation, like

$$x^2 - 2 = 0$$

and apply a rootfinding algorithm.

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By contrast, rootfinding algorithms can only give *sequences* that converge to the root.

Different algorithms will trade off termination, convergence speed, and operation count.

Section 2

Bisection

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If $f : [a, b] \to \mathbb{R}$ *is continuous with* $f(a)f(b) < 0$, *then there exists* $x^\star \in (a, b)$ *with* $f(x^\star) = 0$.

The statement $f(a)f(b) < 0$ is just a fancy way of saying $f(a)$ and $f(b)$ have opposite signs.

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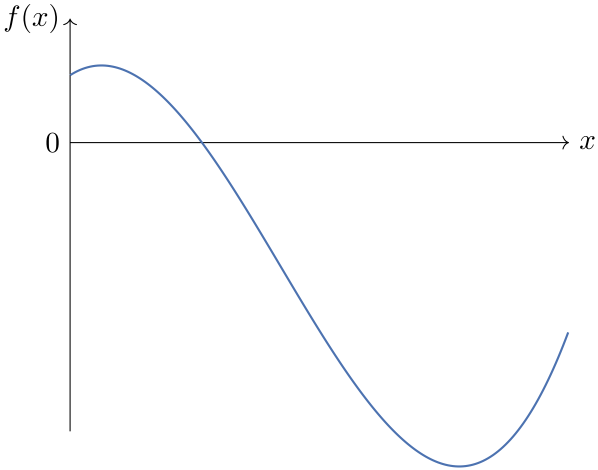
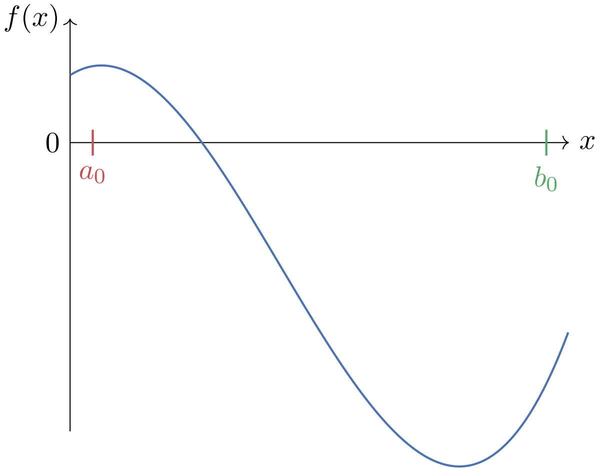
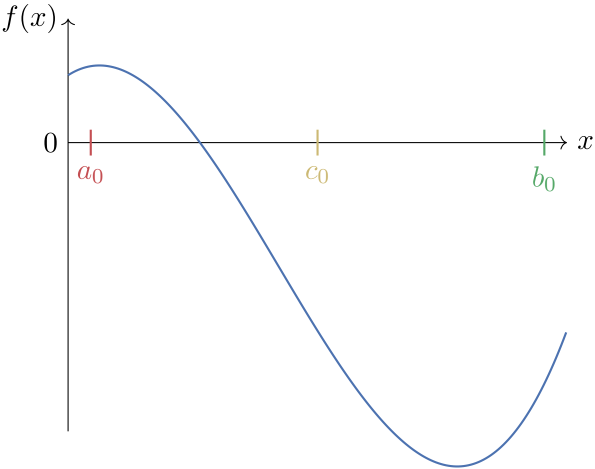
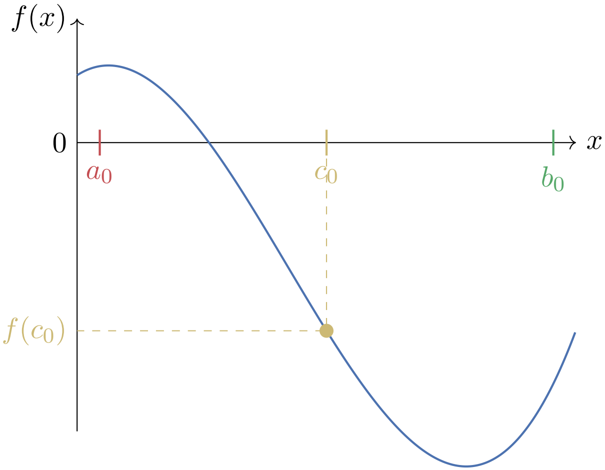
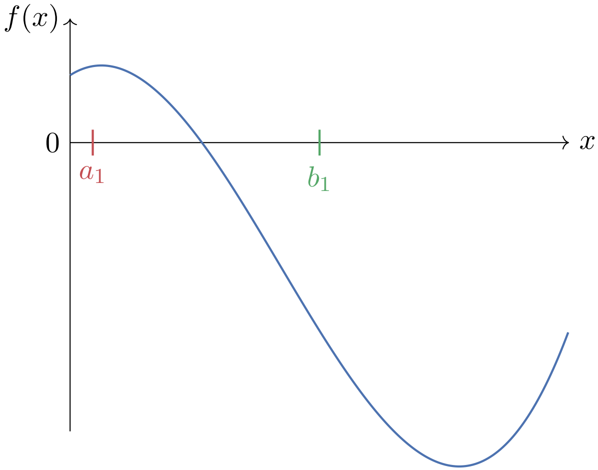

$f(x)$
0
x

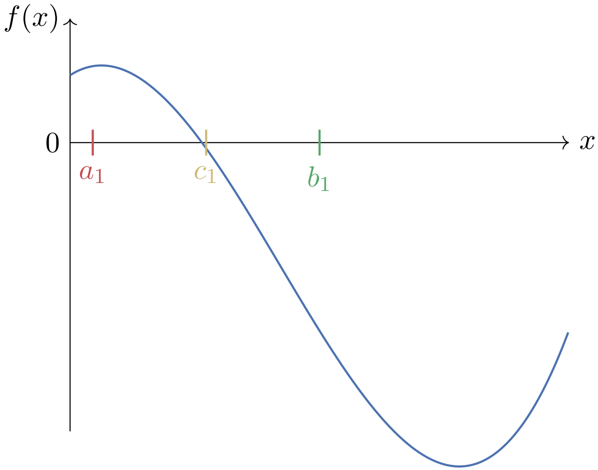

$f(x)$
0
x
a_0
b_0

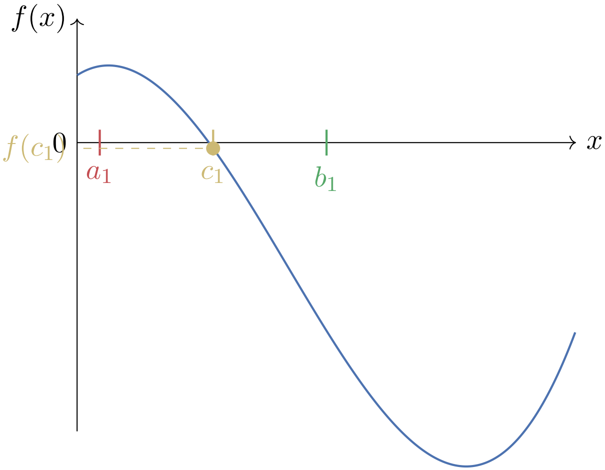

$f(x)$
0
x
a_0
c_0
b_0

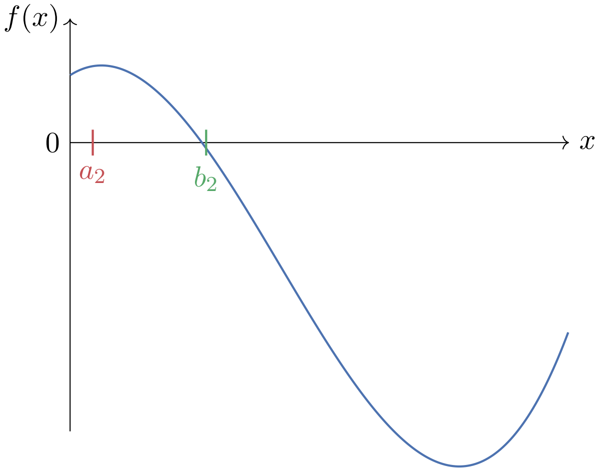


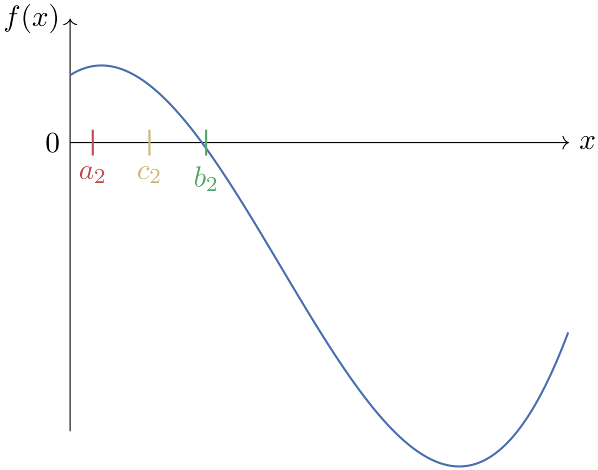
$f(x)$
0
x
a_0
c_0
b_0
$f(c_0)$


$f(x)$
0
x
a_1
b_1

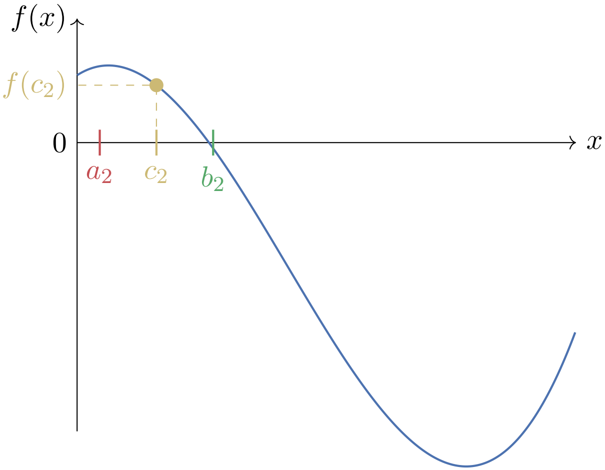

$f(x)$
0
x
a_1
c_1
b_1


$f(x)$
x
0
$f(c_1)$
a_1
c_1
b_1


$f(x)$
0
x
a_2
b_2



$f(x)$
0
x
a_2
c_2
b_2


$f(x)$
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0
x
a_2
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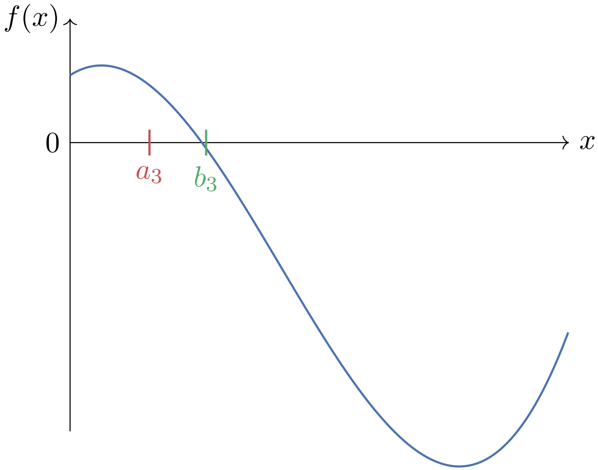
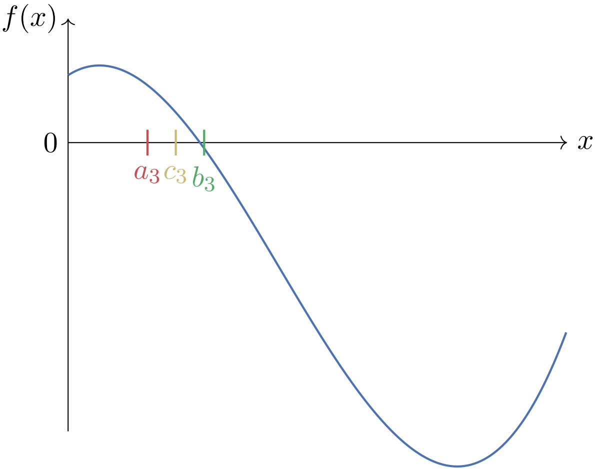
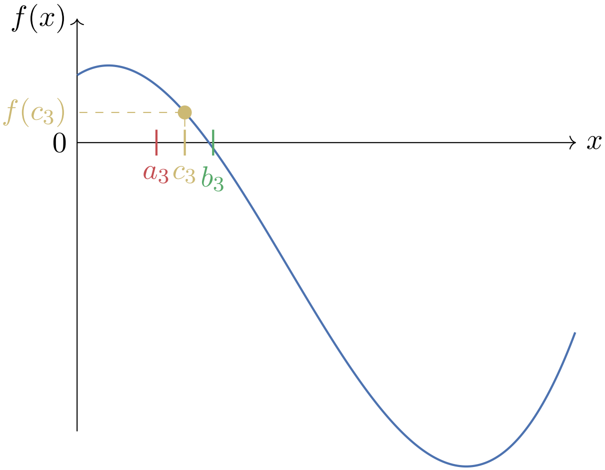
b_2


$f(x)$
0
x
a_3
b_3


$f(x)$
0
x
a_3
c_3
b_3



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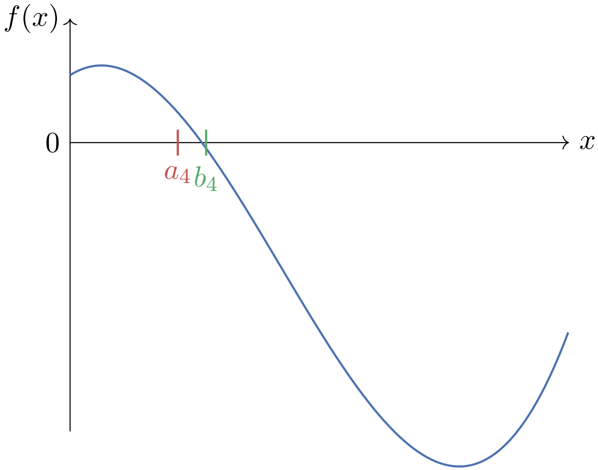
x
a_3
c_3
b_3


$f(x)$
0
x
a_4
b_4

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Note this only uses the *sign* of the output of $f(x)$.

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Augustin-Louis Cauchy FRS
1789–1857

Lemma

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Lemma

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Proof.

In the k-th iteration of the while loop, either the function returns or it shrinks the interval by a factor of 2. For any $\mathrm{tol} > 0$, there exists $k \in \mathbb{N}$ such that $\mathrm{tol} < |b - a|/2^{k+1}$, so the algorithm must terminate. □

Let's do an example. Let's try to solve $x = \cos x$, so $f(x) = x - \cos x$.

Let's start with $[a, b] = [-10, 10]$. $f(-10) \approx -9.16$, $f(10) \approx 10.83$, so we're good to go.

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The true solution is approximately $x \approx 0.739085$, so we're getting there, slowly.

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- ✗ It can be hard to find the initial points $[a, b]$ that bracket a root.

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Later we will study other methods with different sets of advantages and disadvantages.

Section 3

Rate of convergence of a sequence

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Suppose $(x_i) \to x^\star$. We say the sequence converges linearly if there exists $\mu \in (0, 1)$ such that

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For bisection, the sequence of the midpoints of the intervals converges linearly with $\mu = 1/2$.

Can you go faster?

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Definition (Superlinear convergence of a sequence)

Suppose $(x_i) \to x^\star$. We say the sequence converges superlinearly if

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For example, the sequence

$$(\frac{1}{2^{2^n}}) = (\frac{1}{2}, \frac{1}{4}, \frac{1}{16}, \frac{1}{256}, \frac{1}{65535}, \dots) \to 0$$

has the ratio of successive terms going to zero too.

We can further classify superlinear convergence:

Definition (Order of convergence of a sequence)

Suppose $(x_i) \to x^\star$, superlinearly. The sequence converges with order q if

$$\lim_{i \to \infty} \frac{|x_{i+1} - x^\star|}{|x_i - x^\star|^q} = M$$

for some $M > 0$ (not necessarily $M < 1$).

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We will see rootfinding methods with orders of convergence $q = 2$ and $q = 3$. To develop these, we must first understand *fixed point iterations*.

Section 4

Fixed point iterations

So far we have considered rootfinding: find $x^\star \in \mathbb{R}$ such that $f(x^\star) = 0$.

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We can translate between rootfinding problems and fixed point problems. For example, if you want to find the fixed points $g(x) = x$, then you can find the roots of $f(x) := g(x) - x$.

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Transforming between the two problems is useful because there are powerful theorems that apply to finding fixed points. There's even a whole course, C4.6 Fixed Point Methods for Nonlinear PDEs, on this subject.

When can we show fixed points exist?

Theorem (Brouwer's fixed point theorem)

If $g : [a, b] \to [a, b]$ is continuous, then it has a fixed point.

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Warning (endomorphism)

Note that g must send $[a, b]$ to $[a, b]$, i.e. is an *endomorphism*. This result does *not* hold for general $g : [a, b] \to \mathbb{R}$, such as $g(x) = x + 1$.

Proof.

Since $g(x) \in [a, b]$, we have $a \leq g(x) \leq b$ for all $x \in [a, b]$. Thus $f(x) := g(x) - x$ has $f(a) \geq 0$ and $f(b) \leq 0$.

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A root $x^\star$ of $f(x)$ thus exists in (a, b) by Bolzano's Theorem, with $g(x^\star) = x^\star$. □

That's not all! You can get uniqueness of the fixed point under stronger conditions.

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Theorem

If $g : [a, b] \to [a, b]$ is differentiable with $|g'(x)| < 1$ for every $x \in (a, b)$, then g has a ***unique*** *fixed point in (a, b).*

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Theorem (Mean value theorem, 1823)

If $g : [a,b] \to \mathbb{R}$ is differentiable, then there exists some $c \in (a,b)$ such that

$$g'(c) = \frac{g(b) - g(a)}{b - a}.$$

Augustin-Louis Cauchy FRS
1789–1857

Proof.

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Assume without loss of generality that $p < q$. Applying the MVT in $[p, q] \subset [a, b]$, we find that there exists $r \in (p, q)$ such that

$$g'(r) = \frac{g(q) - g(p)}{q - p} = \frac{q - p}{q - p} = 1.$$

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How do we turn this into an algorithm?

Take $x_0 \in [a, b]$ and set $x_{i+1} = g(x_i)$!

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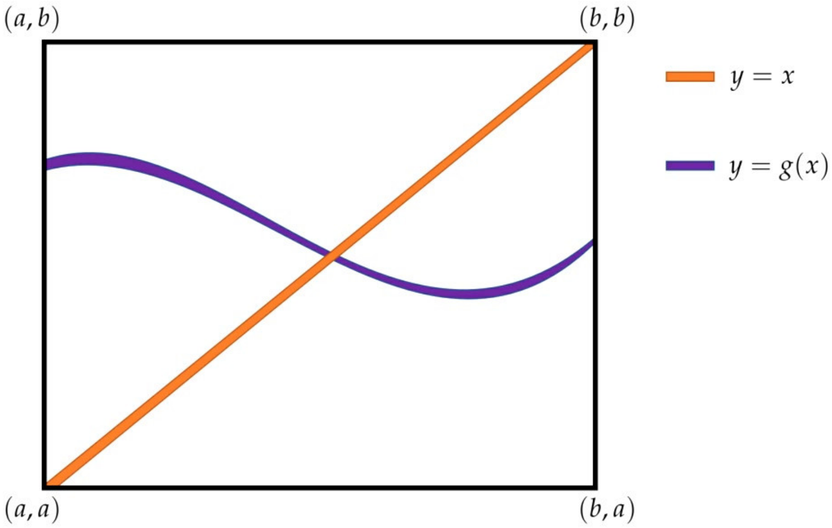
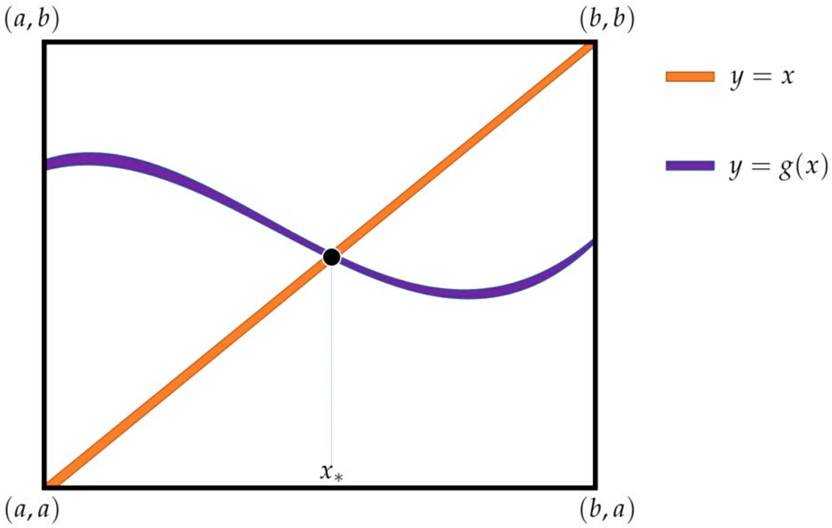
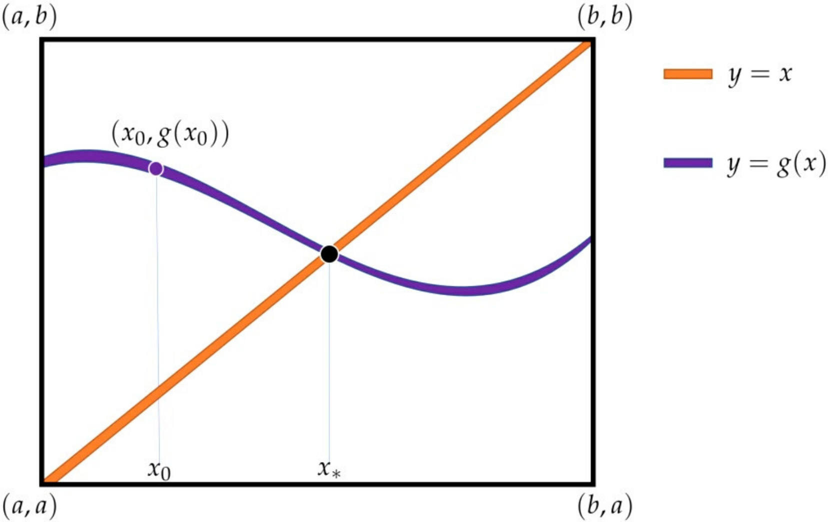
Our goal is to investigate when this converges.


(a, b)
(b, b)
(a, a)
(b, a)
y = x
y = g(x)


(a, b)
(b, b)
$y = x$
$y = g(x)$
x_*
(a, a)
(b, a)



(a,b)
(b,b)
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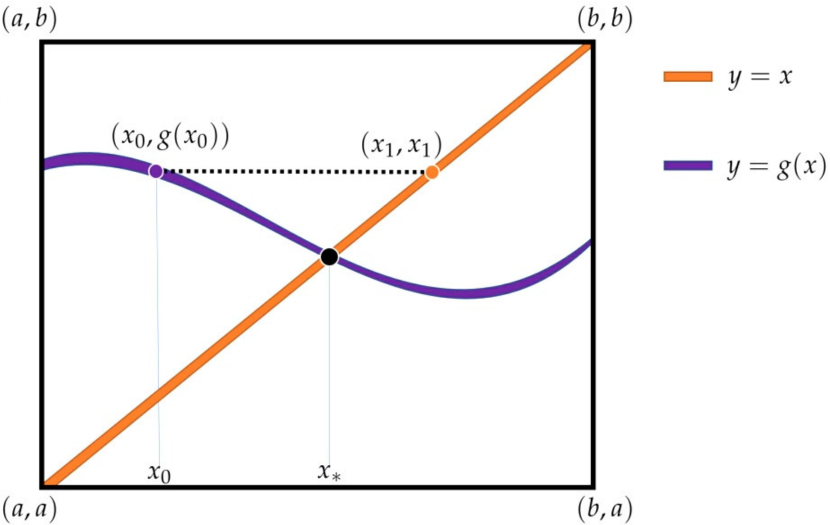

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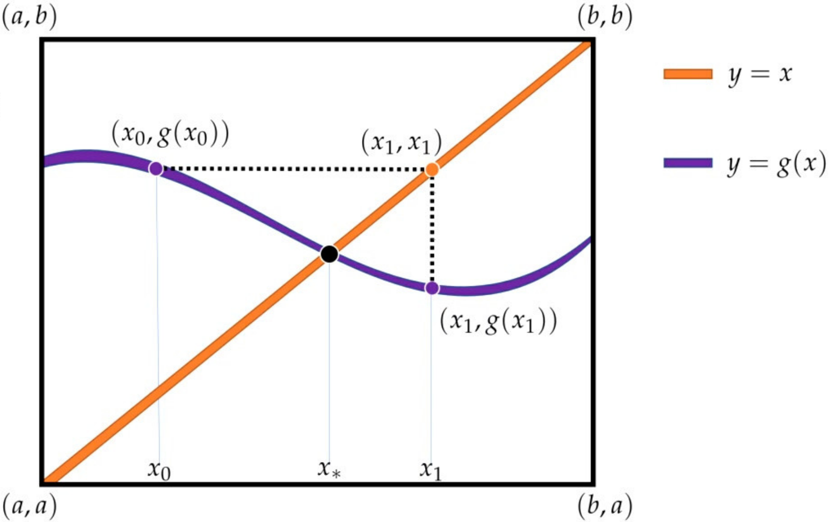

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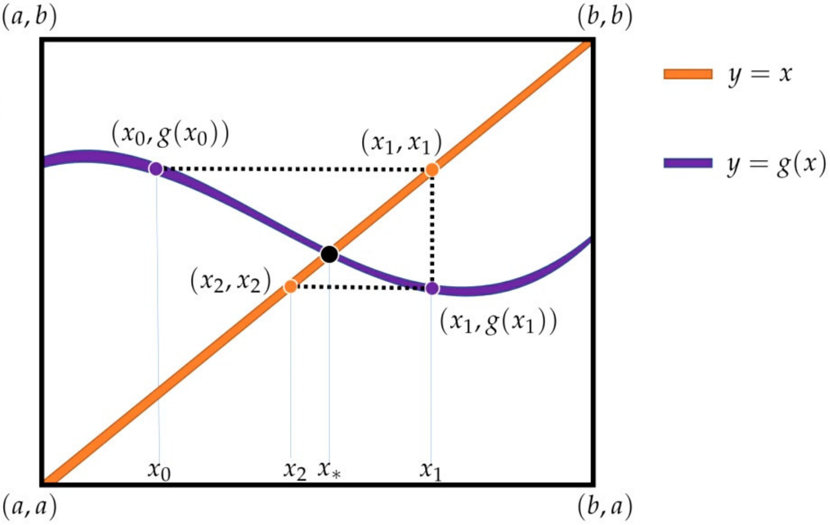

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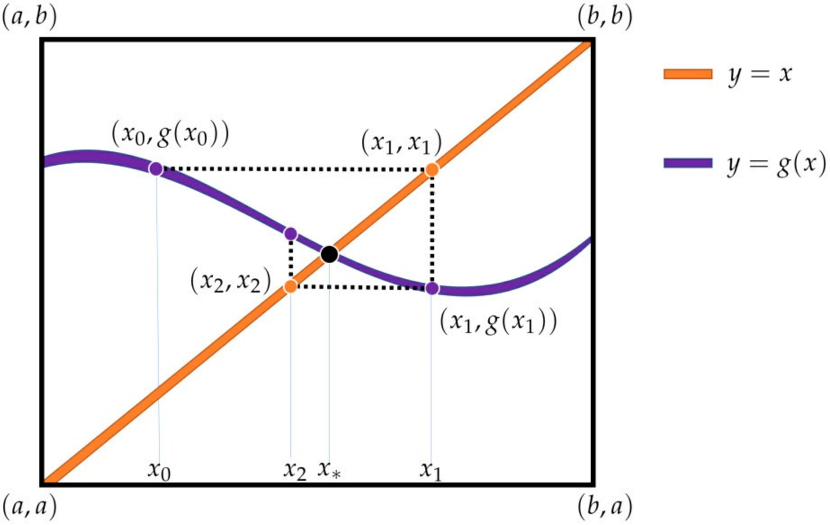

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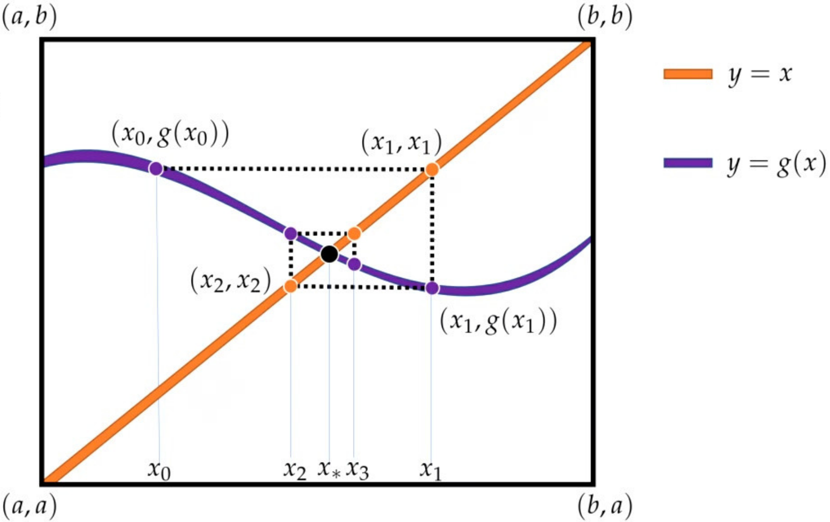

Section 5

The contraction mapping theorem

Let's recall the setting. We have $g : [a, b] \to [a, b]$ with $|g'(x)| < 1$ for $x \in (a, b)$, and we want to find fixed points $x = g(x)$. We know that g has a unique fixed point $x^\star$.

We then proposed the iteration scheme: take any $x_0 \in [a, b]$, and set

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This algorithm doesn't require derivatives. Can we devise conditions for convergence that don't require derivatives? We'll see this next.

Definition (Contraction)

A function $g : [a, b] \to [a, b]$ is called a *contraction* if there exists a constant $0 \le \gamma < 1$ such that

$$|g(x) - g(y)| \le \gamma |x - y|$$

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Any differentiable $g : [a, b] \to [a, b]$ with $|g'(x)| \leq \gamma < 1$ for $x \in (a, b)$ is a contraction. For $x, y \in [a, b]$, by the MVT there exists $c \in (x, y)$ such that

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Not all contractions are differentiable. For example,

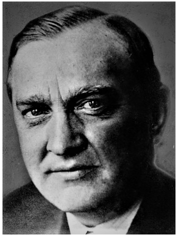
$$g(x) = |x|/2$$

is a contraction with $\gamma = 1/2$, but is not differentiable.

Contraction mapping theorem (1922)

If $g : [a, b] \to [a, b]$ *is a contraction, then it has a unique fixed point* $x^\star$*, and the iteration scheme* $x_{i+1} = g(x_i)$ *converges at least linearly to* $x^\star$ *for any* $x_0 \in [a, b]$.

Banach proved his theorem on more general *complete metric spaces*.



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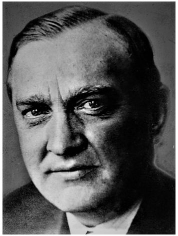

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Banach was a Pole who spent his entire academic career in Lwów (now Lviv).

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If $\gamma = 0$ then $g(x) =$ const which is continuous, so assume $\gamma > 0$. Take arbitrary $\varepsilon > 0$ and choose $\delta = \varepsilon/\gamma$. Then if $|x - y| < \delta$, we have

$$|x - y| < \varepsilon/\gamma \implies \gamma|x - y| < \varepsilon,$$

and since $|g(x) - g(y)| \leq \gamma|x - y|$ by assumption, $|g(x) - g(y)| < \varepsilon$.

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We thus know by Brouwer's theorem that g must have a fixed point.

Proof.

We now show that the fixed point of g is unique. Suppose p and q are two fixed points of g. Then $g(p) = p$ and $g(q) = q$, so

$$|p - q| = |g(p) - g(q)| \leq \gamma |p - q|$$

and since $\gamma < 1$, this can only be satisfied if $|p - q| = 0$, so $p = q$.

Proof.

We now show convergence for arbitrary $x_0 \in [a, b]$. Recall that $x_i = g(x_{i-1})$ and consider

$$|x_i - x^\star| = |g(x_{i-1}) - g(x^\star)| \leq \gamma |x_{i-1} - x^\star|$$

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Since $\gamma < 1$, $\gamma^i \to 0$, while $|x_0 - x^\star|$ is fixed. Thus

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$$\frac{|x_i - x^\star|}{|x_{i-1} - x^\star|} \le \gamma,$$

the convergence is at least linear with rate $\gamma < 1$. □

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Contraction mapping theorem: g a contraction, i.e. with $|g'(x)| \leq \gamma < 1$ for all $x \in (a,b)$ in the differentiable case.

Let's review the conditions for our theorems.

Existence of fixed point: $g : [a, b] \to [a, b]$ continuous.

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Contraction mapping theorem: g a contraction, i.e. with $|g'(x)| \leq \gamma < 1$ for all $x \in (a, b)$ in the differentiable case.

Let's explore some examples on the edges of these results.

First, let's consider

$$g : [0, 1] \to [0, 1], \quad g(x) = x.$$

This is differentiable but has $|g'(x)| = 1$. Clearly this has an infinite number of fixed points.

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You can have a unique fixed point of a differentiable function without being a contraction. An example is

$$g : [0,\pi] \to [0,1] \subset [0,\pi], \quad g : x \mapsto \sin x.$$

This has $|g'(x)| < 1$ for $x \in (0,\pi)$, so has a unique fixed point $x^\star = 0$. But it is not a contraction, since $g'(0) = \cos(0) = 1$; there is no $\gamma < 1$ such that $|g'(x)| \leq \gamma$ on $(0,\pi)$. The fixed point iteration converges, but so slowly as to be absolutely useless.

Section 6

Example

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Let's manipulate f to recast the problem as a fixed point problem. There are many ways to do this.

Fixed point iteration A

$$x^2 - x - 1 = 0$$

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$$x^2 - x - 1 = 0 \implies x^2 = x + 1$$

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Fixed point iteration B

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Fixed point iteration C

$$x^2 - x - 1 = 0$$

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$$x^2 - x - 1 = 0 \implies x(x-1) = 1$$

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Fixed point iteration B

$$x^2 - x - 1 = 0 \implies x = x^2 - 1 =: g_B(x)$$

Fixed point iteration C

$$x^2 - x - 1 = 0 \implies x(x-1) = 1 \implies x = 1/(x-1) =: g_C(x)$$

Comment

Rootfinding with fixed point iteration doesn't typically rely on manual manipulation like this.

We'll see *generic* ways of transforming a rootfinding problem into a fixed point problem that work for very broad classes of functions.

If we run the fixed point iteration with $x_0 = 1.1$, we get

iteration	$g_A(x) = (x+1)/x$	$g_B(x) = x^2 - 1$	$g_C(x) = 1/(x-1)$
1	1.909091	0.210000	10.00000
2	1.523810	-0.955900	0.111111
3	1.656250	-0.086255	-1.125000
4	1.603774	-0.992560	-0.470588
5	1.623529	-0.014825	-0.680000
6	1.615942	-0.999780	-0.595238
7	1.618834	-0.000439	-0.626866
8	1.617729	-1.000000	-0.614679
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Can we explain this?

Let's check if we can find γ and $[a,b]$ such that $g([a,b]) \subset [a,b]$ and $|g'(x)| \leq \gamma < 1$ on (a,b).

Case A: $g(x) = (x+1)/x$

Its derivative is $g'(x) = -1/x^2$. On $[a,b] = [1,2]$ this is increasing, but $g'(1) = -1$. So let's try $[a,b] = [1.1, 2]$. We then have $\gamma = |g'(1.1)| \approx 0.826 < 1$.

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Banach's contraction mapping theorem thus applies.

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Case B: $g(x) = x^2 - 1$

Its derivative is $g'(x) = 2x$. We have $g'(\phi) \approx 3.23 > 1$ and $g'(-\phi^{-1}) \approx -1.23 < -1$. So there can be no interval containing the root that satisfies the criteria.

Let's check if we can find γ and $[a, b]$ such that $g([a, b]) \subset [a, b]$ and $|g'(x)| \leq \gamma < 1$ on (a, b).

Case C: $g(x) = 1/(x - 1)$

Its derivative is $g'(x) = -1/(x-1)^2$, with $g'(\phi) \approx -2.6 < -1$, and $g'(-\phi^{-1}) \approx -0.38$.
Taking $[a, b] = [-0.8, -0.4]$, we have g' is a decreasing function, and $\gamma = |g'(-0.4)| \approx 0.51$.

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On $[-0.8, -0.4]$, g is a decreasing function, so we just need to check the endpoints. We have $g(-0.8) \approx -0.555$ and $g(-0.4) \approx -0.714$, so $g([a, b]) \subset [a, b]$.

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Section 7

Termination criteria

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This reminds us we want a contraction with a small γ: if $\gamma \approx 1$, we will require many iterations to converge.

This is an *a priori* error estimate: we can compute it before ever doing any computations, or choosing x_0. What can we do if we know more?

From the contraction property, we know that

$$|x_i - x_{i-1}| \leq \gamma |x_{i-1} - x_{i-2}|$$

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\end{aligned}$$

In brackets we have the first few terms of the geometric series, which converges because $\gamma < 1$. Taking the limit $J \to \infty$, so $x_J \to x^\star$, we have

$$|x_i - x^\star| \leq \frac{\gamma^i}{1 - \gamma}|x_1 - x_0|.$$

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In brackets we have the first few terms of the geometric series, which converges because $\gamma < 1$. Taking the limit $J \to \infty$, so $x_J \to x^\star$, we have

$$|x_i - x^\star| \leq \frac{\gamma^i}{1-\gamma}|x_1 - x_0|.$$

This is an *a posteriori* bound: you have to do some computation to use it.

Section 8

Another example

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Find some $[a, b]$ so that $g(x) = e^{-x}$ has a unique fixed point in $[a, b]$.

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Also note that $g(1) = e^{-1} < 1$, and $g(x)$ is decreasing, so $g : [0, 1] \to [0, 1]$.

We could thus take an interval with $a > 0$ but close and $b = 1$. Choosing $[a, b] = [1/10, 1]$ works fine. (The actual fixed point is $x^\star \approx 0.567143$.)

Continuing with the same example, how many iterations are required to get within 10^{-3} of the fixed point?

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For the *a priori* bound, solving $\gamma^i < 0.001/0.9$ yields $i > 68$. (To achieve a tolerance of 10^{-6}, $i > 137$ is required.)

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For the *a priori* bound, solving $\gamma^i < 0.001/0.9$ yields $i > 68$. (To achieve a tolerance of 10^{-6}, $i > 137$ is required.)

Let's imagine we start with a lucky guess $x_0 = 0.56$. How does the *a posteriori* bound look? In this case $x_1 \approx 0.57120906$, so we have

$$\frac{\gamma^i}{1-\gamma}|0.57120906 - 0.56| < \mathrm{tol},$$

which gives $i > 47$ for $\mathrm{tol} = 10^{-3}$ and $i > 116$ for $\mathrm{tol} = 10^{-6}$.

Section 9

Accelerating sequence convergence

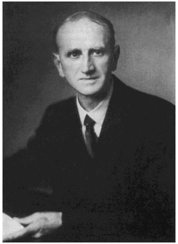
Suppose one has a sequence (x_i) that is linearly converging:

$$\lim_{i\to\infty} \frac{|x_{i+1} - x^\star|}{|x_i - x^\star|} = \mu,$$

with the property that for large enough i,

$$x_i - x^\star, \quad x_{i+1} - x^\star, x_{i+2} - x^\star$$

all have the same sign.



Alexander Aitken FRS FRSL, 1895–1967

Aitken's big idea: use the entries of (x_i) to make a new sequence $(\tilde{x}_i)$ that (hopefully) converges faster!

Assume that the asymptotic limits hold at iterations $i+1$, $i+2$, so that

$$x_{i+1} - x^\star \approx \mu(x_i - x^\star), \quad x_{i+2} - x^\star \approx \mu(x_{i+1} - x^\star).$$

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$$x_{i+1} - x^\star \approx \mu(x_i - x^\star), \quad x_{i+2} - x^\star \approx \mu(x_{i+1} - x^\star).$$

Equating the two expressions for μ and doing some algebra yields

$$x^\star \approx x_i - \frac{(x_{i+1} - x_i)^2}{x_{i+2} - 2x_{i+1} + x_i}$$

so we hope that the expression on the right gives a good approximation to the sequence limit.

Assume that the asymptotic limits hold at iterations $i+1$, $i+2$, so that

$$x_{i+1} - x^\star \approx \mu(x_i - x^\star), \quad x_{i+2} - x^\star \approx \mu(x_{i+1} - x^\star).$$

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Aitken thus defines

$$\tilde{x}_i = x_i - \frac{(x_{i+1} - x_i)^2}{x_{i+2} - 2x_{i+1} + x_i}$$

to yield a new, (hopefully) faster-converging sequence.

Aitken's acceleration is backed up by a theorem.

Aitken's theorem (1926)

Suppose (x_i) is linearly converging with all entries the same sign. Then

$$\lim_{i \to \infty} \frac{\tilde{x}_i - x^\star}{x_i - x^\star} = 0.$$

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Consider Leibniz' formula for π:

$$\pi = 4\sum_{k=0}^{\infty} \frac{(-1)^k}{2k+1}.$$

Set x_i to be the i^{th} partial sum.

To get π to 10 digits, Leibniz' formula requires about 5 billion terms; Aitken's acceleration $(\tilde{x}_i)$ of it requires about 1400.

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To get π to 10 digits, Leibniz' formula requires about 5 billion terms; Aitken's acceleration $(\tilde{x}_i)$ of it requires about 1400.

If you apply Aitken acceleration *again*, to yield $(\tilde{\tilde{x}}_i)$, you can get away with only 70 terms!

Computational Mathematics
Week 3: Newton's method

Patrick E. Farrell

University of Oxford

Let's consider rootfinding again:

$$\text{find } x^\star \in \mathbb{R} \text{ such that } f(x^\star) = 0.$$

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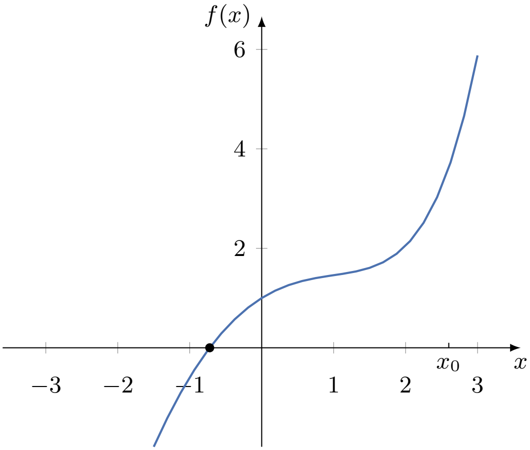
How should we construct $g(x)$ from $f(x)$? One way we've seen is to set

$$g(x) = f(x) + x$$

but we have no reason to think this is a contraction.

Here is a better way to construct $g(x)$.



Start from an initial x_0.

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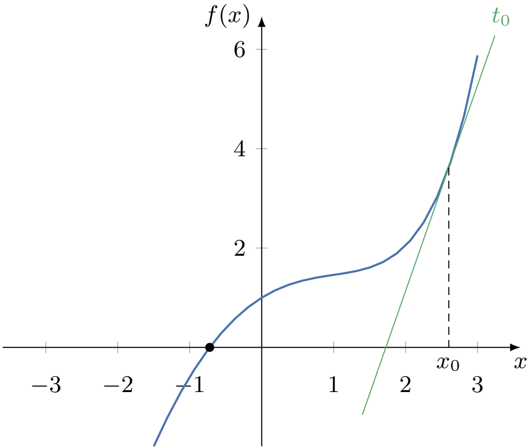

Build a *linear model* of the function.

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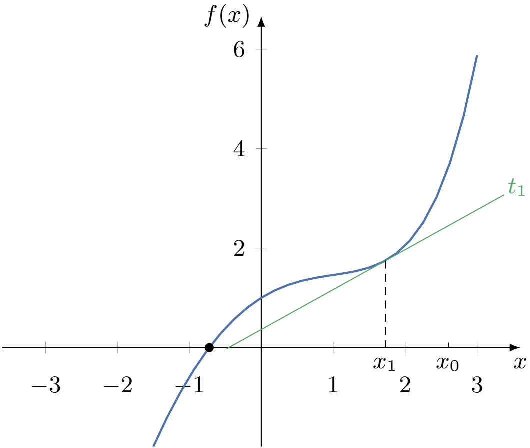

Set x_1 to be the root of the linear model.

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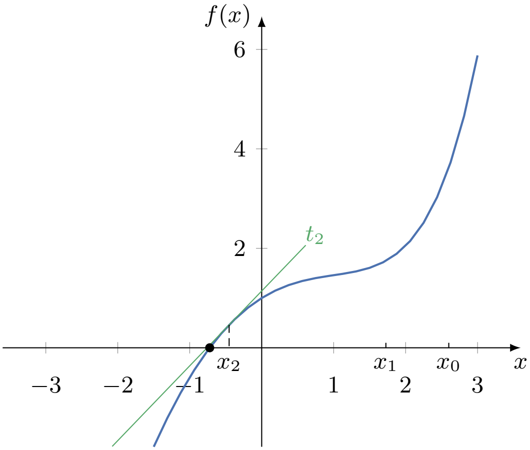

Repeat.

The tangent line joins $(x_i, f(x_i))$ and $(x_{i+1}, 0)$, so we can write its slope as

$$f'(x_i) = \frac{f(x_i) - 0}{x_i - x_{i+1}}$$

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$$f'(x_i) = \frac{f(x_i) - 0}{x_i - x_{i+1}}$$

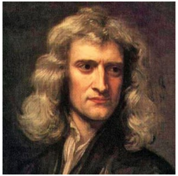
and solving for x_{i+1} yields

$$x_{i+1} = x_i - \left(f'(x_i)\right)^{-1} f(x_i).$$

Newton–Raphson method

$$x_{i+1} = g(x_i) \coloneqq x_i - \left(f'(x_i)\right)^{-1} f(x_i).$$

This is a generic way of constructing a fixed point problem $x = g(x)$ from a rootfinding problem $f(x) = 0$.



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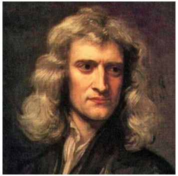

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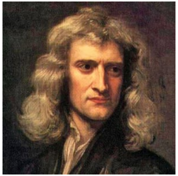

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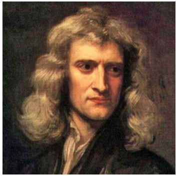

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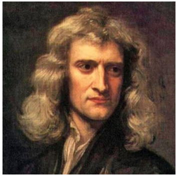

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The extension to computing p-th roots was known to Jamshīd al-Kāshī in Samarkand around 1427.

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Joseph Raphson (1690) simplified the method, but still only applied it to polynomials.

Thomas Simpson (1740) gave the modern description, using calculus, and applied it to general functions.

Newton–Raphson method

$$x_{i+1} = g(x_i) \coloneqq x_i - \left(f'(x_i)\right)^{-1} f(x_i).$$

Comments:

✓ If $f(x_i) = 0$, then $x_{i+1} = x_i$. So roots of f are fixed points of g.

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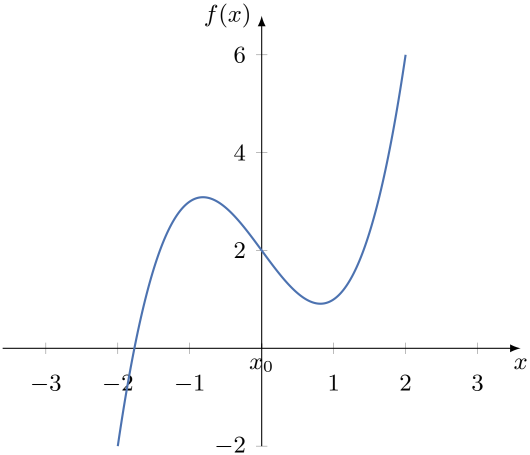
- ✓ If x_0 is close to $x^\star$, Newton's method usually converges *very fast*.
- ✗ If x_0 is far away, the method can diverge or get stuck in a cycle.
- ✓ Newton's method generalises elegantly to higher dimensions.

Consider $f(x) = x^3 - 2x + 2$ with $x_0 = 0$.



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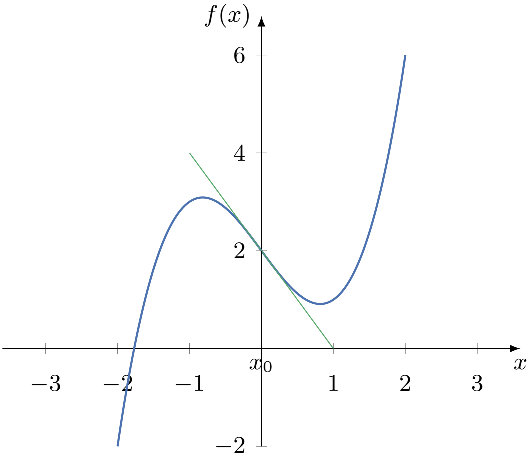

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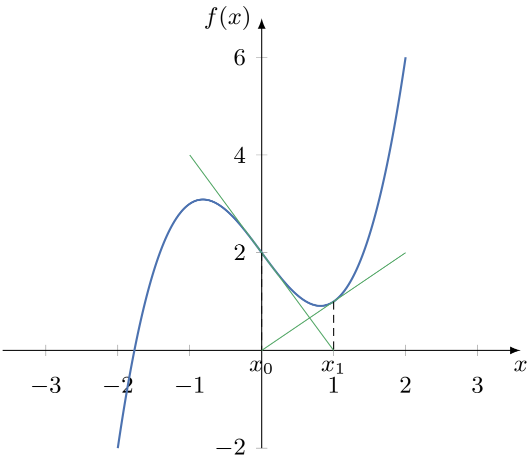

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$$f(x) = (x-4)(x-1)(x+3), \quad x_0 = 2.352836327.$$

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```
In [14]: newton(lambda x: (x-4)*(x-1)*(x+3),
                lambda x: 3*x**2 - 4*x - 11, 2.352836327, 1e-6)
Iteration  0: x = 2.352836e+00 f(x) = -1.192795e+01
Iteration  1: x = -7.829394e-01 f(x) = 1.890641e+01
Iteration  2: x = 2.352836e+00 f(x) = -1.192796e+01
Iteration  3: x = -7.829406e-01 f(x) = 1.890641e+01
...
Iteration  9: x = -8.476712e-01 f(x) = 1.927820e+01
Iteration 10: x = 2.687229e+00 f(x) = -1.259690e+01
Iteration 11: x = -1.449560e+02 f(x) = -3.086271e+06
Iteration 12: x = -9.643403e+01 f(x) = -9.143167e+05
...
Iteration 19: x = -5.622219e+00 f(x) = -1.670889e+02
Iteration 20: x = -4.050607e+00 f(x) = -4.271814e+01
Iteration 21: x = -3.265703e+00 f(x) = -8.235014e+00
Iteration 22: x = -3.023904e+00 f(x) = -6.756020e-01
Iteration 23: x = -3.000221e+00 f(x) = -6.196356e-03
Iteration 24: x = -3.000000e+00 f(x) = -5.385373e-07
Out[14]: -3.0000000192334735
```

Now change from $x_0 = 2.35283632\mathbf{7}$ to $x_0 = 2.35283632\mathbf{3}$.

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In [15]: newton(lambda x: (x-4)*(x-1)*(x+3),
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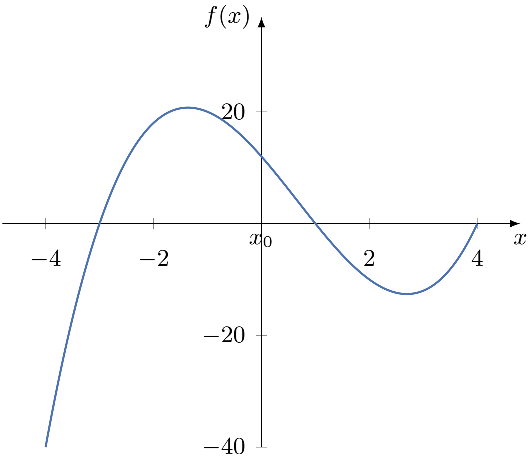
Iteration  7: x = -7.828166e-01 f(x) = 1.890567e+01
Iteration  8: x = 2.352281e+00 f(x) = -1.192584e+01
Iteration  9: x = -7.783146e-01 f(x) = 1.887843e+01
Iteration 10: x = 2.332103e+00 f(x) = -1.184692e+01
Iteration 11: x = -6.205467e-01 f(x) = 1.781690e+01
Iteration 12: x = 1.799380e+00 f(x) = -8.442739e+00
Iteration 13: x = 8.042685e-01 f(x) = 2.379590e+00
Iteration 14: x = 9.981010e-01 f(x) = 2.279200e-02
Iteration 15: x = 9.999997e-01 f(x) = 3.591499e-06
Iteration 16: x = 1.000000e+00 f(x) = 8.926193e-14
Out[15]: 0.9999999999999926
```

Let's draw the first iterations with $x_0 = 2.352836327$.



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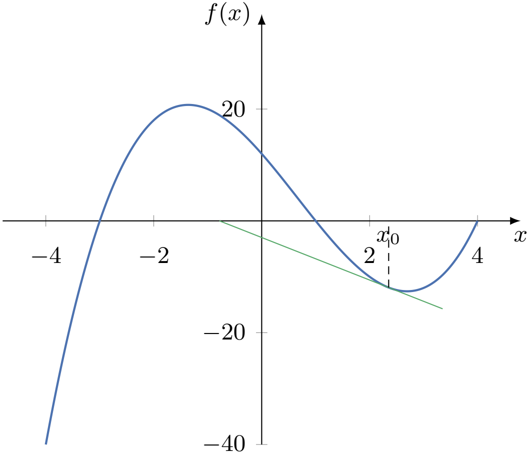

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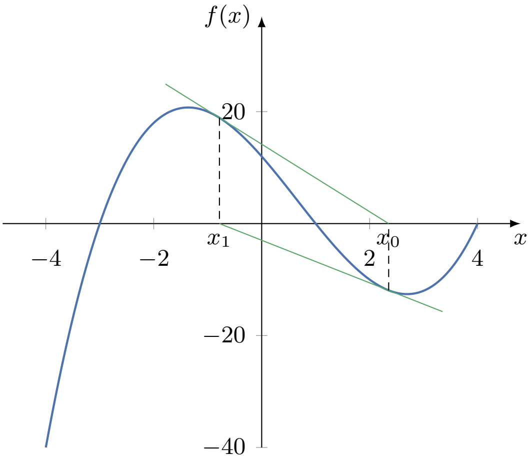

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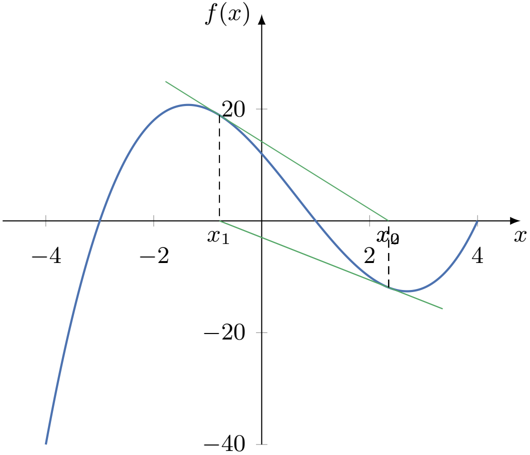

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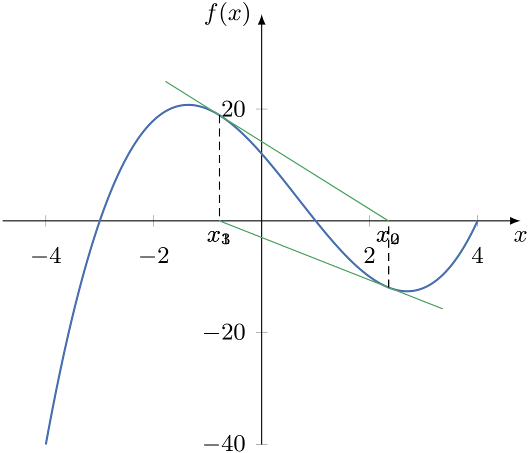

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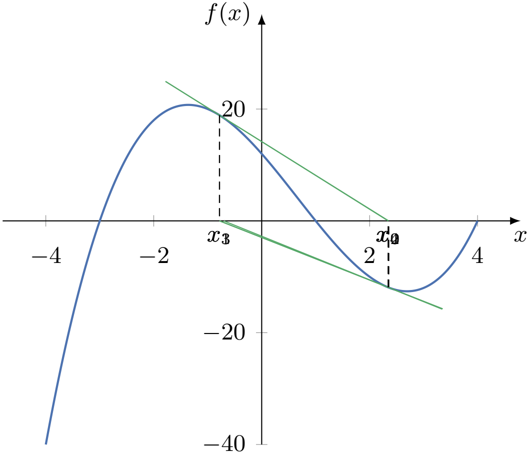

So why is Newton's method a good idea? Let's talk about general fixed point iterations $x_{i+1} = g(x_i)$ converging to $x^\star$ for a moment.

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For a contraction g with contraction factor $\gamma < 1$, we know

$$|x_{i+1} - x^\star| \leq \gamma |x_i - x^\star|,$$

or in other words that we have linear convergence

$$\frac{|x_{i+1} - x^\star|}{|x_i - x^\star|} \leq \gamma < 1.$$

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But Newton's method is special: under mild conditions, when x_i is close to $x^\star$ it will satisfy for some $K > 0$

$$\frac{|x_{i+1} - x^\star|}{|x_i - x^\star|^2} \leq K.$$

Recall that we called this *quadratic* convergence.

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This is much, much faster: roughly speaking, the number of correct digits will *double* at each iteration!

So how can Newton achieve this quadratic convergence?

Recall the Taylor expansion of g around some point a:

$$g(x_i) = g(a) + (x_i - a)g'(a) + \frac{1}{2}(x_i - a)^2 g''(\zeta_i), \quad \text{some } \zeta_i \in (x_i, a).$$

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But $g(x_i) = x_{i+1}$ and $g(x^\star) = x^\star$, so

$$|x_{i+1} - x^\star| = |(x_i - x^\star)g'(x^\star) + \frac{1}{2}(x_i - x^\star)^2 g''(\zeta_i)|$$

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If $f'(x^\star) = 0$, we have a multiple root, and we have to take the limit $x \to x^\star$ and use L'Hôpital's rule to evaluate the fraction.

Take-home message

Newton's method converges quadratically to isolated roots.

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If the root is not isolated, then one generally expects linear convergence, with the exact rate depending on details. For example, on the problem sheets you will prove that if

$$f'(x^\star) = 0, f''(x^\star) \neq 0$$

then one expects linear convergence with rate $1/2$.

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Let's do an exam question. Consider the question from 2017, Paper IV, Q7 (b):

> *The function*
>
> $$p(x) = 27x^3 - 27x^2 + 4$$
>
> *has a root* $\alpha = 2/3$.
>
> *Show that Newton's method to compute approximations to this root, with starting guess* x_0*, can be written as the iteration*
>
> $$x_{k+1} = g(x_k),$$
>
> *where you should find* g *explicitly. Prove or disprove that the sequence generated will converge to* α *for any* $x_0 \in [1/3, 1]$.

We write

$$g(x) = x - \frac{p(x)}{p'(x)}$$
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To check whether the Newton sequence will converge, we investigate the conditions of Banach's contraction mapping theorem.

Let's check the conditions. We compute

$$g'(x) = \frac{2}{3} - \frac{2}{27x^2}, \quad g''(x) = \frac{4}{27x^3}.$$

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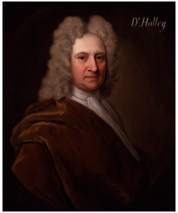
So the conditions of Banach's contraction mapping theorem are satisfied.

There are other fixed-point iterations for rootfinding.

Halley's method (1694)

$$x_{i+1} = g(x_i) := x_i - \frac{2f(x_i)f'(x_i)}{2[f'(x_i)]^2 - f(x_i)f''(x_i)}.$$



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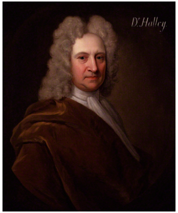

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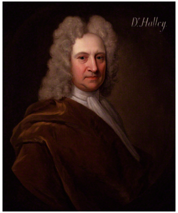

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Halley was Savilian Professor of Geometry here in Oxford, after Wallis.

In a letter in 1712, Taylor wrote

> *While I was thinking of these things, I fell into a general method of applying Dr. Halley's Extraction of roots to all Problems ...And it is comprehended in this Theorem ....*

The theorem he proved was Taylor's theorem!

Brook Taylor FRS, 1685–1731

Section 2

The secant iteration

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The *secant* iteration makes the converse trade: no derivative evaluations, for (slightly) slower convergence.

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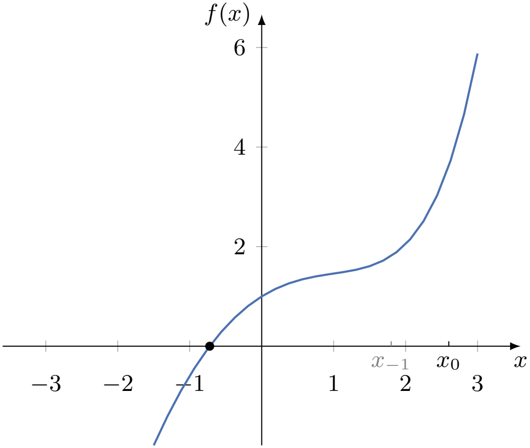
Both the ancient Egyptians and Babylonians used the secant method around 1800 BCE to solve equations like

$$ax + b = c$$

since they didn't know how to move terms from one side to another!

The secant iteration.



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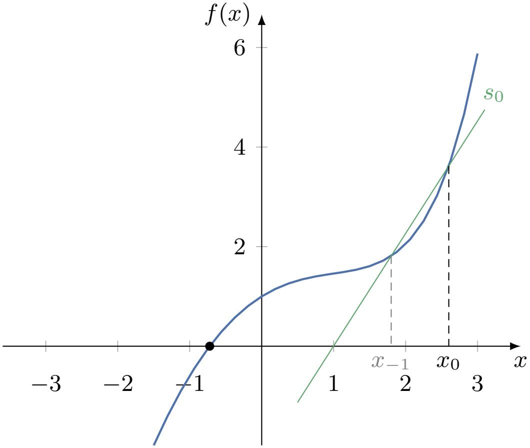

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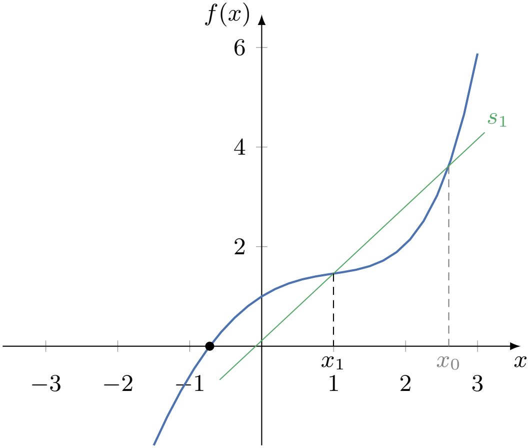

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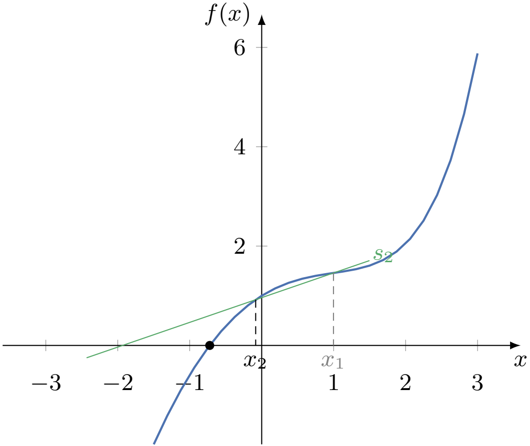

Interestingly, the secant iteration converges with order

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so its convergence is superlinear, but not quite quadratic.

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Comments on the secant method:

- ✗ The method requires more information to start, and depends sensitively on it.
- ✓ In principle the method can be applied to nondifferentiable functions.
- ▶ The generalisation to higher dimensions is different—leading to the quasi-Newton family of methods.

Section 3

Aitken acceleration of fixed-point iterations

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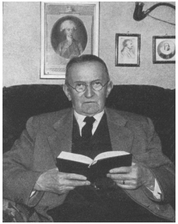
The acceleration only goes one way: we don't re-use the accelerated values in the fixed-point iteration itself.

Steffensen's idea

Do two steps of fixed-point iteration, apply Aitken acceleration, then re-start the fixed-point iteration from there.

This *interleaves* the fixed-point iteration and acceleration.



Johan Frederik Steffensen, 1873–1961

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---

function steffensen(g, x_0, tol)
  $x \leftarrow x_0$
  while $|g(x) - x| > \mathrm{tol}$ **do**
    $x_0 \leftarrow x$
    $x_1 \leftarrow g(x_0)$
    $x_2 \leftarrow g(x_1)$
    $x \leftarrow \left(x_0 x_2 - x_1^2\right) / (x_2 - 2x_1 + x_0)$
  end while
  return $g(x)$
end function

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If you organise the code properly, this requires two evaluations of g per iteration.

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Does this really help?

Yes, it does, under certain conditions:

Steffensen's theorem (1933)

Suppose that $g(x)$ has a fixed point $x^\star$ with $g'(x^\star) \neq 1$. If there exists $\delta > 0$ such that $g \in C^3([x^\star - \delta, x^\star + \delta], \mathbb{R})$, then Steffensen's method gives quadratic convergence for any $x_0 \in [x^\star - \delta, x^\star + \delta]$.

This can achieve quadratic convergence, without derivatives!

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$$g(x) = \frac{x+1}{x}$$

for calculating the golden ratio ϕ.

Fixed-point iteration requires 37 evaluations of g to get ϕ to 16 digits. Steffensen's method requires only 8!

Let's apply Newton's method to

$$f(x) = (x - 1)^2.$$

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This gives

$$g(x) = x - \frac{(x-1)^2}{2x-2}.$$

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Since $f'(1) = 0$, $g'(1) \neq 0$, and we only achieve linear convergence:

```
In [17]: newton(lambda x: (x-1)**2, lambda x: 2*x - 2, 0, 1e-4)
Iteration  0: x = 0.000000e+00 f(x) = 1.000000e+00
Iteration  1: x = 5.000000e-01 f(x) = 2.500000e-01
Iteration  2: x = 7.500000e-01 f(x) = 6.250000e-02
Iteration  3: x = 8.750000e-01 f(x) = 1.562500e-02
Iteration  4: x = 9.375000e-01 f(x) = 3.906250e-03
Iteration  5: x = 9.687500e-01 f(x) = 9.765625e-04
Iteration  6: x = 9.843750e-01 f(x) = 2.441406e-04
Iteration  7: x = 9.921875e-01 f(x) = 6.103516e-05
Out[17]: 0.9921875
```

Converging linearly, you say?

```
In [19]: steffensen(lambda x: x - (x-1)**2/(2*x-2), 2, 1e-12, exact=1)
Iterations  0: fixed point = 2.000000000000000e+00 error = 1.000000000000000e+00
Iterations  2: fixed point = 1.000000000000000e+00 error = 0.000000000000000e+00
```

Steffensen's method gets the answer exact to 16 digits in 2 iterations.

Section 4

Rootfinding for polynomials

We have seen general rootfinding methods that apply to many different kinds of functions.

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Philosophical remark

When designing algorithms, we should always ask: have we used every piece of knowledge we have about the problem?

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When designing algorithms, we should always ask: have we used every piece of knowledge we have about the problem?

For example, if we restrict ourselves to rootfinding for *polynomials*, can we make our algorithms better? The answer is yes.

Section 5

Horner's method

In the literature, Horner's method refers to two different things:

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The evaluation scheme was known in medieval times to Qín Jiŭsháo (c. 1202–1261) and Sharaf al-Dīn al-Ṭūsī (c. 1135-1213), and later to Newton and Lagrange.

In the literature, Horner's method refers to two different things:

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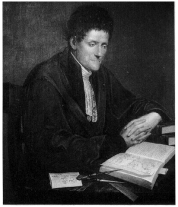
The evaluation scheme was known in medieval times to Qín Jiǔsháo (c. 1202–1261) and Sharaf al-Dīn al-Ṭūsī (c. 1135-1213), and later to Newton and Lagrange.

It's not clear that Horner, a schoolmaster in Bath, even invented the latter method that now bears his name. He was beaten to it by Paolo Ruffini in 1804 and Theophilus Holdred, a London watchmaker, in 1820. The method was published again by Horner in 1830.



Paolo Ruffini, 1765–1822

Let's consider Horner's two methods in order. Suppose we have a polynomial

$$p(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n$$

with n large, e.g. $n = 10,000$. How should we evaluate $p(r)$ for $r \in \mathbb{R}$?

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with n large, e.g. $n = 10,000$. How should we evaluate $p(r)$ for $r \in \mathbb{R}$?

One way would be to evaluate all the terms in the sum separately, and add them up. This would require n additions and

$$0 + 1 + 2 + \cdots + n = \frac{n^2 + n}{2}$$

multiplications. Scaling like n^2 is bad!

Instead, a better way is to write

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This shares the evaluations of powers of x. It only requires n multiplications and n additions!

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$$b_n := a_n$$

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&\vdots \\
b_i &:= a_i + b_{i+1} r \\
&\vdots \\
b_1 &:= a_1 + b_2 r \\
b_0 &:= a_0 + b_1 r.
\end{aligned}$$

We then have $b_0 = p(r)$.

There's more to it than this, however.

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Theorem

Define the polynomial

$$Q(x) := b_n x^{n-1} + b_{n-1}x^{n-2} + \cdots + b_2 x + b_1.$$

Then

$$p(x) = (x - r)Q(x) + b_0.$$

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$$p'(x) = Q(x) + (x - r)Q'(x),$$

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Before proving this, note that indeed $p(r) = b_0$, and

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so in particular

$$p'(r) = Q(r).$$

Proof.

Recall that $p(x) = a_0 + \cdots + a_n x^n$, $b_n = a_n$, and $b_i = a_i + b_{i+1} r$.

Expand

$$(x - r)Q(x) + b_0 =$$

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Expand

$$(x - r)Q(x) + b_0 = (x - r)(b_n x^{n-1} + \cdots + b_1) + b_0$$

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Expand

$$\begin{aligned}(x-r)Q(x) + b_0 &= (x-r)(b_n x^{n-1} + \cdots + b_1) + b_0 \\ &= x(b_n x^{n-1} + \cdots + b_1) - r(b_n x^{n-1} + \cdots + b_1) + b_0\end{aligned}$$

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&= b_n x^n + (b_{n-1} - b_n r)x^{n-1} + \cdots + (b_0 - b_1 r)
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since $a_i = b_i - b_{i+1} r$ for $i < n$. □

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In the context of Newton's method applied to p, we have

$$x_{i+1} = x_i - \frac{p(x_i)}{p'(x_i)}$$

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$$x_{i+1} = x_i - \frac{p(x_i)}{p'(x_i)} = x_i - \frac{p(x_i)}{Q(x_i)}.$$

function horner($[a_0, \cdots, a_n]$, x_0, tol, maxit)

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for $i = 1, \ldots, \text{maxit}$ **do**

$b \leftarrow a_n x + a_{n-1}$ # Horner eval for p

```
function horner([a_0, ..., a_n], x_0, tol, maxit)
    x ← x_0
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        c ← a_n                                  # Horner eval for p'
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      $c \leftarrow cx + b$

      $b \leftarrow bx + a_i$

    end for

    if $|b| < \text{tol}$ **then** # success

      return x

    end if

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function horner([a_0, ..., a_n], x_0, tol, maxit)
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        c ← a_n                                      # Horner eval for p'
        for k = n-1, n-2, ..., 1, 0 do
            c ← cx + b
            b ← bx + a_i
        end for
        if |b| < tol then                            # success
            return x
        end if
        x ← x - b/c                                  # Newton update
    end for
end function
```

We can summarise with the following useful notation:

Definition (Big $\mathcal{O}$ notation)

For $g(n) > 0$, we say

$$f(n) = \mathcal{O}(g(n)) \text{ as } n \to \infty$$

if there exists $M > 0$ and $n_0 \in \mathbb{N}$ such that

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The number of operations to evaluate a degree-n polynomial is:

- $\mathcal{O}(n^2)$ for the naïve way, but
- $\mathcal{O}(n)$ for Horner's evaluation scheme.

This is much, much better at high n!

In fact, Horner's scheme for evaluation has a nice optimality property:

Theorem

Any algorithm for evaluating an arbitrary polynomial must require at least n additions (Ostrowski, 1954) and at least n multiplications (Pan, 1966).

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Since Horner's scheme employs n additions and n multiplications, it is optimal (for arbitrary polynomials).

If you know you'll evaluate a polynomial many times on different inputs, it is possible to preprocess the polynomial into a representation that requires fewer operations (trading offline work for online work).

Section 6

More philosophical remarks

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Philosophical remark

Equivalent expressions can have different algorithmic properties!

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Philosophical remark

Equivalent expressions can have different algorithmic properties!

In Horner's case, we had

$$a_0 + a_1 x + \cdots + a_n x^n = a_0 + x\left(a_1 + x\left(a_2 + \cdots + x\left(a_{n-1} + x a_n\right)\cdots\right)\right).$$

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Algorithmic advances sometimes come by deriving an equivalent expression with better properties.

Think back to our list of questions we ask about algorithms:

- Does the algorithm terminate?
- Does the algorithm give the correct answer?
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There's another very important question we might want to ask:

- Can we parallelise the algorithm?

Every computer nowadays has multiple processing units. (My phone has 8.) Can we use them?

Here's another equivalent expression with different properties:

$$\begin{aligned} &a_0 + a_1 x + \cdots + a_n x^n \\ &\quad = \left(a_0 + a_2 x^2 + a_4 x^4 + \cdots\right) + \left(a_1 x + a_3 x^3 + a_5 x^5 + \cdots\right) \end{aligned}$$

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which we can evaluate in parallel with two independent runs of Horner's method.

More generally, if you have enough terms, you can break p up into $k+1$ polynomials $\{p_j\}_{j=0}^{k}$, each taking the monomial term x^i if

$$i \bmod (k+1) = j.$$

Section 7

Finding all roots of a polynomial

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Once you have found a root $x^\star$ of $p_0(x)$, you can construct

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and apply the scheme again to p_1. Iterating in this way one can find all real roots, if you can construct good initial guesses.

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and apply the scheme again to p_1. Iterating in this way one can find all real roots, if you can construct good initial guesses.

Can we find them all at once, without fussing over guesses?

It turns out that we have *very* fast and powerful algorithms for computing the eigenvalues of diagonalisable matrices:

$$\text{for } A \in \mathbb{R}^{n\times n}, \text{ find all } \lambda_i, v_i \text{ s.t. } Av_i = \lambda v_i, \|v_i\|^2 = 1.$$

It turns out that we have *very* fast and powerful algorithms for computing the eigenvalues of diagonalisable matrices:

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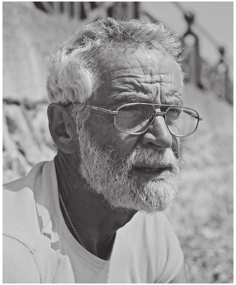
The algorithm is called the QR algorithm, invented independently by Francis (1959) and Kublanovskaya (1961). It is widely regarded as one of the ten most important algorithms of the 20^{th} century.



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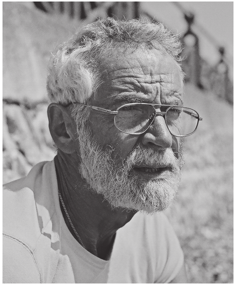

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be our (monic) polynomial. Then we can construct its *companion matrix*

$$C(a) := \begin{pmatrix} 0 & & & & -a_0 \\ 1 & 0 & & & -a_1 \\ 0 & 1 & 0 & & -a_2 \\ & & \ddots & & \vdots \\ & & & 1 & -a_{n-1} \end{pmatrix}.$$

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By construction, we have (proof is by induction):

$$\det(C(a) - \lambda I) = (-1)^n p(\lambda).$$

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We previously saw that Newton's method can get stuck in a cycle for $p(x) = x^3 - 2x + 2$. No problem:

```
In [2]: np.roots([1, 0, -2, -2])
Out[2]:
array([ 1.76929235+0.j,
       -0.88464618+0.58974281j,
       -0.88464618-0.58974281j])
```

Section 8

Representing polynomials

Philosophical remark

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A natural question to ask:

is the map $a \mapsto p$ *stable*?

If we make a perturbation δa to a, how big can the perturbation δp be? For the monomial basis $\{M_i\}$, the answer is *very very big*:

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$$p(x) = \prod_{i=1}^{20}(x - i), \quad x \in [0, 20],$$

then perturb its monomial coefficients by

$$\delta a = [0, -2^{-23}, 0, \ldots, 0].$$

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The resulting δp has

$$\|\delta p\|_\infty := \max\{|\delta p(x)| : x \in [0,20]\} \approx 6.25 \times 10^{17}$$

for a *stability constant* of

$$\frac{\|\delta p\|_\infty}{\|\delta a\|_\infty} \approx 5 \times 10^{24}.$$

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But you'd much rather compute with the latter than the former for small ε.

So what is a good basis for polynomials? An excellent choice on $[a, b]$ is

$$p(x) = \sum_{i=0}^{n} c_i T_i(\hat{x}(x)), \quad \hat{x} = \frac{2(x-a)}{(b-a)} - 1$$

where the *Chebyshev polynomials* $\{T_i : [-1, 1] \to [-1, 1]\}$ satisfy

$$T_0(\hat{x}) = 1, \quad T_1(\hat{x}) = \hat{x}, \quad T_{i+1}(\hat{x}) = 2\hat{x}T_i(\hat{x}) - T_{i-1}(\hat{x}).$$

The role of the $\hat{x}$ is to map the input interval $[a, b]$ to $[-1, 1]$.

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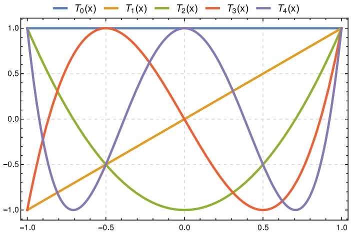

Chebyshev polynomials. Credit: Glosser.ca, Wikipedia

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Theorem

Let $f : [a, b] \to \mathbb{R}$ be analytic with Chebyshev expansion

$$f(x) = \sum_{i=0}^{\infty} c_i T_i(x).$$

Then for a constant $C > 1$

$$\|f - p_n\|_\infty = \mathcal{O}(C^{-n}), \quad p_n(x) = \sum_{i=0}^{n} c_i T_i(x).$$

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Good news

For Chebyshev bases, analogous algorithms exist:

- ✓ the *second barycentric formula*, for $\mathcal{O}(n)$ evaluation, and
- ✓ the *colleague matrix*, for finding all roots with the QR algorithm.

These allow us to work with polynomials with degrees in the millions.

Computational Mathematics
Week 4: Higher-dimensional rootfinding

Patrick E. Farrell

University of Oxford

We have considered several algorithms for rootfinding over $\mathbb{R}$:

$$\text{given } f : \mathbb{R} \to \mathbb{R}, \text{ find } x^\star \in \mathbb{R} \text{ such that } f(x^\star) = 0.$$

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- bisection ($q = 1$, $\mu = 1/2$, when it applies)
- secant method ($q = \phi \approx 1.618$, usually)
- Newton's method ($q = 2$, usually)
- Halley's method ($q = 3$, usually)

In real life, most problems involve more than one variable. So let's consider

$$\text{given } F : \mathbb{R}^N \to \mathbb{R}^N, \text{ find } \mathbf{x}^\star \in \mathbb{R}^N \text{ such that } F(\mathbf{x}^\star) = \mathbf{0}.$$

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Simpson extended Newton's method to this case in his 1740 book *Essays on Several Curious and Useful Subjects in Speculative and Mix'd Mathematicks, Illustrated by a Variety of Examples*.

Thomas Simpson, 1710–1761

Section 2

Derivation of Newton's method

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Consider a Taylor expansion of f. We want to find $x_{i+1} = x_i + \delta x$:

$$f(x_i + \delta x) = f(x_i) + \delta x f'(x_i) + \text{higher-order terms.}$$

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We want to choose the update δx so that $f(x_i + \delta x) = 0$. Setting the left-hand side to zero, and dropping higher-order terms, we get

$$\delta x = -[f'(x_i)]^{-1} f(x_i), \quad x_{i+1} = x_i + \delta x,$$

which we recognise as Newton's scheme written in update form.

Taylor's theorem extends to higher dimensions, with the role of derivative f' replaced by the **Jacobian** matrix. If $F : \mathbb{R}^N \to \mathbb{R}^N$ looks like

$$F(\mathbf{x}) = F\begin{pmatrix} \mathbf{x}^1 \\ \mathbf{x}^2 \\ \vdots \\ \mathbf{x}^N \end{pmatrix} = \begin{pmatrix} F^1(\mathbf{x}^1, \ldots, \mathbf{x}^N) \\ F^2(\mathbf{x}^1, \ldots, \mathbf{x}^N) \\ \vdots \\ F^N(\mathbf{x}^1, \ldots, \mathbf{x}^N) \end{pmatrix},$$

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$$DF(\mathbf{a}) := \begin{bmatrix} \frac{\partial F^1}{x^1}(\mathbf{a}) & \frac{\partial F^1}{x^2}(\mathbf{a}) & \cdots & \frac{\partial F^1}{x^N}(\mathbf{a}) \\ \frac{\partial F^2}{x^1}(\mathbf{a}) & \frac{\partial F^2}{x^2}(\mathbf{a}) & \cdots & \frac{\partial F^2}{x^N}(\mathbf{a}) \\ \vdots & \vdots & & \vdots \\ \frac{\partial F^N}{x^1}(\mathbf{a}) & \frac{\partial F^N}{x^2}(\mathbf{a}) & \cdots & \frac{\partial F^N}{x^N}(\mathbf{a}) \end{bmatrix}.$$

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In practice, we don't actually invert the matrix, but rather

$$\text{solve } DF(\mathbf{x}_i)\delta\mathbf{x} = -F(\mathbf{x}_i),$$

using e.g. an LU factorisation of the matrix.

Newton–Raphson method

$$\mathbf{x}_{i+1} = g(\mathbf{x}_i) := \mathbf{x}_i - \left(DF(\mathbf{x}_i)\right)^{-1} F(\mathbf{x}_i).$$

Comments:

✓ Still a fixed-point method.

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- ✗ If x_0 is far away, the method can diverge or get stuck in a cycle.
- ✓ Newton's method even generalises to infinite dimensions.

Section 3

Example

Let's do an example. Take

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Section 4

Convergence

Definition (Norm of $\mathbf{x} \in \mathbb{R}^N$)

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Definition (Convergence of a vector-valued sequence)

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$$\lim_{i\to\infty} \|\mathbf{x}_i - \mathbf{x}^\star\|_\infty = 0.$$

Definition (Order of convergence of a sequence)

Suppose $(\mathbf{x}_i) \to \mathbf{x}^\star$. The sequence converges with order q if for some $M > 0$

$$\lim_{i\to\infty} \frac{\|\mathbf{x}_{i+1} - \mathbf{x}^\star\|_\infty}{\|\mathbf{x}_i - \mathbf{x}^\star\|_\infty^q} = M.$$

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Theorem (Quadratic convergence of Newton's method)

Let $F \in C^2(\mathbb{R}^N, \mathbb{R}^N)$, i.e. F is continuous with all first and second partial derivatives continuous. Suppose $\mathbf{x}^\star \in \mathbb{R}^N$ is an isolated root of F, i.e. $F(\mathbf{x}^\star) = \mathbf{0}$ with $DF(\mathbf{x}^\star)$ nonsingular. Then if $\mathbf{x}_0$ is close enough to $\mathbf{x}^\star$, the Newton sequence will converge quadratically.

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The core of the proof is that the Jacobian matrix of the associated fixed-point iteration is zero at $\mathbf{x}^\star$.

Section 5

Affine covariance

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Now imagine that we change units or coordinate systems for our outputs F. Instead of solving $F(\mathbf{x}) = \mathbf{0}$, we want to solve $\tilde{F}(\mathbf{x}) = AF(\mathbf{x}) = \mathbf{0}$, where $A \in \mathbb{R}^{N\times N}$ is constant and nonsingular. Of course, this doesn't change the roots $\mathbf{x}^\star$.

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Theorem (Affine covariance)

Premultiplying F by a constant nonsingular $A \in \mathbb{R}^{N\times N}$ does not change the Newton sequence.

Let $\tilde{F}(\mathbf{x}) := AF(\mathbf{x})$. Newton's method applied to $\tilde{F}$ from $\mathbf{x}_0 = \tilde{\mathbf{x}}_0$ generates a sequence

$$\tilde{\mathbf{x}}_0, \tilde{\mathbf{x}}_1, \tilde{\mathbf{x}}_2, \dots .$$

Proof.

For $i = 0$, we have $\mathbf{x}_i = \tilde{\mathbf{x}}_i$ by assumption.

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Assume $\mathbf{x}_i = \tilde{\mathbf{x}}_i$ at iteration i. Then the Newton update for $\tilde{F}$ satisfies

$$-\delta\tilde{\mathbf{x}}_i = [D\tilde{F}(\tilde{\mathbf{x}}_i)]^{-1}\tilde{F}(\tilde{\mathbf{x}}_i) = [ADF(\mathbf{x}_i)]^{-1}AF(\mathbf{x}_i)$$

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Hence $\mathbf{x}_{i+1} = \tilde{\mathbf{x}}_{i+1}$, and the result follows by induction.

We get exactly the same iterates $\mathbf{x}_0, \mathbf{x}_1, \ldots,$ whether we apply Newton to $F(\mathbf{x}) = \mathbf{0}$ or $AF(\mathbf{x}) = \mathbf{0}$.

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Philosophical remark

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Moreover, any sensible strategy for globalising the convergence of Newton's method from poor initial guesses $\mathbf{x}_0$ must also preserve this property. This insight leads to the current state of the art for globalising Newton's method.

Peter Deuflhard, 1944–2019

Section 6

The Newton–Kantorovich theorem

The generalisation of Newton's method to infinite-dimensional (Banach) spaces is called the *Newton–Kantorovich* algorithm.

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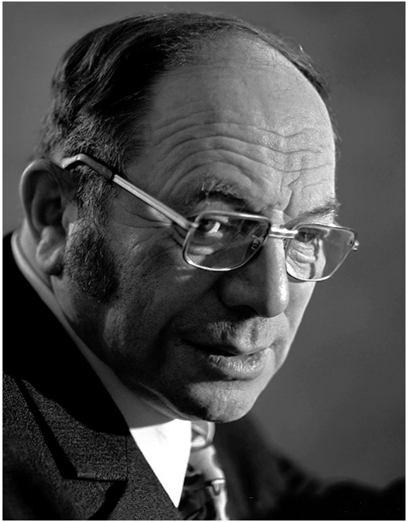

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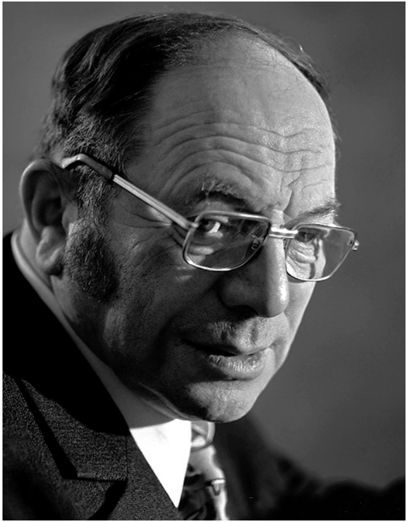

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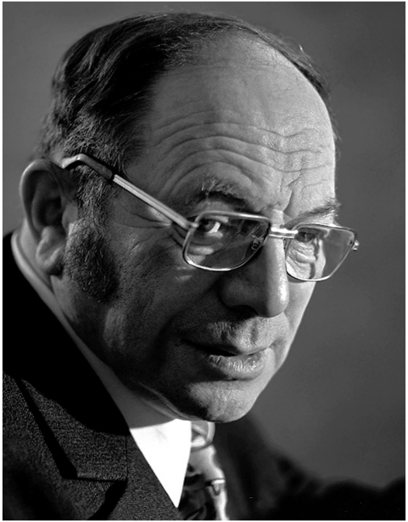

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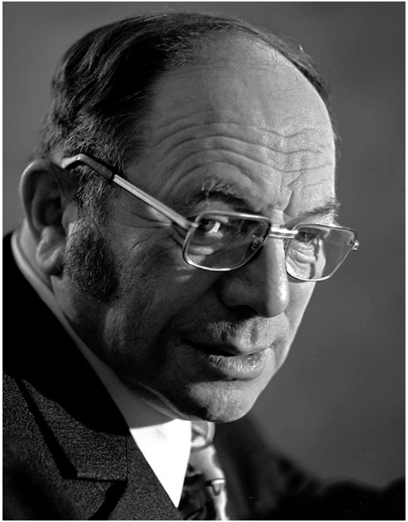

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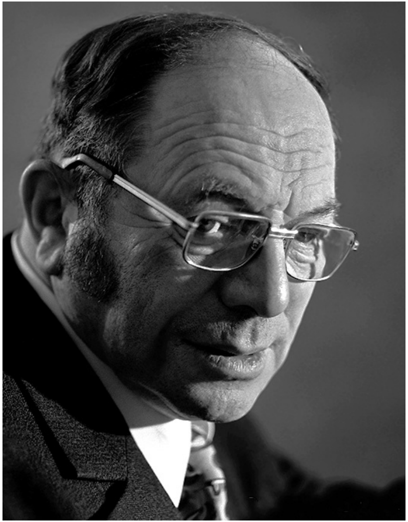

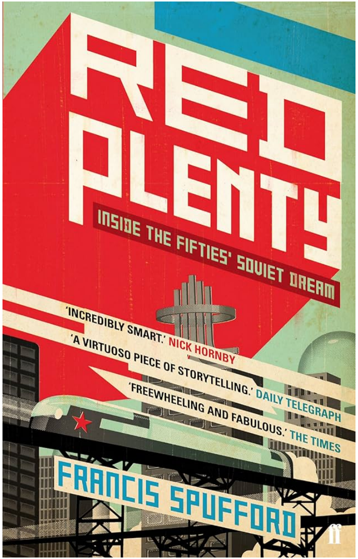
RED PLENTY
INSIDE THE FIFTIES' SOVIET DREAM
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FRANCIS SPUFFORD

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With a good initial guess, and great cleverness, it is possible to devise *computer-assisted proofs* of the existence of solutions to infinite-dimensional nonlinear problems.

Theorem (Kantorovich (1948) in finite dimensions)

Let $F \in C^1(\mathbb{R}^N, \mathbb{R}^N)$ *be the residual of our nonlinear problem, and let* $\mathbf{x}_0 \in \mathbb{R}^N$ *be an initial guess such that the Jacobian* $DF(\mathbf{x}_0)$ *is invertible. Let* $B(\mathbf{x}_0, r)$ *denote the open ball of radius* r *centred at* $\mathbf{x}_0$.

Assume that there exists a constant $r > 0$ *such that*

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(2) For all $\tilde{\mathbf{x}}, \mathbf{x} \in B(\mathbf{x}_0, r)$,

$$\|DF(\mathbf{x}_0)^{-1} \left(DF(\tilde{\mathbf{x}}) - DF(\mathbf{x})\right)\| \leq \frac{1}{r}\|\tilde{\mathbf{x}} - \mathbf{x}\|.$$

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satisfies $\mathbf{x}_i \in B(\mathbf{x}_0, r)$ *for all* i, *and converges to a root* $\mathbf{x}^\star$ *of* F.

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(4) The root $\mathbf{x}^\star$ *is locally unique, i.e.* $\mathbf{x}^\star$ *is the only root of* F *in the ball* $B\overline{(\mathbf{x}_0, r)}$.

Section 7

The Davidenko differential equation

Newton's method applied to $F(\mathbf{x}) = \mathbf{0}$ produces a sequence

$$\mathbf{x}_0, \mathbf{x}_1, \mathbf{x}_2, \ldots, \quad \mathbf{x}_i \in \mathbb{R}^N.$$

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Yes. The *Davidenko differential equation* is

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The Newton iteration is the forward Euler discretisation of the Davidenko differential equation with $\Delta s = 1$:

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}s} \approx \frac{\mathbf{x}(s + \Delta s) - \mathbf{x}(s)}{\Delta s} = -[DF(\mathbf{x}(s))]^{-1} F(\mathbf{x}(s)).$$

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Theorem

For any $\mathbf{x}_0 \in \mathbb{R}^N$, the solution curve of the Davidenko differential equation ends either at

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This shows us that the tangent of the curve—the Newton update $[DF(\mathbf{x})]^{-1}F(\mathbf{x})$—is a special direction to go to find a root, even far away from a solution. It's just that it might be *too long*.

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You can use these ideas to build effective globalisation strategies for Newton's method.

Section 8

Newton fractals

One last beautiful idea about Newton's method in higher dimensions.

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$$\text{find } z \in \mathbb{C} \text{ such that } z^3 - 1 = 0.$$

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We could also think of this as a problem in $\mathbb{R}^2$.

We know this has three solutions,

$$z = 1, \quad z = -1/2 + i\sqrt{3}/2, \text{ and } z = -1/2 - i\sqrt{3}/2.$$

Let's take a subset of the complex plane and colour each point as follows. For a given $z_0 \in \mathbb{C}$, we

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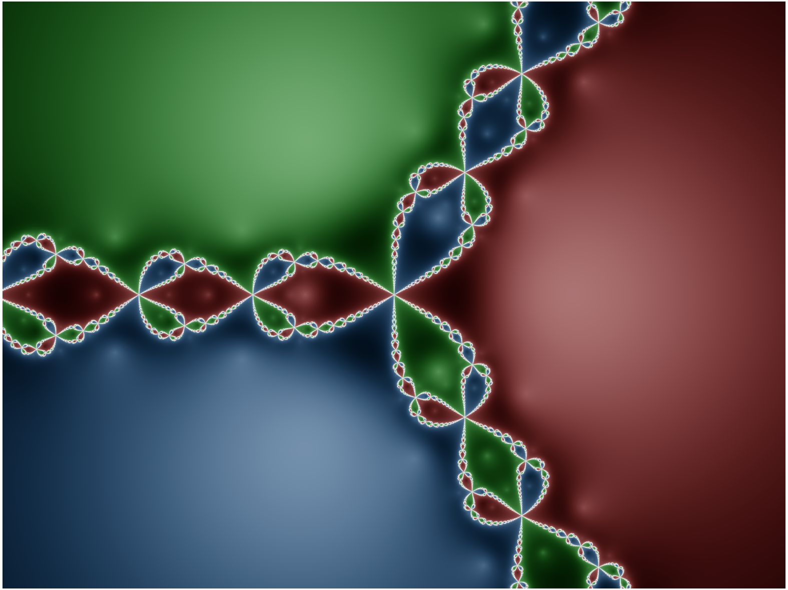
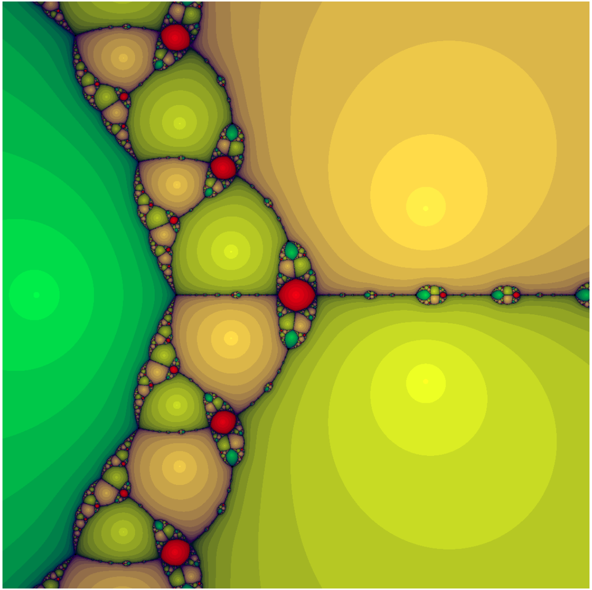
3. shade the colour by how many iterations it took.



The Newton fractal for $z^3 - 1 = 0$.



The Newton fractal for $z^3 - 2z + 2 = 0$.

Some useful websites:

- https://attr.actor/snapshots/dxhdzbzwmylmtywj
- https://newtonfractal.starfree.app/
- https://www.youtube.com/watch?v=-RdOwhmqP5s

Section 9

Algorithms for optimisation problems

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The ideas in this lecture are further explored in ASO Calculus of Variations, B6.2 Optimisation for Data Science, and C6.2 Continuous Optimisation.

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We want an argument $\mathbf{x}^\star$ that satisfies $f(\mathbf{x}^\star) \leq f(\mathbf{x})$ for all $\mathbf{x} \in \mathbb{R}^N$.

Optimisation studies how to find an input $\mathbf{x}^\star$ to a function f that achieves a minimal value. (If you want to maximise $f(\mathbf{x})$, just minimise $-f(\mathbf{x})$.)

Let's consider the optimisation problem: given $f \in C^2(\mathbb{R}^N, \mathbb{R})$,

$$\text{find } \mathbf{x}^\star = \operatorname*{argmin}_{\mathbf{x}\in\mathbb{R}^N} f(\mathbf{x}).$$

We assume f is bounded below (e.g. $f(x) = -x^2$ has no min over $\mathbb{R}$).

We want an argument $\mathbf{x}^\star$ that satisfies $f(\mathbf{x}^\star) \leq f(\mathbf{x})$ for all $\mathbf{x} \in \mathbb{R}^N$.

This is usually too much to ask for, so instead we satisfy ourselves with *local minima* $\mathbf{x}^\star$ such that there is a neighbourhood $\mathcal{N}$ around $\mathbf{x}^\star$ so that

$$f(\mathbf{x}^\star) \leq f(\mathbf{x}) \text{ for all } \mathbf{x} \in \mathcal{N}.$$

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In our case, the optimality conditions are that the *gradient* $g : \mathbb{R}^N \to \mathbb{R}^N$ is zero at a local minimiser:

$$g(\mathbf{x}^\star) := \nabla f(\mathbf{x}^\star) = Df(x^\star)^\top = \begin{pmatrix} \frac{\partial f}{\partial \mathbf{x}^1}(\mathbf{x}^\star) \\ \vdots \\ \frac{\partial f}{\partial \mathbf{x}^N}(\mathbf{x}^\star) \end{pmatrix} = \mathbf{0}.$$

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...and local maxima, and saddle points: any point like these satisfying $g(\mathbf{x}) = \mathbf{0}$ is called a *critical point*.

To develop practical optimisation algorithms, we've already relaxed the problem twice:

$$\text{global minimisers} \subset \text{local minimisers} \subset \text{critical points.}$$

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Local minimisers can be distinguished by studying the *second-order sufficiency conditions*. We won't see these.

Finding global minimisers is so hard that it is its own branch of study, *global* optimisation.

The model problem we're considering in this lecture is quite simplified. In most real optimisation problems, there are *constraints* on the solution:

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\begin{aligned}
\min_{\mathbf{x}\in\mathbb{R}^N} \quad & f(\mathbf{x}) \\
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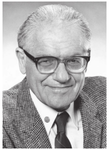
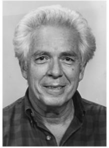


William Karush, 1917–1997



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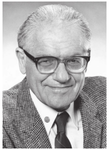
In this lecture we consider the unconstrained problem, since you need to understand that first to attack the constrained one!



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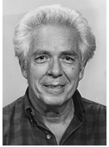

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Section 10

Newton's method for optimisation

Let's see what Newton iteration on the gradient looks like. If we take the Jacobian of the gradient, we get the *Hessian matrix*:

$$Hf(\mathbf{a}) = D\nabla f(\mathbf{a}) := \begin{pmatrix} \frac{\partial^2 f}{\partial x^1 x^1}(\mathbf{a}) & \frac{\partial^2 f}{\partial x^1 x^2}(\mathbf{a}) & \cdots & \frac{\partial^2 f}{\partial x^1 x^N}(\mathbf{a}) \\ \frac{\partial^2 f}{\partial x^2 x^1}(\mathbf{a}) & \frac{\partial^2 f}{\partial x^2 x^2}(\mathbf{a}) & \cdots & \frac{\partial^2 f}{\partial x^2 x^N}(\mathbf{a}) \\ \vdots & \vdots & & \vdots \\ \frac{\partial^2 f}{\partial x^N x^1}(\mathbf{a}) & \frac{\partial^2 f}{\partial x^N x^2}(\mathbf{a}) & \cdots & \frac{\partial^2 f}{\partial x^N x^N}(\mathbf{a}) \end{pmatrix}.$$

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Suppose we're at iterate $\mathbf{x}_i$ and we'd like to minimise f. We don't know how, so we'll replace f with a local quadratic model:

$$f(\mathbf{x}_i + \delta\mathbf{x}) \approx m(\delta\mathbf{x}) := f(\mathbf{x}_i) + \nabla f(\mathbf{x}_i)^\top \delta\mathbf{x} + \frac{1}{2}\delta\mathbf{x}^\top H f(\mathbf{x}_i)\delta\mathbf{x}.$$

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So at every step, Newton's method for optimisation approximates the function with a paraboloid, and minimises that.

Section 11

Quasi-Newton methods

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It is often possible to overcome these issues by exploiting some *structure* in the problem. When minimising energy functions in physics, the matrix is usually *sparse*, which can sometimes be exploited to solve the linear system in time $\mathcal{O}(N)$ instead of $\mathcal{O}(N^3)$.

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But for many problems no such nice structure exists (e.g. neural networks).

The standard practice is to modify the algorithm to

$$\mathbf{x}_{i+1} = \mathbf{x}_i - B_i^{-1}\nabla f(\mathbf{x}_i)$$

for carefully chosen matrices B_i. This is called a *quasi-Newton* scheme.

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The choice most used in practice is the BFGS algorithm (1970).

This builds up an approximation to the Hessian as the iterations proceed.

The BFGS approach demands that the symmetric matrix B_{i+1} satisfy

$$B_{i+1}(\mathbf{x}_{i+1} - \mathbf{x}_i) = \nabla f(\mathbf{x}_{i+1}) - \nabla f(\mathbf{x}_i).$$

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This means we now need to supply B_0. With the right choice of norm, this problem has an explicit solution for B_{i+1} and B_{i+1}^{-1}.

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Diagonal matrices

A diagonal matrix A is positive-definite iff all of its diagonal entries are strictly positive. In this case,

$$\mathbf{x}^T A\mathbf{x} = A_{11}(\mathbf{x}^1)^2 + A_{22}(\mathbf{x}^2)^2 + \cdots + A_{NN}(\mathbf{x}^N)^2 > 0.$$

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BFGS gives a positive-definite Hessian approximation, if B_0 is.

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Since $\phi_i'(0) < 0$, this means that there exists $t > 0$ such that

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We therefore modify the algorithm to

$$\mathbf{x}_{i+1} = \mathbf{x}_i - t_i^\star B_i^{-1} \nabla f(\mathbf{x}_i),$$

where $t_i^\star$ is an (approximate) minimiser of $\phi(t)$.

We end the course with a final example. Consider the problem

$$\text{find } (x,y)^\star = \underset{(x,y)\in\mathbb{R}^2}{\operatorname{argmin}} \; f(x,y) := 100(y-x^2)^2 + (1-x)^2.$$

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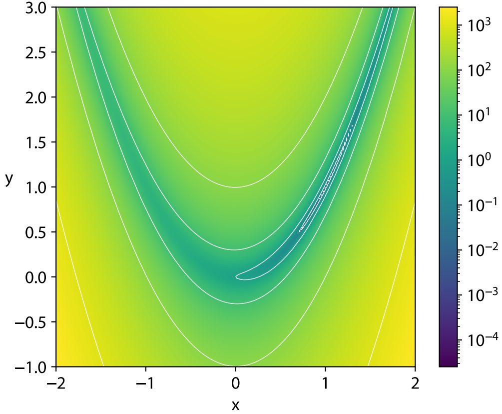
This is the *Rosenbrock* function and has unique minimiser $(x,y)^\star = (1,1)$.



We solve this from $(x_0, y_0) = (-1.2, 1)^\top$ with gradient descent, Newton's method, and BFGS, with a Wolfe line search, until $\|\nabla f(x)\| < 10^{-5}$.

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Gradient descent	Newton's method	BFGS
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$\|(x, y) - (x, y)^\star\|$ for the last 4 iterations.

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Gradient descent took 5264 iterations, Newton's method 21, and BFGS 34.