Mathematical representations, Computational aspects Fitting, minimization, finding extrema, random numbers

... and more

The book of nature is written in mathematics.
Without it, it is impossible to understand anything and one risks getting lost in an obscure labyrinth

Galileo Galilei (1564-1642)

Nowadays, very little is done with pencil and paper, and computer programs (codes) are used for all kinds of purposes.

First Rule of computational studies:

GIGO : "Garbage In - Garage Out"
This means any program will give you a
nonsensical output (result) if you supply a nonsensical input (data)

It is always difficult to assess whether a program does what you think it does, or should do, and whether it does it consistently and reliably.

This is why you always need to check your results carefully:
eg: does it behave as you expect? (do you know what to expect?)
how do they change if you change your input data slightly (stability)

For this, you need to know the scientific background of the methods used and the approximations made in the calculations.

As simple example for this, we shall look at two applications:

- Fitting
- Minimization
- Monte Carlo Methods

Fitting

We have a number N of (x_i, y_i) points and want to find the coefficients of a function $y = f(x)$ that is the "best possible" (?) representation of the points.

– We **invent** a function $f(x)$ that we think should be suitable, eg a linear one
  $f(x) = a + b \cdot x$ with the two parameters a and b to be determined.

– We must decide: what is "best possible"
  Choice 1: the (vertical) distances between y_i and $f(x_i)$ should be minimal,
  i.e. we try to find the minimum of

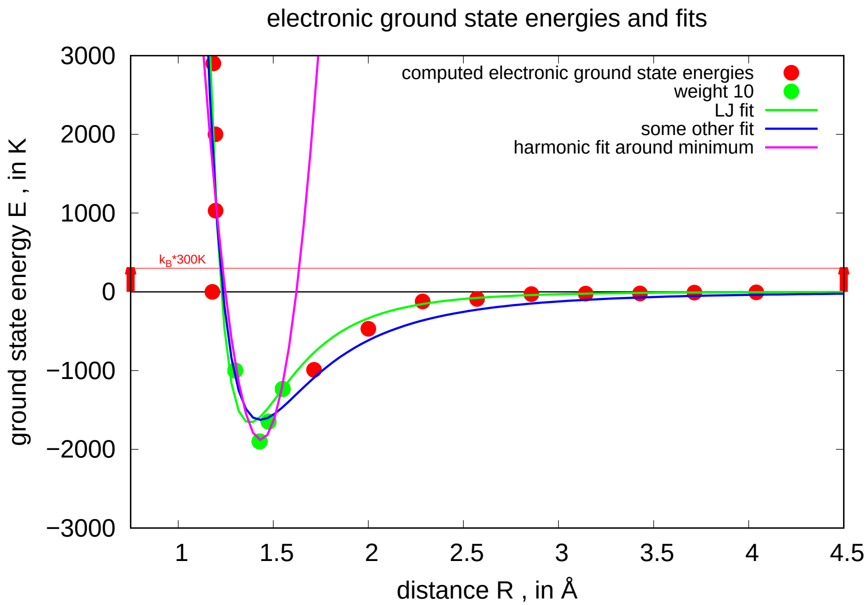
$$\sum_i^N \mid y_i - f(x) \mid \quad \text{or} \quad \sum_i^N (y_i - f(x))^2$$

  Choice 2: the relative error should be minimal

$$\sum_i^N \mid \frac{(y_i - f(x))}{y_i} \mid$$

or (Choices 3 - N) any other criterion we may deem useful, taking eg. into account that there may be different Δys and Δxs in our data points

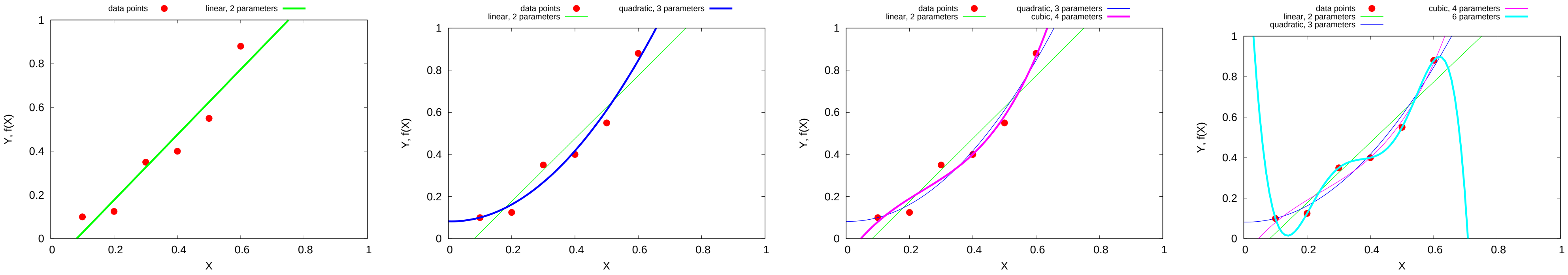
One trick is to give data points deemed more important, or with smaller uncertainties, a higher weight.
The figure shows how the fits to potential energy points (eg. from OC) change (a bit) when the points around the minimum are given a higher weight.



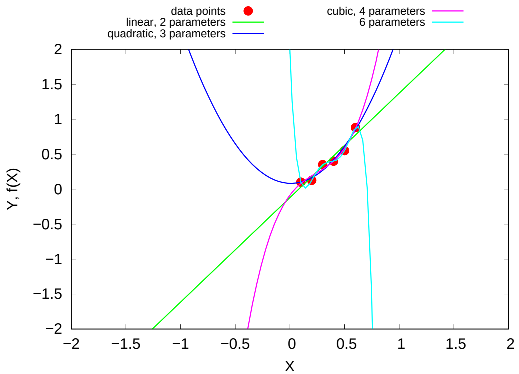
"Fitting" is a particular case of a more general mathematical problem:
finding extrema (minima, maxima) of complicated functions
We will come to this later

Of course, when we have N points, we can always find a function that will fit the N points exactly (eg a polynomial of order N). Such fits are usually **meaningless** and **useless**

The sense and nonsense of fitting



same fits, different ranges



The mathematically 'best' fit is not necessarily the physically 'best' fit (overfitting)
One must carefully select the fitting function $f(x)$, best based on a physical model

These plots and fits were made with the free software `gnuplot`*, which is highly recommended*

How do fit programs work

Linear fit vs. **non-linear** fit

Linear: the fitting coefficients to be determined (eg $c_1, c_2, c_3, ...$) appear only linearly in $f(x)$
(or $f(x, y, z, ...)$, eg $f(x) = c_1 \cdot x + c_2 \cdot x^2$
This works almost always (except for numerical problems), there is an analytical solution
see https://en.wikipedia.org/wiki/Linear_regression for details

Non-linear: the fitting coefficient appear non-linearly, eg $f(x) = \cos(c_1 \cdot x) * \exp(-c_2 \cdot x)$
see https://en.wikipedia.org/wiki/Nonlinear_regression
This can be tricky, even very tricky, there are many methods (*may be we can look at a few*)
convergence may be difficult to achieve, one finds many local minima, but
not the global one, etc etc

→ gradient methods
→ Monte Carlo methods
→ neural networks
This is an active field of research

Famous historic examples of minimization problems

– The traveling salesman problem

A salesman has to visit N customers in different places,

How can he minimize his travels

https://en.wikipedia.org/wiki/Travelling_salesman_problem

related:

– The Königsberg Bridge Problem (Immanuel Kant (1724-1804))

Kant wanted to find out whether he could make a walk starting from his home and returning to his home, crossing each bridge only once

https://en.wikipedia.org/wiki/Seven_Bridges_of_Königsberg

The most famous story about reproducing experiments accurately and their correct description

– The earth is the center of the universe. Since Ptolemy $\approx 100 - 170$ there were mathematical expression (cycles,epicycles ...), which, based on this view, described and predicted the positions of the (then known) planets reasonably well

– Nicolaus Copernicus (1474-1543) said: The sun is in the center.
But this model did not always give the planet positions very accurately

– Tycho Brahe (1546-1601) re-measured the planet motions extremely carefully. He concluded that both Ptolomy and Copernicus were "wrong" and made a new, very sophisticated model (some planets go around the sun, others go around the earth)

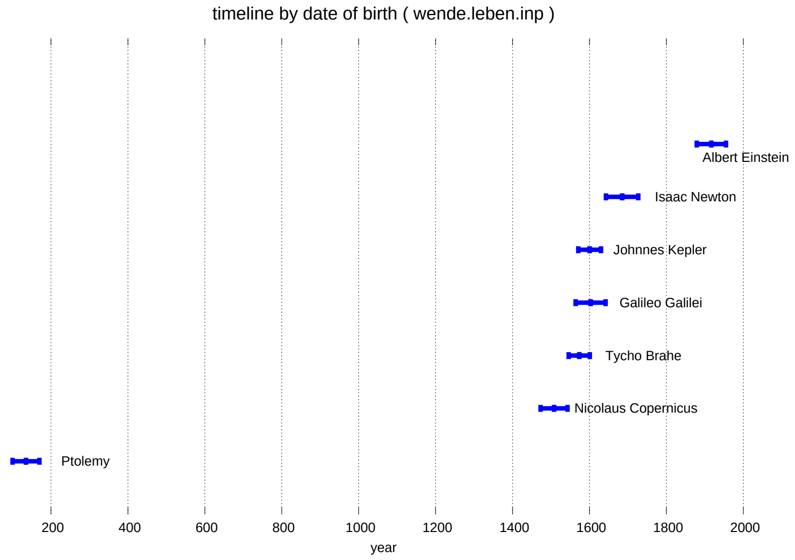
– Johannes Kepler (1571-1630) said: The planetary orbit are not circles, but ellipses.
This fitted Tycho's data well.

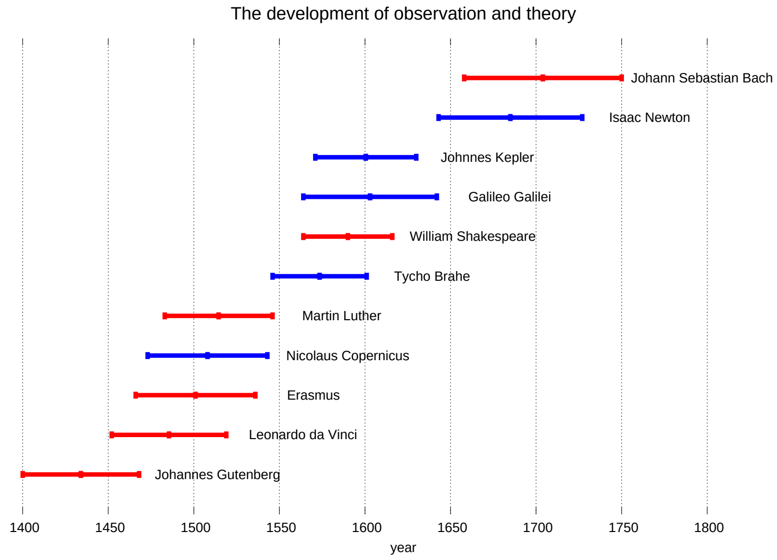
– Galileo Galilei (1564-1642) observed Jupiter's moons going around their planet

– Isaac Newton (1643-1727) found the **law** that underlies all these observations
(and the apple falling on his head)

Note:
Ptolemy was Greek (or Egyptian), Copernicus was Polish (or German), Tycho was Danish, Kepler was Austrian, Galileo was Italian, Newton was English, science is international

Timelines


timeline by date of birth (wende.leben.inp)
Albert Einstein
Isaac Newton
Johnnes Kepler
Galileo Galilei
Tycho Brahe
Nicolaus Copernicus
Ptolemy
200
400
600
800
1000
1200
1400
1600
1800
2000
year


The development of observation and theory
Johann Sebastian Bach
Isaac Newton
Johnnes Kepler
Galileo Galilei
William Shakespeare
Tycho Brahe
Martin Luther
Nicolaus Copernicus
Erasmus
Leonardo da Vinci
Johannes Gutenberg
1400
1450
1500
1550
1600
1650
1700
1750
1800
year

Random numbers

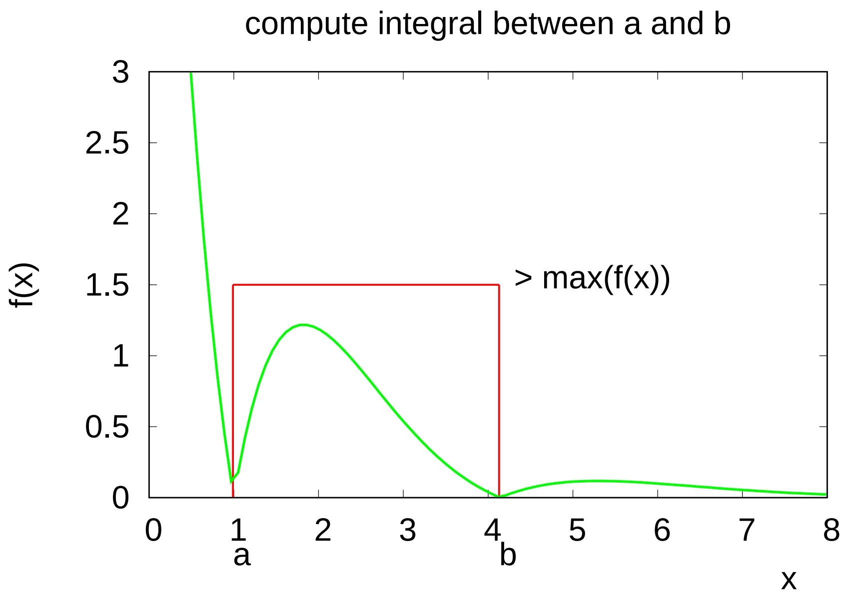
see https://en.wikipedia.org/wiki/Random_number

(Pseudo-)random numbers are used in many ways in numerical mathematics
We will look at a few applications:
1) Calculating integrals
2) Fitting
3) Monte Carlo (MC) Simulations (in CHE501)

1) The best known example is:
You are given a pseudo random number generator that generates
real number equidistributed between 0 and 1
Determine the value of π

http://www.stealthcopter.com/blog/2009/09/python-calculating-pi-using-random-numbers/
https://theabbie.github.io/blog/estimate-pi-using-random-numbers.html
and many other sites

For a general integral $\int_a^b f(x)\ \mathrm{d}x$ you embed $f(x)$ in a surface $(b-a)\cdot\max(f(x))$, scale and shift your random numbers (to be between a and b for x and between 0 and $\max(f(x))$ for y) and count the random points below $f(x)$ $\Rightarrow$ next page



The number of random points below the curve between a and b, divided by the total number of points, is proportional to the surface under the curve (ie its integral) and the surface of the red square

2) Fitting

Finding a minimum (or a maximum) in many-dimensional space is very difficult

Example: We have an energy E that depends on the positions of many (10, 100, 1000) particles (molecules):

$$E(x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, ...)$$

Question: for which positions is the energy minimal?

One way to do it: random moves (Monte Carlo)
(i) Select (very carefully!) a starting point $(x_1^0, y_1^0, z_1^0, x_2^0, y_2^0, z_2^0, x_3^0, y_3^0, z_3^0, ...)$
(ii) Change one variable (coordinate) randomly, not too much and not too little
(iii) Recompute the energy with the changed coordinate
(iv) If the new energy is lower, keep the new (changed) coordinate,
if not, keep the old coordinate
(v) go back to (ii)

This is a 'trial and error' method
it will probably find a minimum,but not necessarily the global (lowest) one

3) Monte Carlo (MC) simulations

Many methods using random numbers are called 'Monte Carlo', like eg the minimum search method we just discussed

This is not to be confused with the Monte Carlo simulations in statistical mechanics that we will discuss in che501