Mathematics for Informatics

Numerical Mathematics: introduction, computer arithmetics (lecture 9 of 12)

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Winter 2025/2026

created: August 25, 2025, 13:53

Numerical mathematics

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The following mathematical problems are often involved:

1. solution of systems of linear equations,
2. solution of differential equations,
3. calculation of integrals,
4. evaluations of function values,
5. estimation of errors in calculations,
6. ...

Typically, a computer calculation is involved.

From the history

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This does not mean that approximation methods do not work. In the vast majority of cases they work well, but it is important to know how reliable they are.

Category of errors

We will use different **approximations** to design the algorithm. We will therefore make various kind of mistakes, which can be divided according to their origin:

1. errors in the **model**: the mathematical model to solve the problem is somehow simplified.
2. errors in the **data**: data often come from measurements that do not have absolute accuracy.
3. errors in the **algorithm**: we don't have to have an algorithm that finds the exact solution in a finite number of steps.
4. **rounding** errors: errors occur during the calculation itself (e.g., during arithmetic operations).

Apart from data errors, we will give examples of all other kinds of errors. We start with rounding errors, which are given by the fact that the algorithm need a computer to do the hard work.

Representation with floating point

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For non-integers, one can use the **scientific notation**. In the binary base a number x is represented as

$$x = \pm m \cdot 2^e.$$

m - **mantissa/significand** having a fixed number of digits / fixed length; these digits are also called **significant digits**.

e - **exponent** having a fixed number of digits / fixed length.

IEEE-754

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precision	length of m	d = length of e	b
`binary32` / single precision	23	8	127
`binary64` / double precision	52	11	1023
`binary128` / quadruple precision	112	15	16383

- if $e = 2^d - 1$ and $m \neq 0$, then $x = \texttt{NaN}$ (Not a Number)
- if $e = 2^d - 1$ and $m = 0$ and $s = 0$, then $x = +\texttt{Inf}$
- if $e = 2^d - 1$ and $m = 0$ and $s = 1$, then $x = -\texttt{Inf}$
- if $0 < e < 2^d - 1$, then $x = (-1)^s \cdot (1.m)_2 \cdot 2^{e-b}$ (so-called **normalized numbers**)
- if $e = 0$ and $m \neq 0$, then $x = (-1)^s \cdot (0.m)_2 \cdot 2^{-b+1}$ (so-called **subnormal/unnormalized numbers**)
- if $e = 0$ and $m = 0$ and $s = 0$, then $x = 0$
- if $e = 0$ and $m = 0$ and $s = 1$, then $x = -0$

Machine numbers (1/3)

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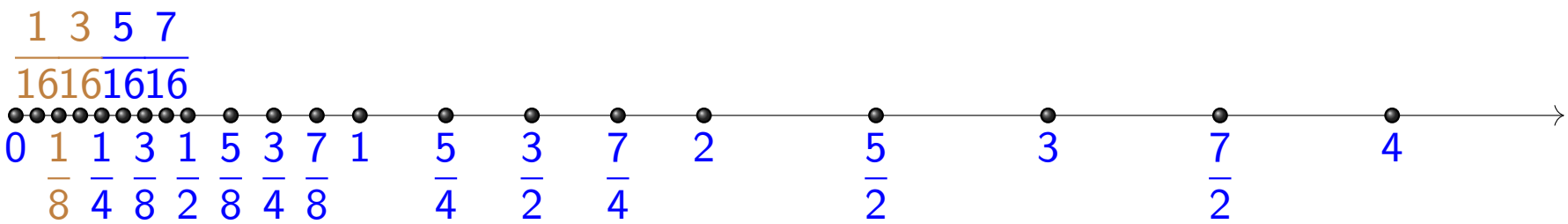
Example: take m of length 2 bits, e of length 3 bits, and $b = 3$.

We obtain the following set of numbers (we consider only positive elements)

$$\left\{0, \frac{1}{16}, \frac{1}{8}, \frac{3}{16}, \frac{1}{4}, \frac{5}{16}, \frac{3}{8}, \frac{7}{16}, \frac{1}{2}, \frac{5}{8}, \frac{3}{4}, \frac{7}{8}, 1, \frac{5}{4}, \frac{3}{2}, \frac{7}{4}, 2, \frac{5}{2}, 3, \frac{7}{2}, 4, 5, 6, 7, 8, 10, 12, 14\right\}$$

Subnormal numbers are in brown.



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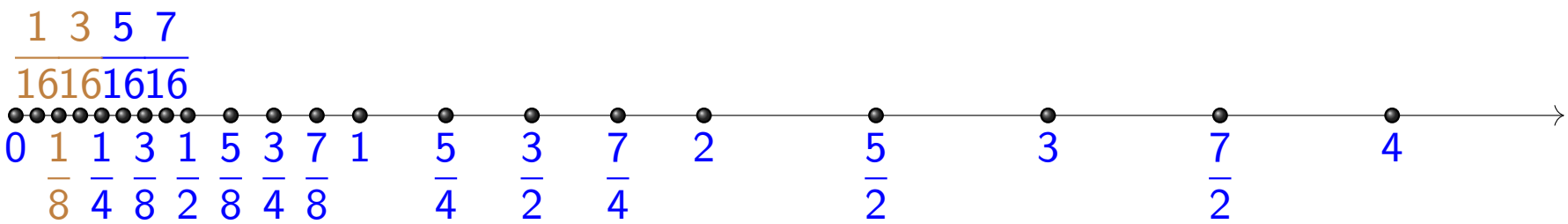

The set of all machine numbers with a given precision has little in common with the set of real numbers. It resembles more to a finite subset of integers.

Machine numbers (2/3)

Denote the set of machine numbers by F.

The set F has the largest and the smallest positive elements as follows:

precision	max. no.	min. pos. normalized	min. pos. subnormal
single	$(2-2^{-23})\cdot 2^{127}$ $\approx 3.4\cdot 10^{38}$	2^{-126} $\approx 1.2\cdot 10^{-38}$	$2^{-126-23}=2^{-149}$ $\approx 1.4\cdot 10^{-45}$
double	$(2-2^{-52})\cdot 2^{1023}$ $\approx 1.8\cdot 10^{308}$	2^{-1022} $\approx 2.2\cdot 10^{-308}$	$2^{-1022-52}=2^{-1074}$ $\approx 4.9\cdot 10^{324}$

Machine numbers (3/3)

F is characterized by the **machine epsilon** ε_F, which is the difference between 1.0 and the smallest number in F larger than 1.

For single precision we have $\varepsilon_F = 2^{-23}$, for double 2^{-52}.

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Proposition

The distance between any two neighboring normalized numbers in F is at least $\frac{\varepsilon_F}{2}$ and at most ε_F.

Representation of real numbers (1/3)

Let $fl : \mathbb{R} \to F$ be the mapping which assigns to any $x \in \mathbb{R}$ the closest machine number.

The "closest" is given by the method chosen: rounding ("ties to even"), chopping (rounding towards 0),...

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When trying to represent a number which is out of the representable range, an **overflow** or **underflow** is returned.

Definition

Let a number α be an approximate value of a number a.

- *The **absolute error** is the value $|\alpha - a|$.*
- *For $a \neq 0$, the **relative error** is $\dfrac{|\alpha - a|}{|a|}$.*

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In single precision, suppose that a number $x \in \mathbb{R}$ lies in the normalized range, i.e.,

$$x = q \cdot 2^{\ell}, \quad \text{where } 1 \leq q < 2 \text{ and } -126 \leq \ell \leq 127.$$

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If $x = (1.b_1 b_2 \cdots b_{22} b_{23} b_{24} \cdots)_2 \cdot 2^{\ell}$ then $fl(x) = (1.b_1 b_2 \cdots b_{23}) \cdot 2^{\ell}$.

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The absolute error and the absolute errors are respectively:

$$|x - fl(x)| \leq 2^{-23+\ell} \qquad \text{and} \qquad \frac{|x - fl(x)|}{|x|} \leq \frac{2^{-23+\ell}}{q \cdot 2^{\ell}} \leq 2^{-23}.$$

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Proposition

Let $x \in \mathbb{R}$ be greater than the smallest normalized number of F and smaller than the greatest normalized number of F. We have

$$fl(x) = x(1+\delta), \quad \text{where } |\delta| \leq \mathbf{u},$$

Arithmetic operations - error

Proposition

Let $x, y \in F$ and $\odot$ be the operation of addition, multiplication or division. If there is no overflow or underflow, then we have

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In general: If we operate with more numbers, it is better to start with the smallest ones.

Arithmetic operations - a demonstration

Let $f : \mathbb{R}^2 \mapsto \mathbb{R}$ be a mapping given by

$$f(x, y) = 333.75y^6 + x^2 \left(11x^2y^2 - y^6 - 121y^4 - 2\right) + 5.5y^8 + \frac{x}{2y}.$$

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Let us evaluate $f(77617, 33096)$:

`SageMath` (precision 23 bits)	1.17260
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The exact solution is $-\frac{54767}{66192} \approx -0.827396$.

[S. M. Rump: *Algorithms for verified inclusions - theory and practice*, ..., 1988]

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Let us calculate the relative error.

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That is a lot in comparison to

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Proposition

Let x and y be normalized machine numbers and $x>y>0$.
*If $2^{-p}\leq 1-\frac{y}{x}\leq 2^{-q}$ for some positive integers p and q, then **at most** p and **at least** q significant binary bits are lost when performing the operation $x-y$.*

Loss of significant digits (3/3)

Cancellation can be avoided by using the following techniques:

- rationalizing the problem, i.e., using rational numbers and avoiding the subtraction in floating points arithmetics,
- using series expansions (such as Taylor series),
- using other identities,. . .

Errors - conclusion

Origins of errors:

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A few final notes:

- increased precision may not lead to a more precise result,
- cancellation can be useful - it may cancel rounding errors,
- few operations with small numbers do not imply a small error.

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There are some alternatives:

- Exact arithmetics: $\mathbb{Z}$, $\mathbb{Q}$ or $GF(p)$ (it is not always possible or suitable).
- Interval arithmetics (we work with intervals instead of points). (IEEE 1788-2015).
- Unum.