Computational Mathematics
Lecture 1

Patrick E. Farrell

University of Oxford

Section 1

Computational mathematics by example

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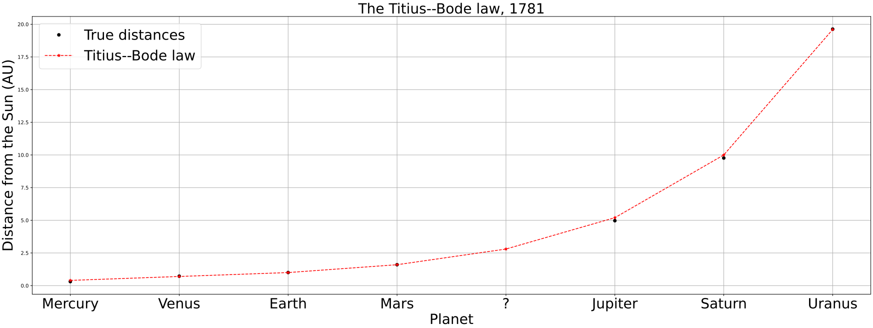

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On 1 January 1801, Giuseppe Piazzi discovered Ceres, almost exactly where the Titius–Bode law predicted!

But he could only observe it for 41 days before it was lost behind the Sun—not long enough to compute its orbit. How could it be found again?

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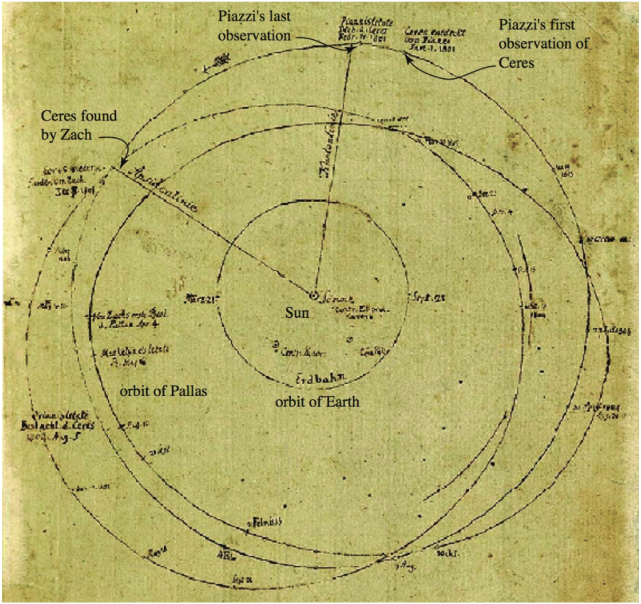
Gauss knew that orbits are approximately ellipses with the sun at one focus, which left him with six parameters to estimate from Piazzi's 22 observations.

Gauss calculated for weeks on end; he published his prediction for Ceres' location in September 1801. On December 7, astronomers found Ceres again, almost exactly where he predicted.



Annotated sketch from Gauss' papers. Courtesy Georg-August-Universität Göttingen.

It is possible to find two squares that sum to a square:

$$3^2 + 4^2 = 5^2,$$

and three cubes that sum to a cube:

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So, in 1769, Euler conjectured that

$$\exists\, k > 1, n > 1, a_1, \ldots, a_n, b \in \mathbb{N}_+ : a_1^k + a_2^k + \cdots a_n^k = b^k \implies k \leq n.$$

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In 1966, Leon J. Lander and Thomas R. Parkin discovered a counterexample:

COUNTEREXAMPLE TO EULER'S CONJECTURE ON SUMS OF LIKE POWERS

BY L. J. LANDER AND T. R. PARKIN

Communicated by J. D. Swift, June 27, 1966

A direct search on the CDC 6600 yielded

$$27^5 + 84^5 + 110^5 + 133^5 = 144^5$$

as the smallest instance in which four fifth powers sum to a fifth power. This is a counterexample to a conjecture by Euler [1] that at least n nth powers are required to sum to an nth power, $n > 2$.

REFERENCE

1. L. E. Dickson, *History of the theory of numbers*, Vol. 2, Chelsea, New York, 1952, p. 648.

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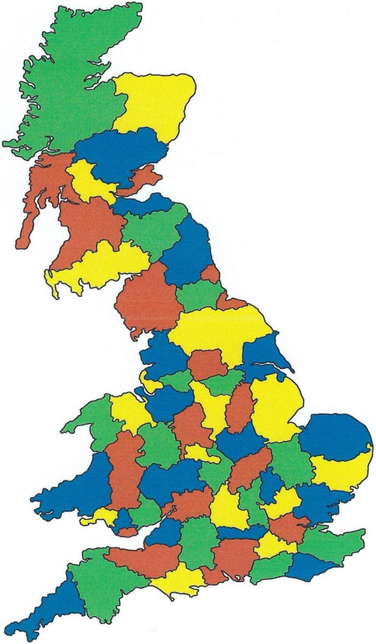
This is equivalent to colouring a *graph*: each region is a vertex, and adjacent regions are connected with an edge.



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While the proof was wrong, the basic strategy was right.

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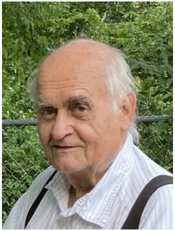
Kenneth Appel, 1932–2013



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With a computer, they found an unavoidable set with 1834 cases, and programmed it to mechanically check that in each case the graph can be coloured with four colours.

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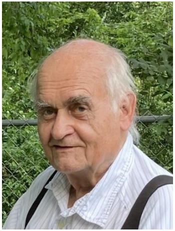

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Since then, many theorems have been proven with computer-assisted proofs, among them

- Kepler's conjecture on packing cannonballs;
- Keller's conjecture on tiling Euclidean space;
- Feigenbaum's conjecture in dynamical systems.

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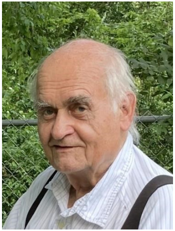

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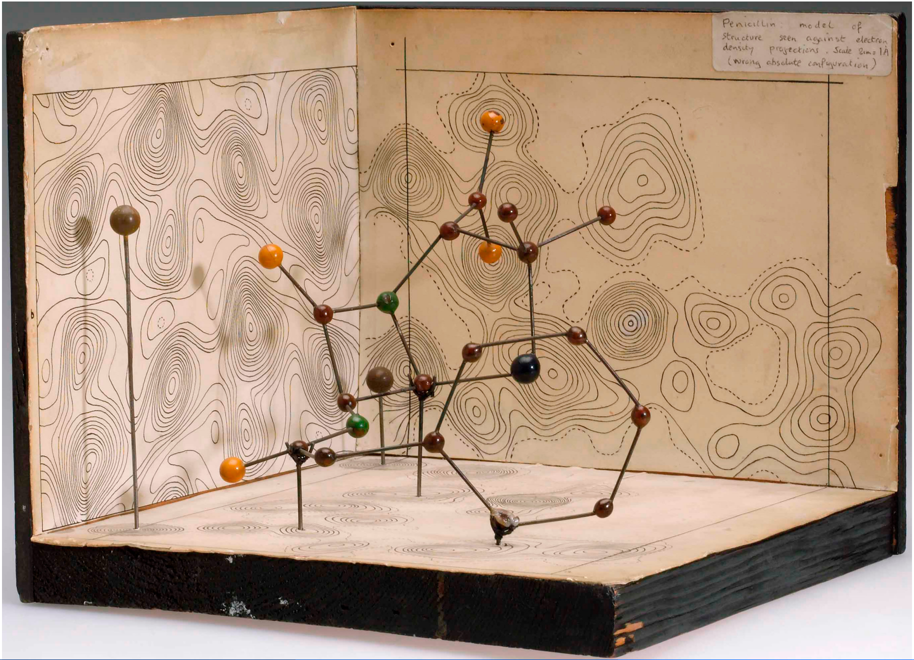
Penicillin: model of
structure seen against electron
density projections. Scale 2cm = 1Å
(wrong absolute configuration)

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In 1964 she won the Nobel Prize in Chemistry for her identification of penicillin and vitamin B_{12}.

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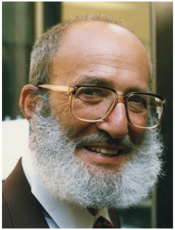
Computational mathematics is an ancient subject; it did not begin with the invention of computers. Instead, *computers were invented to speed up computational mathematics!*

In 1985, Paul Halmos wrote

> *When you try to prove a theorem, you don't just list the hypotheses, and then start to reason. What you do is trial and error, experimentation, guesswork. You want to find out what the facts are.*



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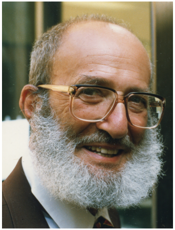

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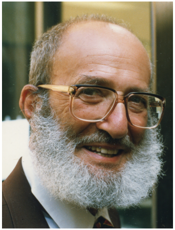

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As G. H. Hardy wrote,

> *The theory of numbers, more than any other branch of mathematics, began by being an experimental science. Its most famous theorems have all been conjectured, sometimes a hundred years or more before they were proved; and they have been suggested by the evidence of a mass of computations.*

Godfrey Hardy, 1877–1947

Section 2

Practicalities

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On a pragmatic point, a very large fraction of Oxford mathematics graduates will pursue careers where programming is useful, if not essential. These include

- mathematical research;
- scientific research;
- quantitative finance;
- teaching;
- data science;
- management consulting.

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5–6 MT	7	8	I.2
7–8 MT	10	-	I.3
1–2 HT	12–13	-	I.4

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There are four two-hour demonstration sessions for this course; three this term, and one next term. In demonstration session n you start problem sheet n, and return it for marking in demonstration session $n+1$.

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(Optionally) bring your laptops along to the next lecture to follow along with installation.

$\rightarrow$ the Lander–Parkin counterexample

Computational Mathematics
Lecture 2

Patrick E. Farrell

University of Oxford

How to submit problem sheets

A brief tour of the course

- Week 3–4 MT
- Week 5–6 MT
- Week 7–8 MT
- Week 1–2 HT

Software installation

Section 1

How to submit problem sheets

$\rightarrow$ using `publish.py`

Section 2

A brief tour of the course

Week 3–4 MT teaches

- arithmetic,
- conditionals,
- iteration.

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Bolzano's theorem (1817)

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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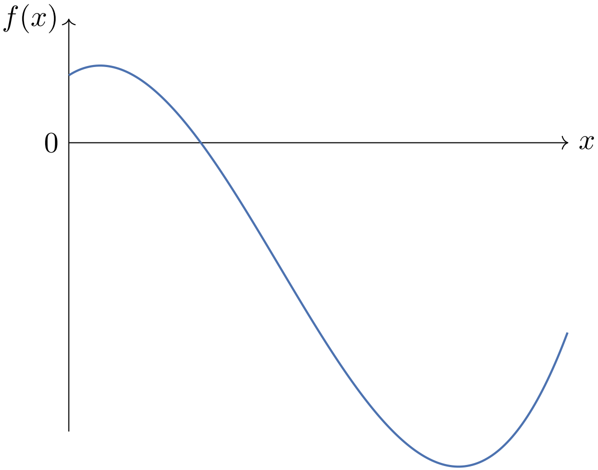
$f(x)$
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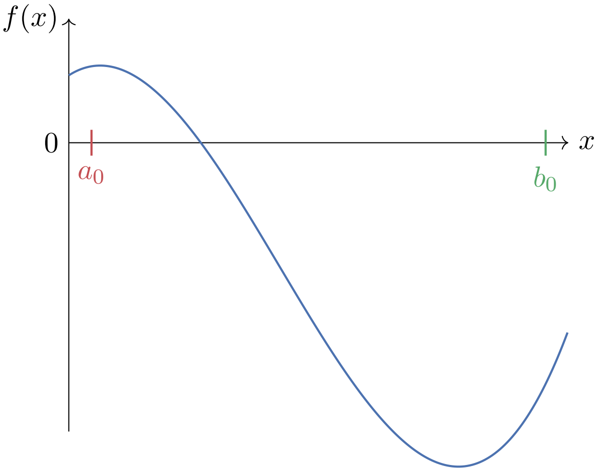
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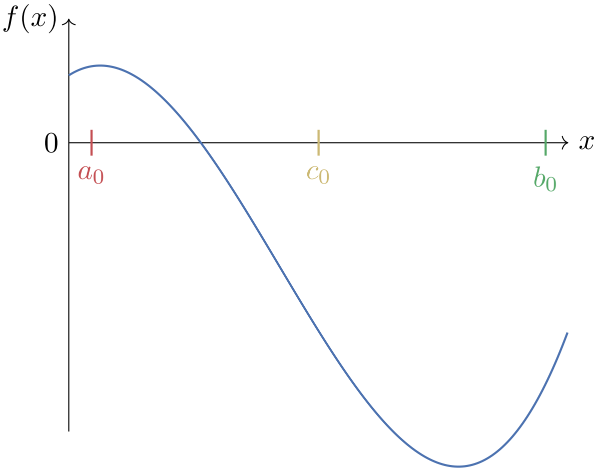
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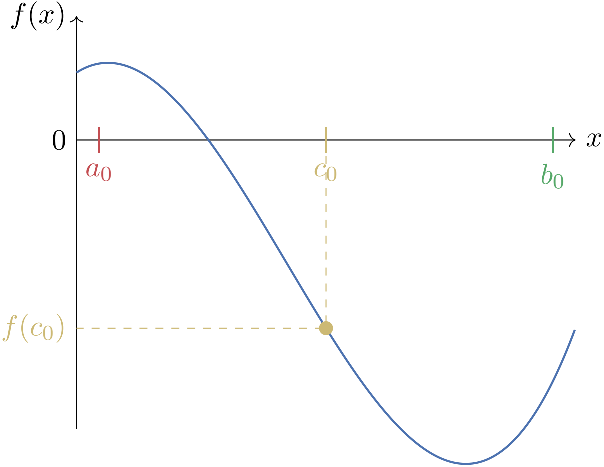
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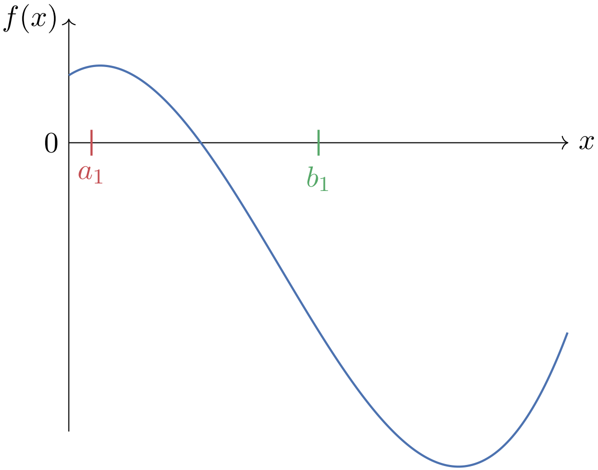
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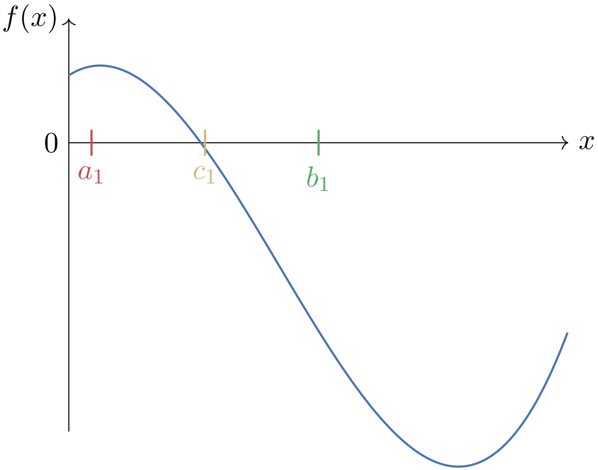
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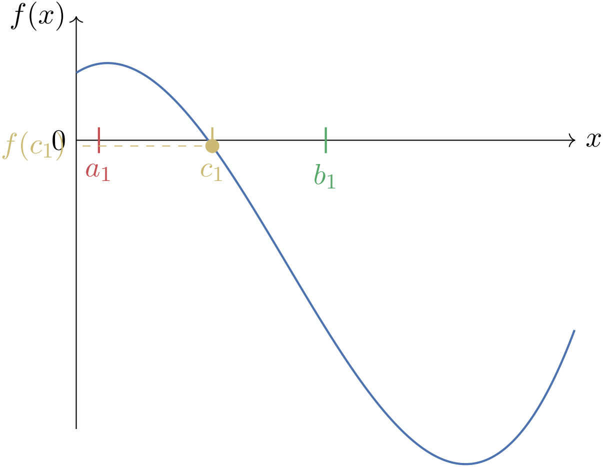
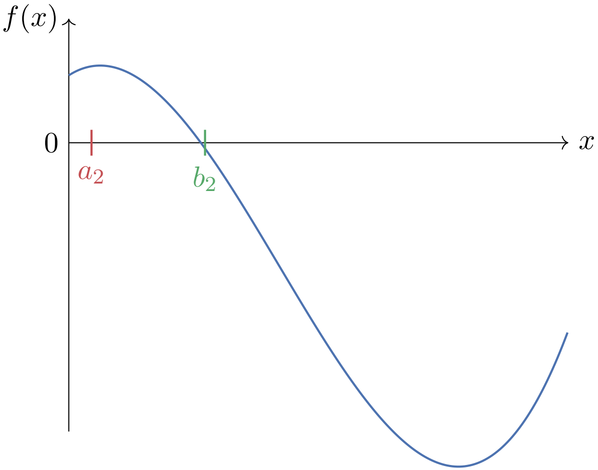
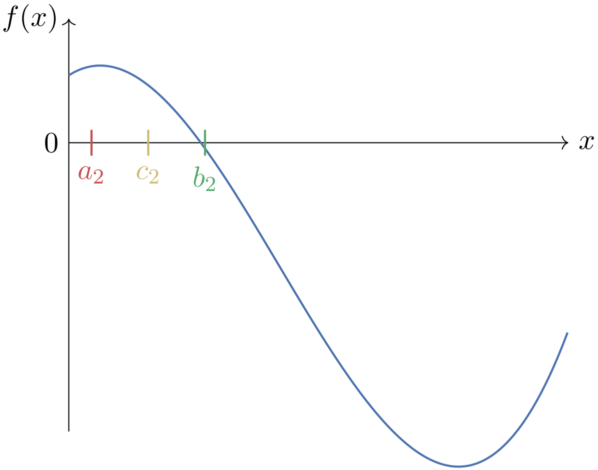
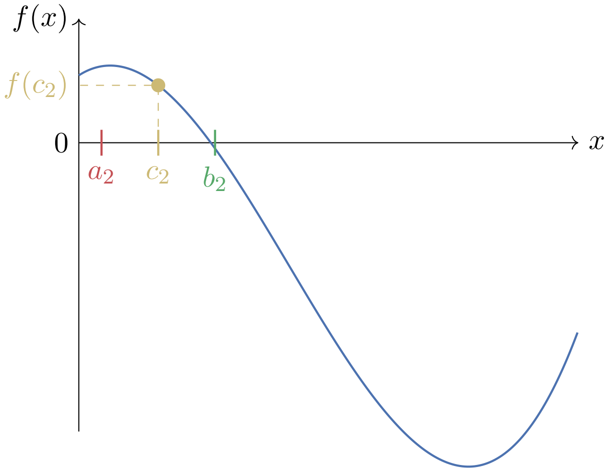
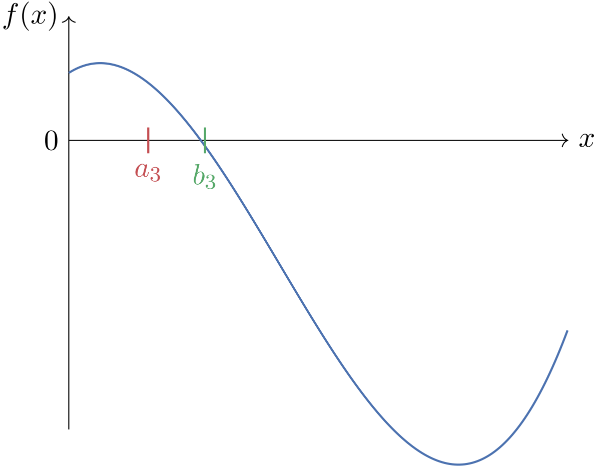
c_1
b_1


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

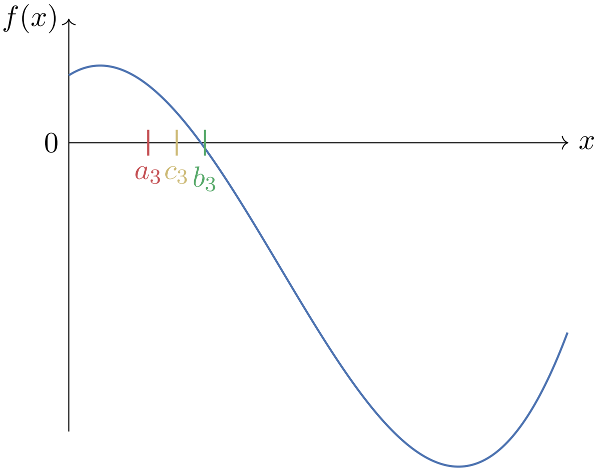

$f(x)$
0
x
a_2
b_2

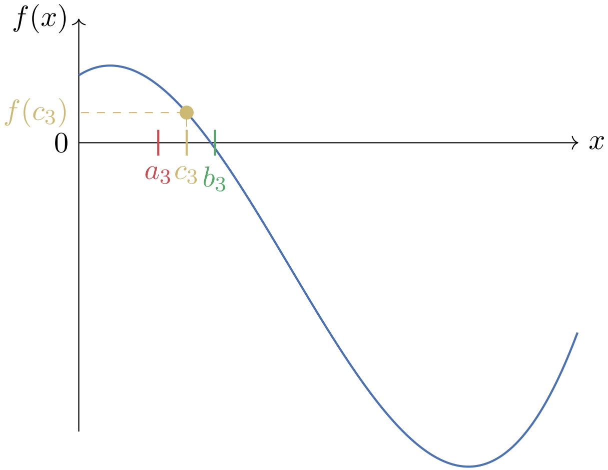

$f(x)$
0
x
a_2
c_2
b_2

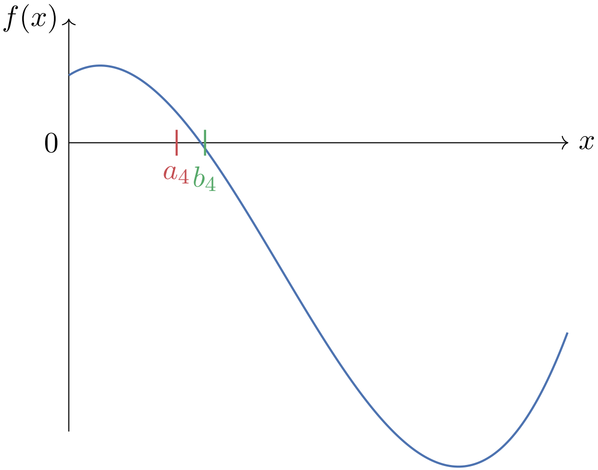

$f(x)$
$f(c_2)$
0
x
a_2
c_2
b_2



$f(x)$
0
x
a_3
b_3


$f(x)$
0
x
a_3
c_3
b_3


$f(x)$
$f(c_3)$
0
x
a_3
c_3
b_3


$f(x)$
0
x
a_4
b_4

$\rightarrow$ `bisection.py`

How can we use this to compute an approximation to π?

Week 5–6 MT teaches

- lists, tuples
- dictionaries, sets,
- functions,
- plotting.

Week 5–6 MT ends with a naïve code for *primality testing*, checking whether a given integer is prime or not.

Week 5–6 MT ends with a naïve code for *primality testing*, checking whether a given integer is prime or not.

$\rightarrow$ `isprime.py`

Can we make `isprime(9999991111111)` faster?

Week 7–8 MT introduces *symbolic computing*, the use of computers to automate the kind of mathematical manipulations you do on paper.

This includes expanding and simplifying expressions, differentiating and integrating functions, calculating limits, and solving equations.

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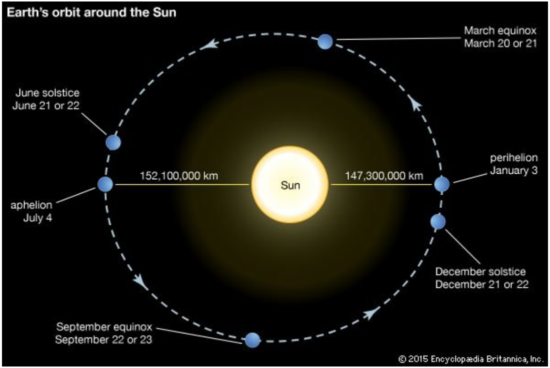
In 1843, describing Charles Babbage's Analytical Engine, Ada Lovelace wrote

> *Many persons who are not conversant with mathematical studies imagine that because the business of the engine is to give its results in numerical notation, the nature of its processes must consequently be arithmetical and numerical rather than algebraic and analytical. This is an error. The engine can arrange and combine its numerical quantities exactly as if they were letters or any other general symbols; and in fact it might bring out its results in algebraic notation were provisions made accordingly.*

Ada Lovelace, 1815–1852

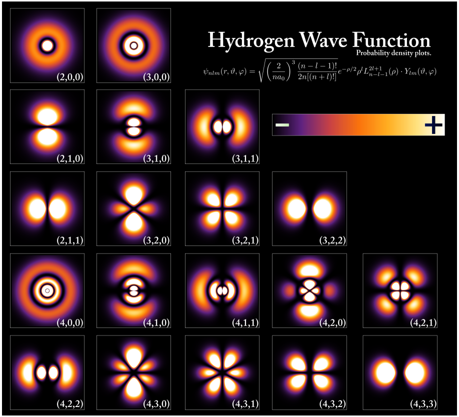
In the associated problem sheet, we use symbolic computing to

- derive the equations for the orbit of the Earth around the Sun;



In the associated problem sheet, we use symbolic computing to

- derive the equations for the orbit of the Earth around the Sun;
- explore the wave function of the hydrogen atom.

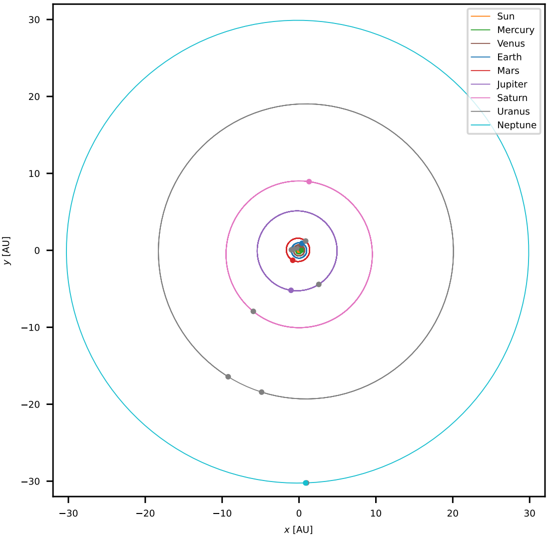


Week 1–2 HT introduces *numerical* computing, a powerful expansion of the conception of what it means to solve a mathematical problem.

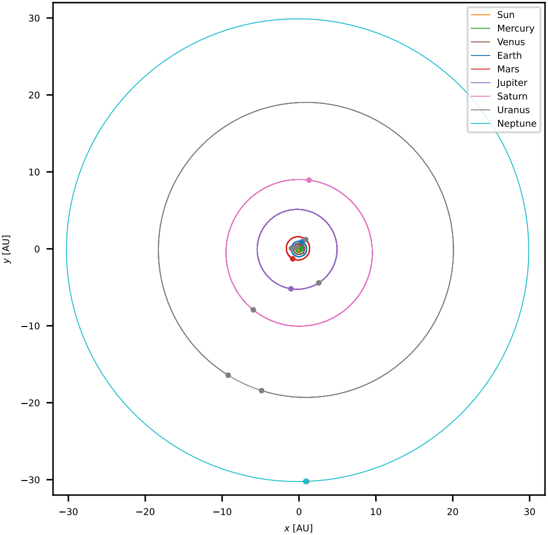
We will study

- numerical linear algebra,
- numerical quadrature of integrals,
- least squares and curve-fitting,
- numerical solution of ODE initial value problems.

Week 1–2 HT ends with a code for numerically simulating the solar system.



Week 1–2 HT ends with a code for numerically simulating the solar system.



→ `solar.py`

Section 3

Software installation

$\rightarrow$ Windows