# Bi7740: Scientific computing

## Introductory considerations

Vlad Popovici
popovici@iba.muni.cz

Institute of Biostatistics and Analyses
Masaryk University, Brno

*There is nothing more practical than a good theory.*
Kurt Lewin (1890–1947)

# Outline

Bibliography:


- HEATH M.T. (2002). Scientific Computing. An introductory survey. McGraw-Hill, 2nd edition. ISBN: 0-07-239910-4 Good accompanying materials at `http://www.cs.illinois.edu/~heath/scicomp/`, including slides and demos! Used as basis for the first part of the course.
- KEPNER J. (2009). Parallel Matlab for Multicore and Multinode Computers. SIAM Publishing. ISBN: 978-0-898716-73-3
- GENTLE J.E. (2005). Elements of Computational Statistics. Springer. ISBN:978-0387954899
- HŘEBÍČEK, J. et al. Vědecké výpočty v matematické biologii (Scientific computing in mathematical biology). Brno: Akademické nakladatelství CERM, 2012. 117 pp. Neuveden. ISBN 978-80-7204-781-9.

Computing environments for the course:

- MATLAB, `http://www.mathworks.com` - commercial
- GNU OCTAVE, `https://www.gnu.org/software/octave/` - "quite similar to MATLAB"
- R, `http://www.r-project.org` - "environment for statistical computing and graphics"

WARNING: Some pieces of code shown during the course may not represent the optimal implementation in the given language. They are merely a device for demonstrating some principles.

# Scientific computing

Wikipedia:

"Computational science (also scientific computing or scientific computation) is concerned with constructing mathematical models and quantitative analysis techniques and using computers to analyze and solve scientific problems."

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Basically: find numerical solutions to mathematically-formulated problems.

(J. Hadamard) A problem is well posed if its solution

- exists
- is unique
- has a behavior that changes continuously with the initial conditions;

otheriwse, it is ill posed.
Inverse problems are often ill posed.
Example: 3D to 2D projection.

- continuous domain → discrete domain
- well-posed but ill-conditioned problems: small errors in input lead to large variations in the solution
- improve conditioning by regularization

# General computational approach

- continuous domain $\to$ discrete domain
- infinite $\to$ finite
- differential $\to$ algebraic
- nonlinear $\to$ (combination of) linear
- accept approximate solutions, but control for the error

# Approximations

- Modeling approximations:
  - "model" = approximation of the nature
  - data - inexact measurements or previous results
- Implementation/computational approximations:
  - discretization of the continuous domain; truncation
  - rounding
- errors in input data
- errors propagated by the algorithm
- accuracy of the final result

# Example: area of the Earth

- model: sphere
- $A = 4\pi r^2$
- $r = ?$
- $\pi = 3.14159\ldots$
- rounded arithmetic

# Errors

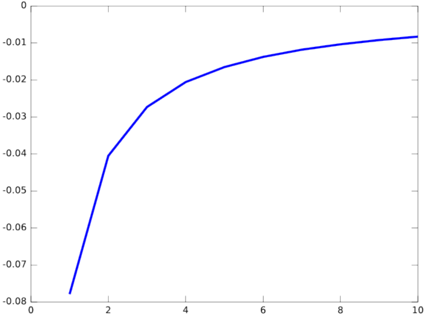
- Absolute error: approximate value - true value
- Relative error:
$$\frac{\text{absolute error}}{\text{true value}}$$
- $\rightarrow$ approximate value $=$ (1 $+$ relative error) $\times$ (true value)
- if the relative error is $\sim 10^{-d}$, it means that $\hat{x}$ has about $d$ exact digits: there exists $\tau = \pm(0.0\ldots 0 n_{d+1} n_{d+2}\ldots)$ such that $\hat{x} = x + \tau$
- true value is usually not known $\rightarrow$ use estimates or bounds on the error
- relative error can be taken relative to the approximate value

# Example/exercise - Implement!

Stirling's approximation for factorials:

$$S_n = \sqrt{2\pi n}\left(\frac{n}{e}\right)^n \approx n!, \qquad n = 1, 2, \ldots$$

where $e = \exp(1)$.
Relative error $(S_n - n!)/n!$:



# Errors: data and computational

- compute $f(x)$ for $f : \mathbb{R} \to \mathbb{R}$
  - $x \in \mathbb{R}$ is the true value
  - $f(x)$ true/desired result
  - $\hat{x}$ approximate input
  - $\hat{f}$ approximate result
- total error:

$$\begin{aligned}\hat{f}(\hat{x}) - f(x) &= (\hat{f}(\hat{x}) - f(\hat{x})) + (f(\hat{x}) - f(x)) \\ &= \text{computational error} + \text{propagated data error}\end{aligned}$$

- *the algorithm has no effect on propagated error*

# Computational error

is sum of:

- truncation error = (true result) - (result of the algorithm using exact arithmetic)
  Example: considering only the first terms of an infinite Taylor series; stopping before convergence
- rounding error = (result of the algorithm using exact arithmetic) - (result of the algorithm using limited precision arithmetic)
  Example: $\pi \approx 3.14$ or $\pi \approx 3.141593$

# Finite difference approximation

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h} \approx \frac{f(x+h) - f(x)}{h}, \text{ for some small } h > 0$$

- truncation error: $f'(x) - \frac{f(x+h)-f(x)}{h} \leq Mh/2$ where $|f''(t)| \leq M$ for $t$ in a small neighborhood of $x$ (HOMEWORK, 5p)
- rounding error: $2\epsilon/h$, for $\epsilon$ being the precision
- total error is minimized for $h \approx 2\sqrt{\epsilon/M}$

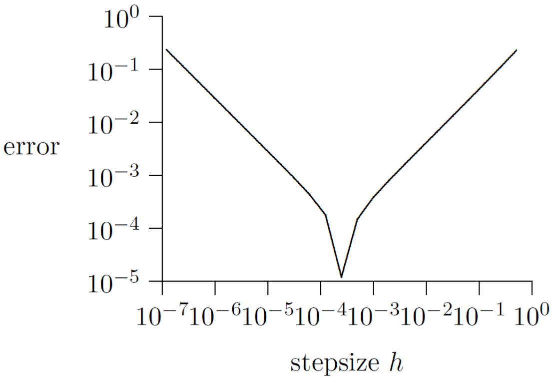



Figure : Total computational error as a tradeoff between truncation and rounding error (from *Heath - Scientific computing*)

# Error analysis

For $y = f(x)$, for $f : \mathbb{R} \to \mathbb{R}$ an approximate $\hat{y}$ result is obtained.

- forward error: $\Delta y = \hat{y} - y$
- backward error: $\Delta x = \hat{x} - x$, for $f(\hat{x}) = \hat{y}$

$$\begin{tikzcd} x \arrow[r, "f"] \arrow[d, leftrightarrow, "\text{backward error}"'] \arrow[dr, "\hat{f}"] & y \arrow[d, leftrightarrow, "\text{forward error}"] & = f(x) \\ \hat{x} \arrow[r, "f"] & \hat{y} & = \hat{f}(x) = f(\hat{x}) \end{tikzcd}$$

Compute $f(x) = e^x$ for $x = 1$. Use the first 4 terms from Taylor expansion:

$$\hat{f}(x) = 1 + x + \frac{x^2}{2} + \frac{x^3}{6}$$

- take "true" value: $f(x) = 2.716262$ and compute $\hat{f}(x) = 2.666667$, then
- forward error: $|\Delta y| = 0.051615$, or a relative f. error of about 2%
- backward error: $\hat{x} = \ln \hat{f}(x) = 0.989829 \Rightarrow |\Delta x| = 0.019171$, or a relative b. error of 2%
- these are two perspectives on assessing the accuracy

# Exercise

Consider the general Taylor series with limit $e$:

$$\sum_{n=0}^{\infty} \frac{1}{n!} = e$$

How many terms are needed for an approximation of $e$ to three decimal places?

# Backward error analysis

- idea: approximate result is the exact solution of a modified problem
- how far from the original problem is the modified version?
- how much error in the input data would explain all the error in the result?
- an approximate solution is good if it is an exact solution for a nearby problem
- backward analysis is usually easier

# Sensitivity and conditioning

- insensitive (well-conditioned) problem: relative changes in input data causes similar relative change in the result
- large changes in solution for small changes in input data indicate a sensitive (ill-conditioned) problem;
- condition number:

$$\text{cond} = \frac{\text{absolute relative change in solution}}{\text{absolute relative change in input}} = \frac{|\Delta y/y|}{|\Delta x/x|}$$

- if cond >> 1 the problem is sensitive

- condition number is a scale factor for the error:

$$\text{relative forward err} = \text{cond} \times \text{relative backward err}$$

- usually, only upper bounds of the cond. number can be estimated, cond $\leq C$, hence

$$\text{relative forward err} \leq C \times \text{relative backward err}$$

- $\hat{x} = x + \Delta x$
- forward error: $f(x + \Delta x) - f(x) \approx f'(x)\Delta x$, for small enough $\Delta x$
- relative forward error: $\approx \frac{f'(x)\Delta x}{f(x)}$
- $\Rightarrow$ cond $\approx \left|\frac{xf'(x)}{f(x)}\right|$

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Example: tangent function is sensitive in neighborhood of $\pi/2$

- $\tan(1.57079) \approx 1.58058 \times 10^5$; $\tan(1.57078) \approx 6.12490 \times 10^4$
- for $x = 1.57079$, cond $\approx 2.48275 \times 10^5$

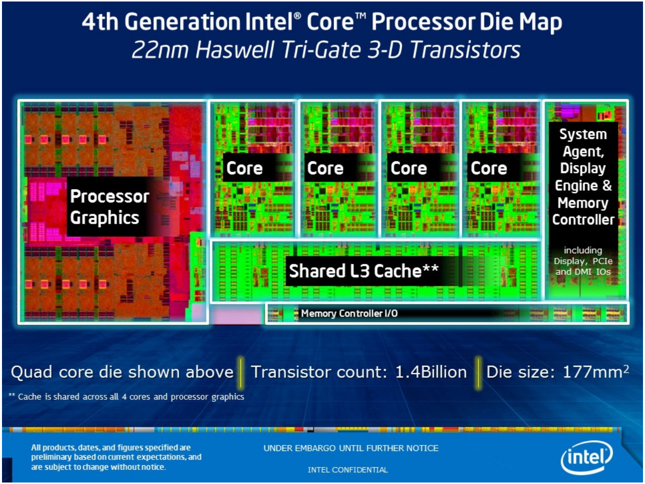
# Stability

- an algorithm is stable if is relatively insensitive to perturbations during computation
- stability of algorithms is analogous to conditioning of problems
- backward analysis: an algorithm is stable if the result produced is the exact solution of a nearby problem
- stable algorithm: the effect of computational error is no worse than the effect of small error in input data

# Accuracy

- accuracy closeness of the result to the true solution of the problem
- depends on the conditioning of the problem AND on the stability of the algorithm
- stable algorithm + well-conditioned problem = accurate results

# CPUs


4th Generation Intel® Core™ Processor Die Map
22nm Haswell Tri-Gate 3-D Transistors
Processor Graphics
Core
Core
Core
Core
System Agent, Display Engine & Memory Controller
including Display, PCIe and DMI IOs
Shared L3 Cache**
Memory Controller I/O
Quad core die shown above
Transistor count: 1.4Billion
Die size: 177mm2
** Cache is shared across all 4 cores and processor graphics
All products, dates, and figures specified are preliminary based on current expectations, and are subject to change without notice.
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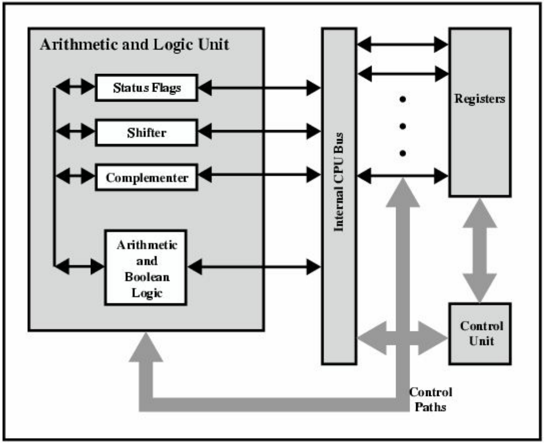

Arithmetic and Logic Unit
Status Flags
Shifter
Complementer
Arithmetic and Boolean Logic
Internal CPU Bus
Registers
Control Unit
Control Paths

# Number representation

- internally, all data are represented in binary format (each digit can be either 0 or 1, e.g. 1011001...)
- bit, nybble, byte
- word → specific to architecture: 1, 2, 4, or 8 bytes
- integers:
  - unsigned ($\geq 0$): on $n$ bits: $0, \ldots, 2^n - 1$. The stored representation (for 1 byte) is $b_7 b_6 b_5 b_4 b_3 b_2 b_1 b_0$ for a value $x = \sum_{i=0}^{7} b_i 2^i$.
  - signed: 1 bit for sign, rest for the absolute value; $-2^{n-1}, \ldots, 0, \ldots, 2^{n-1} - 1$. The stored representation (for 1 byte) is $b_7 b_6 b_5 b_4 b_3 b_2 b_1 b_0$ for a value $x = b_7(-2^7) + \sum_{i=0}^{6} b_i 2^i$.

# Floating-point numbers

- like in scientific notation: mantissa $\times$ radix$^{\text{exponent}}$, e.g. $2.35 \times 10^3$
- formally

$$x = \pm \left( b_0 + \frac{b_1}{\beta} + \frac{b_2}{\beta^2} + \cdots + \frac{b_{p-1}}{\beta^{p-1}} \right) \times \beta^E$$

  where
  $\beta$ is the radix (or base)
  $p$ is the precision
  $L \leq E \leq U$ are the limits of the exponent
  $0 \leq b_k \leq \beta$
- mantissa: $m = b_0 b_1 \dots b_{p-1}$; fraction: $b_1 b_2 \dots b_{p-1}$
- the sign, mantissa and exponent are stored in fixed-sized fields (the radix is implicit for a given system, $\beta = 2$ usually)

Normalization:

- $b_0 \neq 0$ for all $x \neq 0$
- mantissa $m$ satisfies $1 \leq m < \beta$
- ensures unique representation, optimal use of available bits

Internal representation (on 64 bits - "double precision", binary representation):

$$x = \boxed{\text{sign} \mid \text{exponent} \mid \text{fraction}} = \boxed{b_{63}}\boxed{b_{62} \ldots b_{52}}\boxed{b_{51} \ldots b_0}$$

Properties:

- only a finite number of discrete values can be represented
- total number of floating point numbers representable in normalized format is

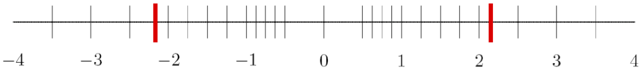
$$2(\beta - 1)\beta^{p-1}(U - L + 1) + 1$$

  (Q: can you justify the result?)
- undeflow level (smallest number): $UFL = \beta^L$
- overflow level (largest number): $OFL = \beta^{U+1}(1 - \beta^{-p})$
- not all real numbers can be represented exactly:
  - *machine numbers*
  - rounding $\rightarrow$ rounding error

Example: let $\beta = 2, p = 3, L = -1, U = 1$, there are 25 distinct numbers that can be represented:


- $UFL = 0.5_{10}$; $OFL = 3.5_{10}$
- note the non-uniform coverage
- $\forall x \in \mathbb{R}$, $fl(x)$ is the floating point representation; $x - fl(x)$ is the rounding error

# Rounding rules




- *chop* = round toward zero: truncate the base–$\beta$ representation after $p$ – 1st digit
- *round to nearest*: $fl(x)$ is the closest machine number to $x$

# Machine precision

- machine precision, $\epsilon_{\text{mach}}$
  - with chopping: $\epsilon_{\text{mach}} = \beta^{1-p}$
  - with rounding to nearest: $\epsilon_{\text{mach}} = \frac{1}{2}\beta^{1-p}$
- called also *unit roundoff*: the smallest number $\epsilon$ such that $fl(1+\epsilon) > 1$
- maximum relative error of representation

$$\left|\frac{fl(x) - x}{x}\right| \le \epsilon_{\text{mach}}$$

- usually $0 < UFL < \epsilon_{\text{mach}} < OFL$

# Machine precision - example

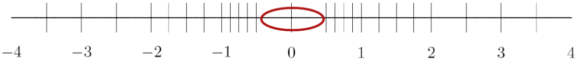
For $\beta = 2, p = 3, L = -1, U = 1$,

- $\epsilon_{\text{mach}} = (0.01)_2 = (0.25)_{10}$ with chopping
- $\epsilon_{\text{mach}} = (0.001)_2 = (0.125)_{10}$ with rounding to nearest

The usual case (IEEE fp systems):

- $\epsilon_{\text{mach}} = 2^{-24} \approx 10^{-7}$ in single precision
- $\epsilon_{\text{mach}} = 2^{-53} \approx 10^{-16}$ in double precision
- $\rightarrow$ about 7 and 16 decimals of precision, respectively
- (in R: p-value $< 2.2e - 16$)

# Gradual underflow




- to improve representation of numbers around 0 - use subnormal (or denormalized) numbers
- when exponent is at minimum, alow leading digits to be 0
- subnormals are less precise
- $\rightarrow$ gradual underflow

# Special values

IEEE standard:

- Inf: infinity; the result of $1/0$
- NaN: the result of $0/0$ or $Inf/Inf$
- special representation of the exponent field

# Floating-point arithmetic

- *addition/subtraction*: denormalization might be required: $3.52 \times 10^3 + 1.97 \times 10^5 = 0.0352 \times 10^5 + 1.97 \times 10^5 = 2.0052 \times 10^5 \rightarrow$ might cause loss of some digits
- *multiplication/division*: the result may not be representable
- overflow is more serious than underflow: how to approximate large numbers?
- for underflow, the result may be approximated by 0
- in FP arithm. addition and multiplication are commutative but *not* associative: if $\epsilon$ is slightly smaller than $\epsilon_{\text{mach}}$, then $(1 + \epsilon) + \epsilon = 1$, but $1 + (\epsilon + \epsilon) > 1$
- ideally, $x \operatorname{flop} y = fl(x op y)$; IEEE standard ensures this for within range results

## Example: divergent series

$$\sum_{n=1}^{\infty} \frac{1}{n}$$

- in FP arithm, the sum of the series is finite;
- depending on the system, this is because:
  - after a while, the sum overflows
  - $1/n$ underflows
  - for all $n$ such that
    $$\frac{1}{n} < \epsilon_{\text{mach}} \sum_{k=1}^{n-1} \frac{1}{k}$$
    the sum does not change anymore

# Cancellation

- subtracting 2 numbers of the same magnitude usually cancels the *most significant* digits:
  $1.92403 \times 10^2 - 1.92275 \times 10^2 = 1.28000 \times 10^{-1} \rightarrow$ only 3 significant digits
- let $\epsilon > 0$ be slightly smaller than $\epsilon_{\text{mach}}$, then $(1 + \epsilon) - (1 - \epsilon)$ yields 0 in FP arithmetic, instead of $2\epsilon$.

# Cancellation - example

For the quadratic equation, $ax^2 + bx + c = 0$, the two solutions are given by

$$x_{1,2} = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

Problems:

- for very large/small coefficients, the terms $b^2$ or $4ac$ may over-/underflow $\rightarrow$ rescale coeficients by $\max\{a, b, c\}$.
- cancellation between $-b$ and $\sqrt{\cdot}$ can be avoided by computing one root using $x = \frac{2c}{-b \mp \sqrt{b^2 - 4ac}}$

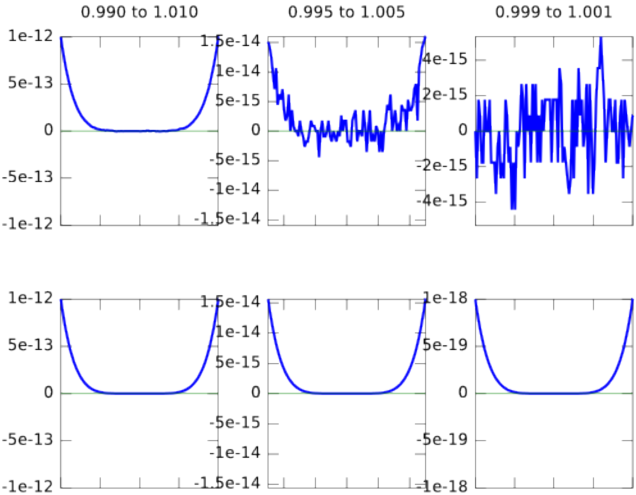
Exercise: let $x_1 = 2000, x_2 = 0.05$ be the roots of a quadratic equation. Compute the coefficients and then use the above formulas to retrieve the roots. Try `roots()` function in MATLAB.

# Cancellation - another example

$P(X) = (X-1)^6 = X^6 - 6X^5 + 15X^4 - 20X^3 + 15X^2 - 6X + 1.$
What happens around $X = 1$?

```
epsilon = [.01, .005, .001];
for k=1:3
  x   = linspace(1-epsilon(k), 1+epsilon(k), 100);
  px  = x.^6 - 6*x.^5 + 15*x.^4 - 20*x.^3 + 15*x.^2  ...
      - 6*x + 1;
  px0 = (x - 1).^6;
  subplot(2, 3, k);
  plot(x, px, '-b', x, zeros(1,100), '-r');
  axis([1-epsilon(k), 1+epsilon(k), -max(abs(px)), ...
       max(abs(px))]);
  subplot(2, 3, k+3);
  plot(x, px0, '-b', x, zeros(1, 100), '-r' );
  axis([1-epsilon(k), 1+epsilon(k), -max(abs(px0)), ...
       max(abs(px0))]);
end
```

# ...mathematically equivalent, but numerically different...



HOMEWORK

Let $\mathbf{x} = [a, b] \in \mathbb{R}^2$ and let $p$ be its Euclidean norm, $p = \sqrt{a^2 + b^2}$. However, using this formula is prone to under- and over-flow errors.

- show that $\min\{|a|, |b|\} \leq p \leq \sqrt{2} \max\{|a|, |b|\}$
- implement in MATLAB a procedure that would avoid unnecessary under-/over-flows Hint: $p = c\sqrt{(a/c)^2 + (b/c)^2}$. Find a suitable $c$...

# In MATLAB...

- you can change the format of FP in output using `format` option
- $\epsilon_{\text{mach}}$ is returned by the function `eps()`:
  - single precision: `eps(single(1))` gives $1.1921e-07 = 2^{-23}$
  - double precision: `eps(double(1))` gives $2.2204e-16 = 2^{-52}$
- to obtain the smallest or largest single/double precision numbers, use `realmin('single')`, `realmin('double')`, `realmax('single')`, `realmax('double')`
- you have the special constants `Inf` and `NaN`