Numerical errors in computer simulations

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Chemical Process Intensification group
Eindhoven University of Technology

Numerical Methods (6BER03), 2024-2025

Today's outline

- Introduction
- Roundoff and truncation errors
- Break errors
- Loss of digits
- (Un)stable methods
- Symbolic math
- Summary

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Start your spreadsheet program (Excel, ...)

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Cell	Value
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(repeat until A30)

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What's happening?

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(repeat until A30)

What's happening?

Enter:

Cell	Value
A1	`2`

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(repeat until A30)

Enter:

Cell	Value
A1	`2`
A2	`=(A1*10)-18`
A3	`=(A2*10)-18`
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(repeat until A30)

What's happening?

Example 2

Start Python

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Investigate the result of `np.sin(1e40 * np.pi)`

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Create a vector `v` containing the powers of 10, e.g., from 10^0 up to 10^{40}, and solve `np.sin(v * np.pi)`:

```python
import numpy as np
import matplotlib.pyplot as plt

v = np.logspace(0, 40, 41)
y = np.sin(v * np.pi)
plt.loglog(v, np.abs(y)) # Double log plot, values on y-axis must be positive.
plt.show()
```

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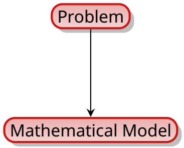
- Errors in the mathematical model (physics)

Verification and validation

Problem

Verification and validation



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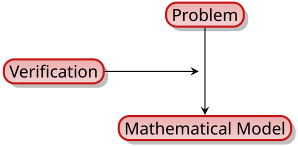
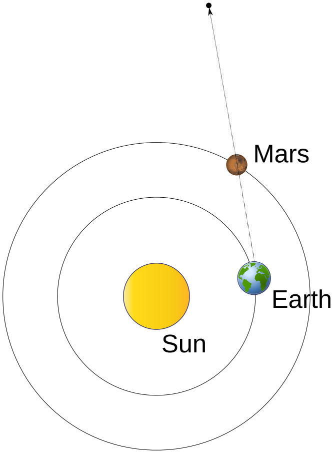


Verification

Verification is the process of mathematically and computationally assuring that the model computes the equations you intended to implement.

Verification of the physical model



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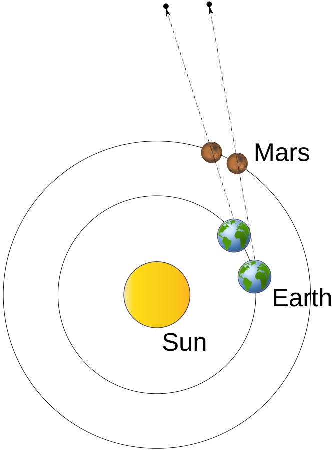

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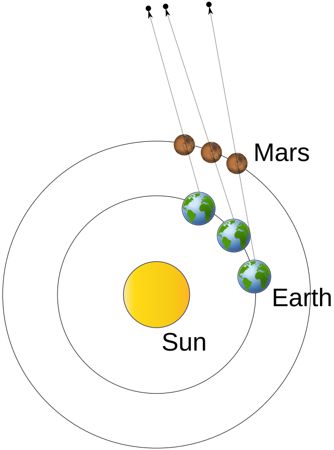

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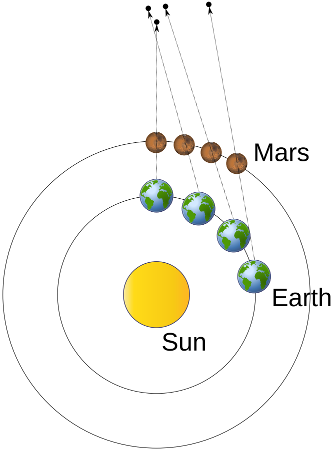

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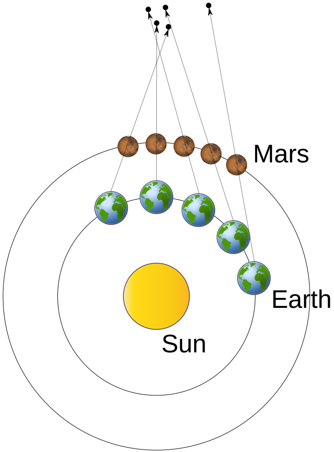

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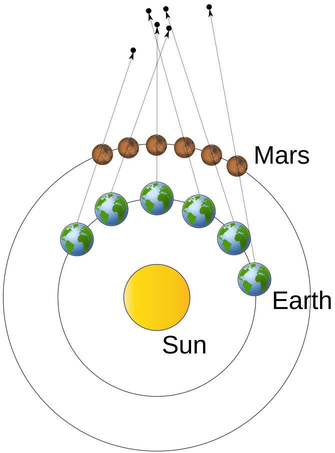

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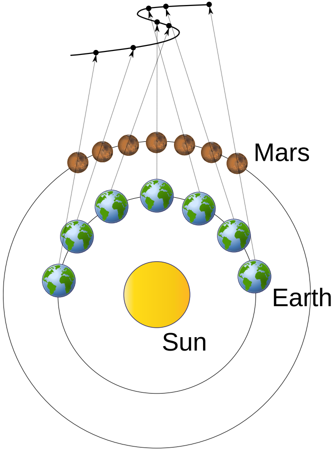

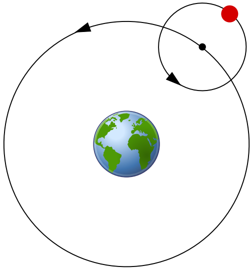

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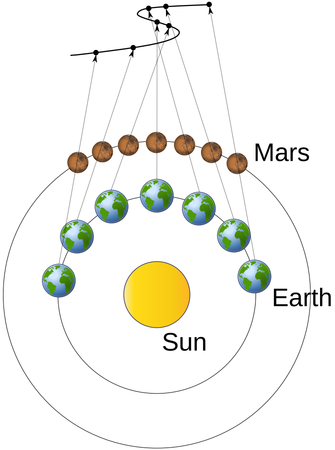

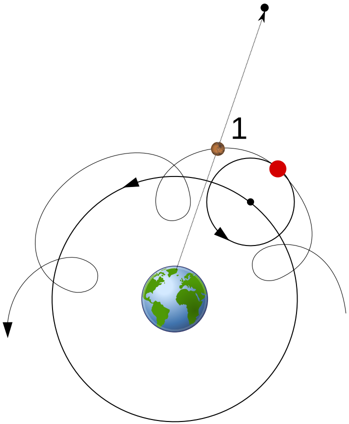

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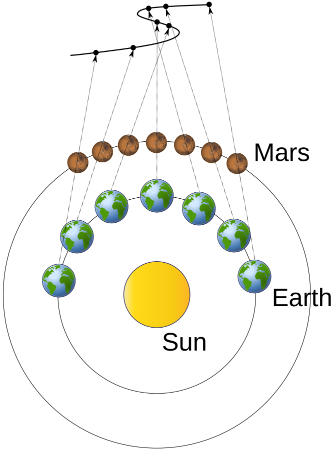

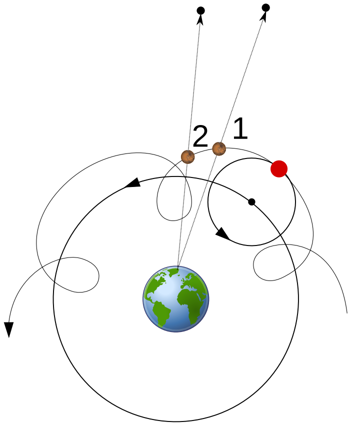

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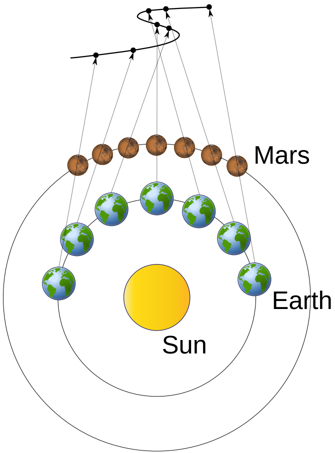

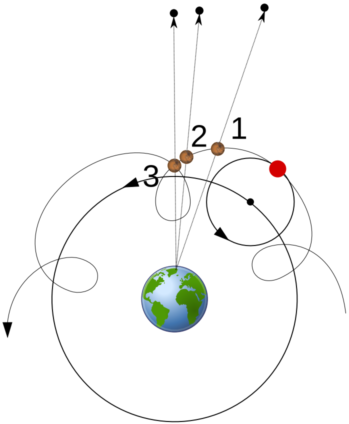

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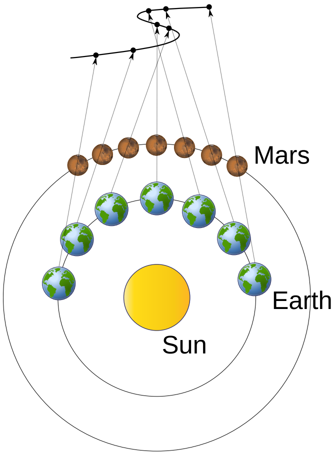

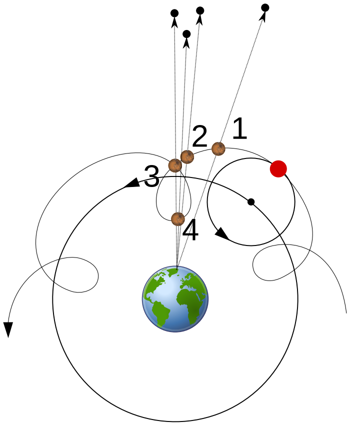

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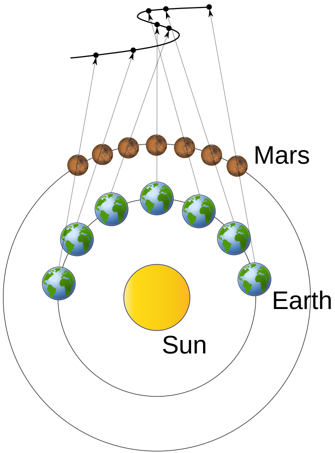

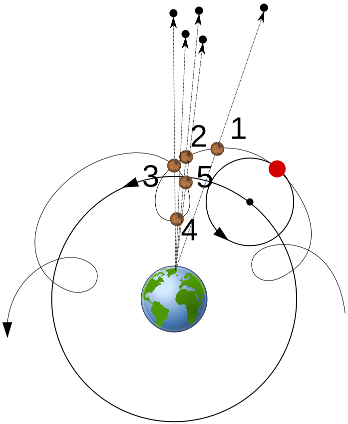

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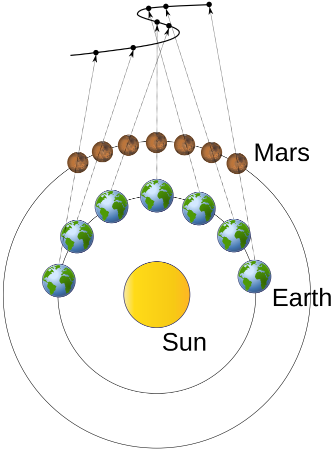

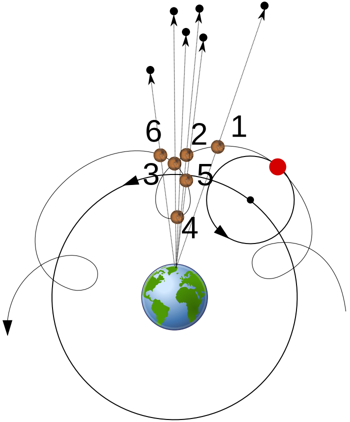

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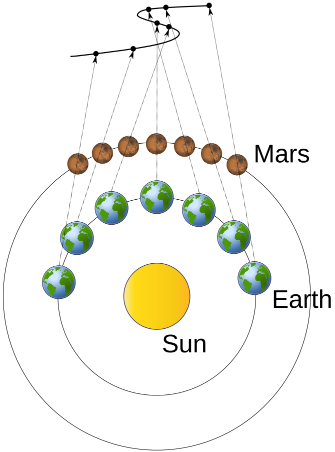

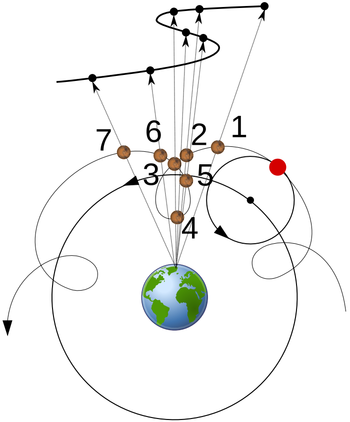

- The perceived orbit of Mars from Earth shows a zig-zag (in contrast to the Sun, Mercury, Venus)
- Even though they were not 'right', Earth-centered models (Ptolemy) were still valid

Be aware of your uncertainties

Aleatory uncertainty

Uncertainty that arises due to inherent randomness of the system, features that are too complex to measure and take into account

Epistemic uncertainty

Uncertainty that arises due to lack of knowledge of the system, but could in principle be known

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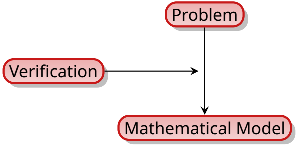

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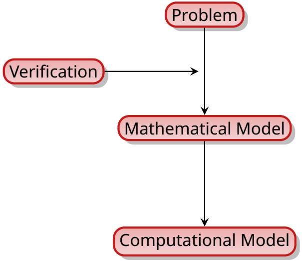

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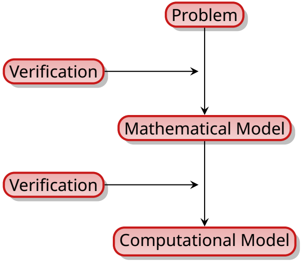

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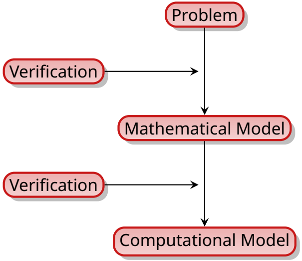

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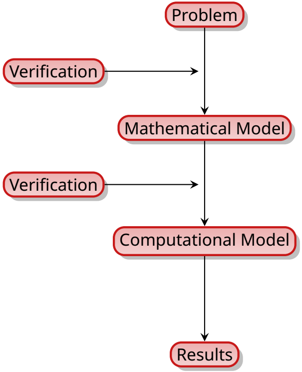

Verification and validation

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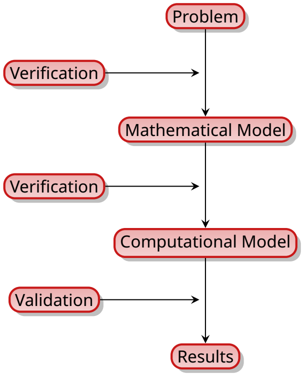
Validation

Validation is the process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model



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Significant digits

A numerical result $\tilde{x}$ is an approximation of the real value x.

- Absolute error

$$\delta = |\tilde{x} - x|, x \neq 0$$

- Relative error

$$\frac{\delta}{\tilde{x}} = |\frac{\tilde{x} - x}{\tilde{x}}|$$

- Error margin

$$\tilde{x} - \delta \leq x \leq \tilde{x} + \delta$$

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- $\tilde{x}$ has m significant digits if the absolute error in x is smaller or equal to 5 at the $(m+1)$-th position:

$$10^{q-1} \leq |\tilde{x}| \leq 10^{q}$$

$$|x - \tilde{x}| = 0.5 \times 10^{q-m}$$

- For example:

$$x = \frac{1}{3}, \tilde{x} = 0.333 \Rightarrow \delta = 0.00033333\ldots$$

3 significant digits

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$$(4521)_{10} = 4 \times 10^3 + 5 \times 10^2 + 2 \times 10^1 + 1 \times 10^0$$

Representation of numbers

- You could use another basis, computers often use the basis 2:

$(4521)_{10} =$

$=($

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$=(10$

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$$= (100$$

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$$=(10001$$

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$$\ldots 1 \times 2^{7} +$$

$$=(100011$$

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$$\dots 1 \times 2^{7} + 0 \times 2^{6} +$$

$$= (1000110$$

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$$=(10001101$$

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$$\dots 1 \times 2^{7} + 0 \times 2^{6} + 1 \times 2^{5} + 0 \times 2^{4} + \dots$$

$$=(100011010$$

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$$
\begin{aligned}
(4521)_{10} = & 1 \times 2^{12} + 0 \times 2^{11} + 0 \times 2^{10} + 0 \times 2^{9} + 1 \times 2^{8} + \dots \\
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& \dots 1 \times 2^{3} + \\
& = (1000110101
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&\ldots 1\times 2^{3} + 0\times 2^{2} + 0\times 2^{1} + 1\times 2^{0} \\
&\quad =(1000110101001)_2
\end{aligned}
$$

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(4521)_{10} = {} & 1 \times 2^{12} + 0 \times 2^{11} + 0 \times 2^{10} + 0 \times 2^{9} + 1 \times 2^{8} + \ldots \\
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& \ldots 1 \times 2^{3} + 0 \times 2^{2} + 0 \times 2^{1} + 1 \times 2^{0} \\
& = (1000110101001)_2
\end{aligned}
$$

- In general:

$$(c_m \ldots c_1 c_0)_q = c_0 q^0 + c_1 q^1 + \ldots + c_m q^m, c \in \{0, 1, 2, \ldots, q-1\}$$

Representation of numbers

- Numbers are stored in binary in the memory of a computer, in segments of a specific length (called a *word*).
- We distinguish multiple types of numbers:
  - Integers: $-301, -1, 0, 1, 96, 2293, \ldots$
  - Floating points: $-301.01, 0.01, 3.14159265, 14498.2$
- A binary integer representation looks like the following bit sequence:

$$z = \sigma\left(c_0 2^0 + c_1 2^1 + \ldots + c_{\lambda-1} 2^{\lambda-1}\right)$$

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Addition:

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- Multiplication and division are more expensive, and more elaborate

Exercise

Try the following commands in Python:

Command	Result
`np.iinfo(np.int32).min`	`-2147483648`

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`print(":.16f".format(f))`	`0.1000000000000000`
`print(":.20f".format(f))`	`0.10000000000000000555`

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- How can a computer identify an overflow? Usually through error reporting mechanisms within the language. Python's numpy library, for instance, will throw an OverflowError when an operation results in a number larger than what can be represented by the current data type.

Representation of real (floating point) numbers

- Formally, a real number is represented by the following bit sequence

$$x = \sigma\left(2^{-1} + c_2 2^{-2} + \ldots + c_m 2^{-m}\right) 2^{e-1023}$$

  Here, σ is the sign of x and e is an integer value.

- A floating point number hence contains sections that contain the sign, the exponent and the mantissa

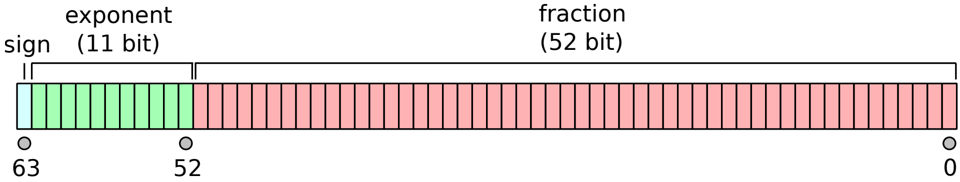

Image: Wikimedia Commons CC by-SA

Representation of real (floating point) numbers

- Example: $\lambda = 3$, $m = 2$, $x = \frac{2}{3}$

$$x = \pm\left(2^{-1} + c_2 2^{-2}\right)2^e$$

  - $c_0 \in \{0, 1\}$
  - $e = \pm a_0 2^0$
  - $a_0 \in \{0, 1\}$
- Truncation: $fl(x) = 2^{-1} = 0.5$
- Round off: $fl(x) = 2^{-1} + 2^{-2} = 0.75$

Today's outline

Trigonometric, Logarithmic, and Exponential computations

- Processors can do logic and arithmetic instructions
- Trigonometric, logarithmic and exponential calculations are “higher-level” functions: exp, sin, cos, tan, sec, arcsin, arccos, arctan, log, ln, ...
- Such functions can be performed using these “low level” instructions, for instance using a Taylor series:

$$\sin(x) = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)!} x^{2n+1} = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \dots$$

$$e^x = \sum_{n=0}^{\infty} \frac{x^n}{x!} = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!} + \dots$$

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- These operations involve many multiplications and additions, and are therefore *expensive*
- Computations can only take finite time, for infinite series, calculations are interrupted at N

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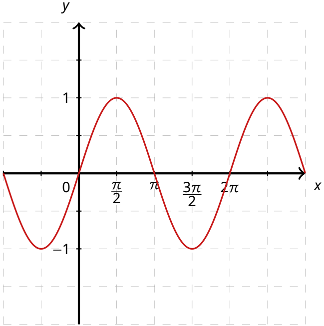
Algorithm for sine-computation

A computer may use a clever algorithm to limit the number of operations required to perform a higher-level function. A (fictional!) example for the computation of $\sin(x)$:



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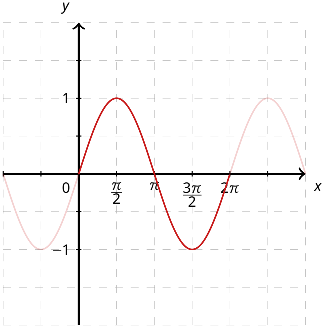

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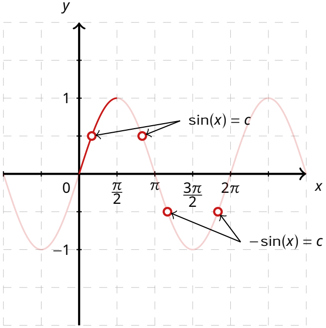

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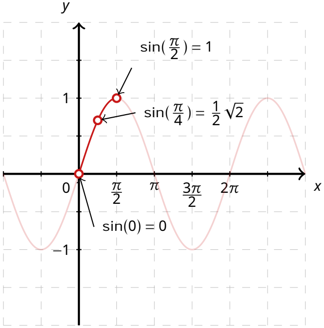

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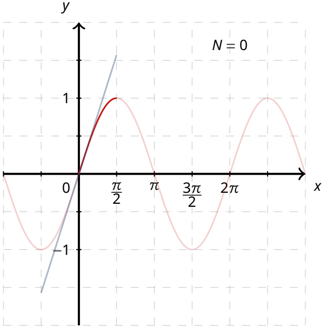

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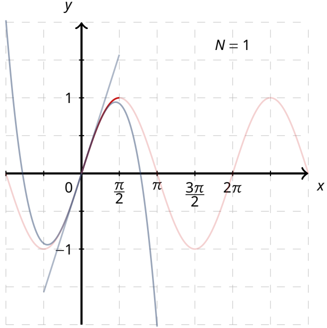

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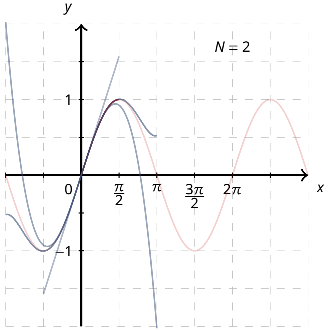

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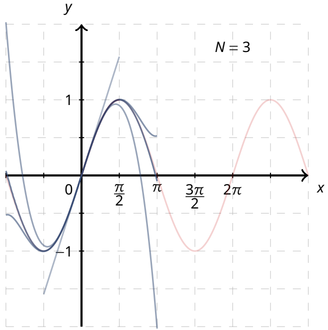

Today's outline

- Introduction
- Roundoff and truncation errors
- Break errors
- Loss of digits
- (Un)stable methods
- Symbolic math
- Summary

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Loss of digits

- During operations such as $+$, $-$, $\times$, $\div$, an error can add up
- Consider the summation of x and y

$$\tilde{x} - \delta \leq x \leq \tilde{x} + \delta \quad \text{and} \quad \tilde{y} - \varepsilon \leq y \leq \tilde{y} + \varepsilon$$

$$(\tilde{x} + \tilde{y}) - (\delta + \varepsilon) \leq x + y \leq (\tilde{x} + \tilde{y}) + (\delta + \varepsilon)$$

Loss of digits: Example 1

$x = \pi, \tilde{x} = 3.1416$

$y = 22/7, \tilde{y} = 3.1429$

Loss of digits: Example 1

$$\left.\begin{array}{l} x = \pi, \tilde{x} = 3.1416 \\ y = 22/7, \tilde{y} = 3.1429 \end{array}\right\} \Rightarrow \left.\begin{array}{l} \delta = \tilde{x} - x = 7.35 \times 10^{-6} \\ \varepsilon = \tilde{y} - y = 4.29 \times 10^{-5} \end{array}\right\}$$

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$$x+y=\tilde{x}+\tilde{y}\pm(\delta+\varepsilon)\approx 6.2845-5.025\times 10^{-5}$$

$$x-y=\tilde{x}-\tilde{y}\pm(\delta+\varepsilon)\approx -0.0013+3.55\times 10^{-5}$$

- The absolute error is small ($\approx 10^{-5}$), but the relative error is much bigger (0.028).
- Adding up the errors results in a loss of significant digits!

Loss of digits: Example 2

- Calculate e^{-5}
  - Use the Taylor series
  - Calculate the first 26 terms ($N = 26$)
- Now repeat the calculation, but use for each calculation only 4 digits. What do you find?
- Without errors you would find: $e^{-5} = 0.006738$
- If you only use 4 digits in the calculations, you'll find 0.00998

Loss of digits: Example 2

- Calculate e^{-5}
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Badly (ill) conditioned problems

We consider a system $F(x,y)$ that computes a solution from input data. The input data may have errors:

$$\xrightarrow{x} \boxed{F(x,y) = 0} \xrightarrow{y}$$ (Without errors)

Badly (ill) conditioned problems

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$$x \longrightarrow \boxed{F(x,y) \;=\; 0} \xrightarrow{\quad y \quad} \text{(Without errors)}$$

$$x+\delta x \longrightarrow \boxed{F(x+\delta x, y+\delta y) = 0} \xrightarrow{\quad y+\delta y \quad} \text{(With errors)}$$

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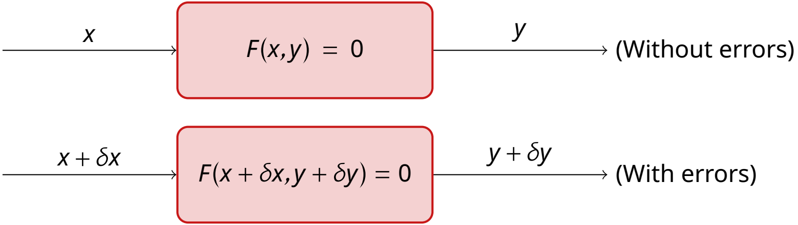

$$y(x+\delta x) - y(x) \approx y'(x)\delta x$$

Propagated error on the basis of Taylor expansion

$$C = \max_{\delta x}\left(\left|\frac{\delta y/y}{\delta x/x}\right|\right)$$

Condition criterion, $C < 10$ error development small

Badly (ill) conditioned problems: Example

Solve the following linear system in Python using double and single precision:

$$A = \begin{bmatrix} 1.2969 & 0.8648 \\ 0.2161 & 0.1441 \end{bmatrix}, \quad x = \begin{bmatrix} 0.8642 \\ 0.1440 \end{bmatrix}$$

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Double precision

```python
import numpy as np

# Double precision
A = np.array([[1.2969, 0.8648], [0.2161,
     0.1441]], dtype=np.float64)
x = np.array([0.8642, 0.1440], dtype=np.float64)
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Single precision

```python
import numpy as np

# Single precision
A = np.array([[1.2969, 0.8648], [0.2161,
     0.1441]], dtype=np.float32)
x = np.array([0.8642, 0.1440], dtype=np.float32)
y = np.linalg.solve(A, x)
print("y =")
print(y)
```

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Badly (ill) conditioned problems: Example

- Python does not automatically warn about bad condition number. You need to compute and check it manually using NumPy:

```
if np.linalg.cond(A)> threshold: raise("Ill conditioned error")
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- The `cond` number is the condition number computed using NumPy.
- A small error in A (the matrix) results in a big error in the solution. This is called an ill-conditioned problem.

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- **(Un)stable methods**
- Symbolic math
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(Un)stable methods

- The condition criterion does not tell you anything about the quality of a numerical solution method!
- It is very well possible that a certain solution method is more sensitive for one problem than another
- If the method propagates the error, we call it an *unstable method*. Let's look at an example.

The Golden mean

The Golden Mean is a well known ratio and one of the solutions of $\phi^2 = \phi + 1$, such that $\phi = \frac{1+\sqrt{5}}{2}$, and $\phi - 1 = \phi^{-1}$. Many relations to compute ϕ have been established (which pose often an interesting source for creating small test programs).

- Let's evaluate the following recurrent relationship:

$$y_{n+1} = y_{n-1} - y_n$$

$$y_0 = 1, \quad y_1 = 1 - \phi = \phi^{-1} = \frac{2}{1+\sqrt{5}}$$

- Alternatively, a closed form power law relation exists, which again computes y_n:

$$y_n = x^{-n}, \quad n = 0, 1, 2, \ldots, \quad x = \frac{1+\sqrt{5}}{2}$$

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The Golden mean

Recurrent version

```python
import numpy as np

def golden_mean_recurrent(Ntot):
    # Initialize the series with the given
        initial conditions
    y = np.zeros(Ntot)
    y[0] = 1
    y[1] = 2 / (1 + np.sqrt(5))

    # Perform the recurrence to fill in the rest
        of the series
    for n in range(2, Ntot):
        y[n] = y[n-1] - y[n-2]
    return y
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Power law version

```python
import numpy as np

def golden_mean_powerlaw(Ntot):
    # Initialize the constant value
    x = (1 + np.sqrt(5)) / 2

    # Generate a range of values from 0 to Ntot and apply the power law
    y = x ** -np.arange(0, Ntot + 1)

    return y
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- Compare the outcomes: `plot(goldenMeanPowerlaw(40)- goldenMeanRecurrent(40))`

The Golden mean

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- Compare the outcomes: `plot(goldenMeanPowerlaw(40)- goldenMeanRecurrent(40))`
- See what happens if you use single precision (add `dtype=np.float32` to line 5 (`np.zeros`) and line 8 (`np.arange`)).

The Golden mean

n	Recurrent	Power law
0	1.0000	1.0000
1	0.6180	0.6180
2	0.3820	0.3820
3	0.2361	0.2361
...	...	...
37	$1.714 \cdot 10^{-08}$	$1.851 \cdot 10^{-08}$
38	$1.366 \cdot 10^{-08}$	$1.144 \cdot 10^{-08}$
39	$3.485 \cdot 10^{-08}$	$7.071 \cdot 10^{-09}$
40	$1.017 \cdot 10^{-08}$	$4.370 \cdot 10^{-09}$

- The recurrent approach enlarges errors from earlier calculations!

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Example 1: Explanation

Recall example 1, where the errors blew up our computation of 0.1, whereas they did not for 2. Why did we see these results?

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- The number 0.1 is not exactly represented in binary
  - A tiny error can accumulate up to catastrophic proportions!
- The number 2 does have an exact binary representation

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Example 2 (large sine series)

The `np.sin(1e40*np.pi)` result gives poor results because 1e40 has an error margin on the order of floating-point machine epsilon, which is roughly 1×10^{-16} in Python (double-precision floating-point format). In Python, as in many computing environments, the number of $2 \cdot \pi$ cycles is still much larger than $10^{40} \cdot 10^{-16}$. Also, π is not stored with an infinite number of digits, which further contributes to the imprecision.

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Example 3

Start your calculation program of choice (Excel, Python, ...)

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Calculate the result of y:

$$y = e^{\pi} - \pi$$

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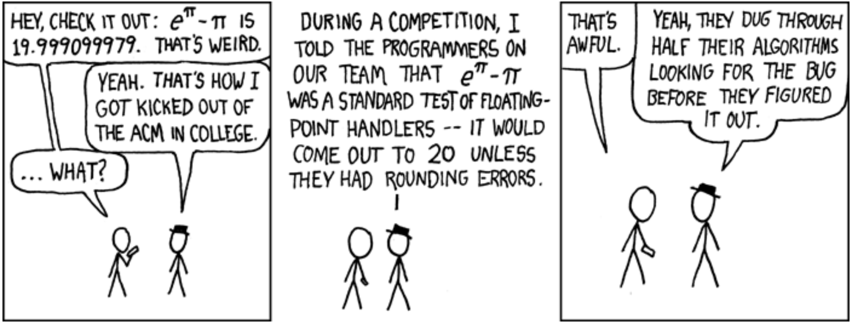

Image: xkcd

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Symbolic math packages

Definition

The use of computers to manipulate mathematical equations and expressions in symbolic form, as opposed to manipulating the numerical quantities represented by those symbols.

- Symbolic integration or differentiation, substitution of one expression into another
- Simplification of an expression, change of subject etc.
- Packages and toolboxes:

Symbolic math packages

Mathematica	Well known software package, license available via TU/e
Maple	Well known, license available via TU/e
Wolfram|Alpha	Web-based interface by Mathematica developer. Less powerful in mathematical respect, but more accessible and has a broad application range (unit conversion, semantic commands).
Sage	Open-source alternative to Maple, Mathematica, Magma, and MATLAB.
Matlab	Symbolic math toolbox
Python	SymPy

Symbolic math: simplify

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

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```python
from sympy import symbols, simplify

x = symbols('x') # Alt: from sympy.abc import x,y,z
f = (x - 1)*(x + 1)*(x**2 + 1) + 1
f_simplified = simplify(f)
print(f_simplified)
```

Symbolic math: simplify

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```
f_simplified = x**4
```

Symbolic math: integration and differentiation

$$f(x) = \frac{1}{x^3 + 1}$$

Symbolic math: integration and differentiation

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```python
from sympy import symbols, simplify, integrate, diff

x = symbols('x')
f = 1/(x**3+1)
my_f_int = integrate(f, x)
my_f_diff = diff(my_f_int, x)
my_f_diff_simplified = simplify(my_f_diff)
print(my_f_diff_simplified)
```

Symbolic math: integration and differentiation

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```

```
my_f_diff_simplified = 1/(x**3 + 1)
```

Symbolic math: exercises

Exercise 1

Simplify the following expression:

$$f(x) = \frac{2\tan x}{(1+\tan^2 x)}$$

Symbolic math: exercises

Exercise 1

Simplify the following expression:

$$f(x) = \frac{2\tan x}{(1+\tan^2 x)} = \sin 2x$$

```python
from sympy import symbols, trigsimp, tan

x = symbols('x')
expr = 2*tan(x)/(1 + tan(x)**2)
simplified_expr = trigsimp(expr)
```

Symbolic math: exercises

Exercise 2

Calculate the *value* of p:

$$p = \int_0^{10} \frac{e^x - e^{-x}}{\sinh x} dx$$

Symbolic math: exercises

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```python
from sympy import exp, sinh, integrate, symbols

x = symbols("x")
f = ((exp(x)- exp(-x))/sinh(x)).simplify()
p = integrate(f, (x, 0, 10))
print(p)
```

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Symbolic math: exercises

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p = 20

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Symbolic math: root finding

A root finding method searches for the values where a function reaches zero. We will cover the numerical methods later, here we show how to use root finding with symbolic math in Python.

Symbolic math function

$$f(x) = \frac{3}{x^2 + 3x} - 2$$

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```python
from sympy import solve, symbols

x = symbols("x")
f = 3 / (x**2 + 3*x) - 2
solutions = solve(f, x)
print(solutions)
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```
solutions = [-3/2 + sqrt(15)/2, -sqrt(15)/2 - 3/2]
```

Today's outline

Summary

- Numerical errors may arise due to truncation, roundoff and break errors, which may seriously affect the accuracy of your solution
- Errors may propagate and accumulate, leading to smaller accuracy
- Ill-conditioned problems and unstable methods have to be identified so that proper measures can be taken
- Symbolic math computations may be performed to solve certain equations algebraically, bypassing numerical errors, but this is not always possible.

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