E7441: Scientific computing

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RECETOX

Outline

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

Outline

Bibliography:

- KONG Q., SIAUW T., BAYEN A. (2020). Python programming and numerical methods. Academic Press. ISBN: 9780128195499
- HEATH M.T. (2002). Scientific Computing. An introductory survey. McGraw-Hill, 2nd edition. ISBN: 0-07-239910-4 Good accompanying materials at https://heath.cs.illinois.edu/scicomp/notes/index.html, 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

Computing environments for the course:

- PYTHON 3, https://www.python.org - with NUMPY and SCIPY packages
- recommended: JUPYTERLAB for exercises
- suggestion: install PYTHON and related packages using a distribution like ANACONDA or MAMBA for easier integration of dependencies
- 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;

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

- continuous domain $\rightarrow$ 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 → discrete domain
- infinite → finite
- differential → algebraic
- nonlinear → (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

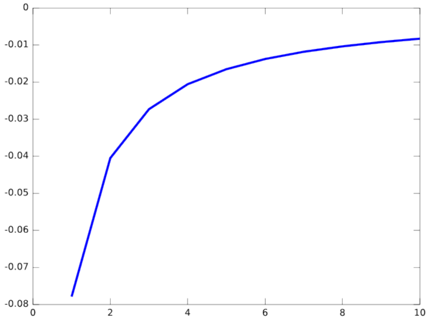
- Absolute error: approximate value ($\hat{x}$) - true value (x)
- Relative error:
$$\frac{\text{absolute error}}{\text{true value}}$$
- $\rightarrow$ approximate value $=$ (1 $+$ relative error) $\times$ (true value)
- if the relative error is $\sim 10^{-d}$, it means that $\hat{x}$ has about d exact digits: there exists $\tau = \pm(0.0\dots0n_{d+1}n_{d+2}\dots)$ 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 - Homework!

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)
- rounding error: $2\epsilon/h$, for ϵ being the precision
- total error is minimized for $h \approx 2\sqrt{\epsilon/M}$

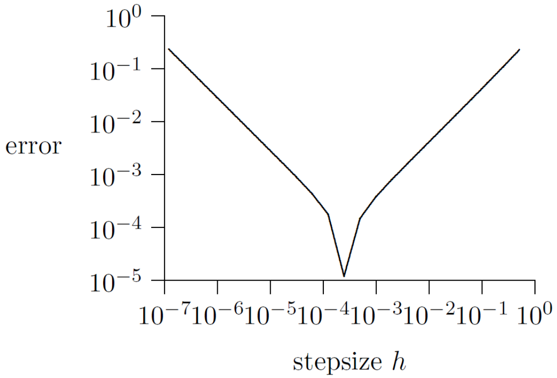


Figure: Total computational error as a tradeoff between truncation and rounding error (from *Heath - Scientific computing*)

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 $f(\hat{x}) = \hat{y}$

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

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 $\text{cond} >> 1$ 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, $\text{cond} \leq C$, 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 Δx
- 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 $\approx 2.48275 \times 10^5$

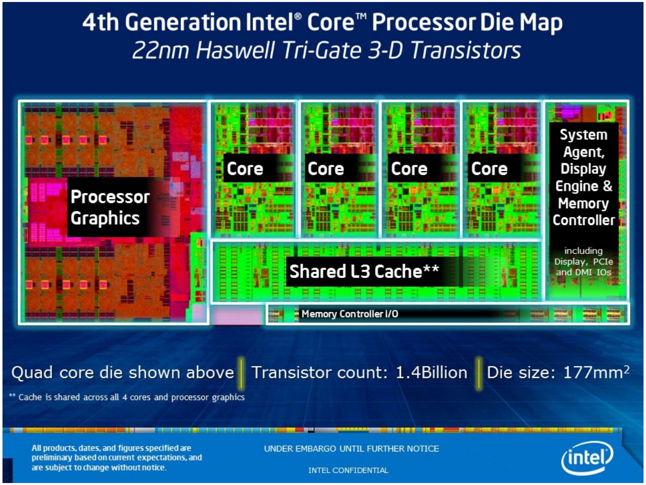
Stability

- 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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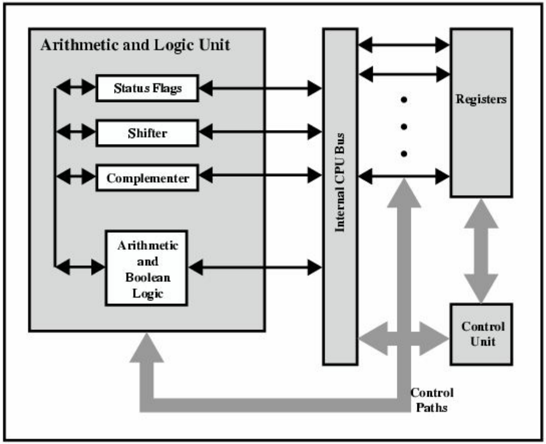

Arithmetic and Logic Unit
Status Flags
Shifter
Complementer
Arithmetic and Boolean Logic
Internal CPU Bus
Registers
Control Unit
Control Paths

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 $\rightarrow$ specific to architecture: 1, 2, 4, or 8 bytes
- integers:
  - unsigned (≥ 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. 2.35×10^3
- 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
  β 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

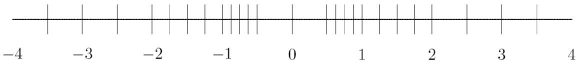
Internal representation (on 64 bits - "double precision", binary representation):

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

Properties:

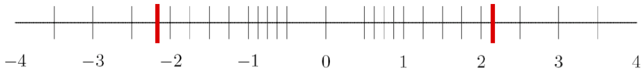
- only a finite number of discrete values can be represented
- total number of floating point numbers representable in normalized format is
$$2(\beta - 1)\beta^{p-1}(U - L + 1) + 1$$
- undeflow level (smallest number): $UFL = \beta^L$
- overflow level (largest number): $OFL = \beta^{U+1}(1 - \beta^{-p})$
- not all real numbers can be represented exactly:
  - *machine numbers*
  - rounding → 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–β representation after $p-1$st digit
- *round to nearest*: $fl(x)$ is the closest machine number to x

Machine precision

- machine precision, ϵ_{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 ϵ such that $fl(1+\epsilon) > 1$
- maximum relative error of representation

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

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

Machine precision - example

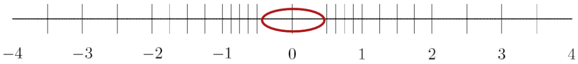
For $\beta = 2, p = 3, L = -1, U = 1$,

- $\epsilon_{\text{mach}} = (0.01)_2 = (0.25)_{10}$ 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
- → 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 ϵ is slightly smaller than ϵ_{mach}, then $(1+\epsilon)+\epsilon = 1$, but $1 + (\epsilon + \epsilon) > 1$
- ideally, $x \text{ flop } y = fl(x \ op \ y)$; 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 ϵ_{mach}, then $(1 + \epsilon) - (1 - \epsilon)$ yields 0 in FP arithmetic, instead of 2ϵ.

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 `numpy.roots()` function in Python.

Cancellation - another example

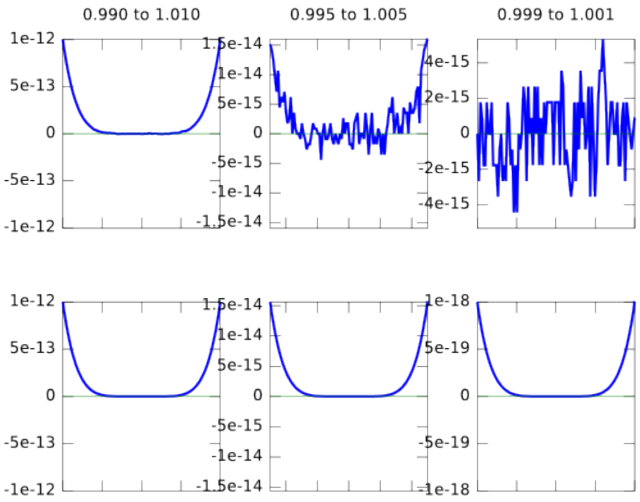
$P(X) = (X-1)^6 = X^6 - 6X^5 + 15X^4 - 20X^3 + 15X^2 - 6X + 1$. What happens around $X = 1$?

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

epsilon = [0.01, 0.005, 0.001]
for k in range(3):
    x = np.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
    plt.subplot(2, 3, k+1)
    plt.plot(x, px, '-b', x, np.zeros(100), '-r')
    plt.axis([1 - epsilon[k], 1 + epsilon[k], -max(abs(px)),
                                  max(abs(px))])
    plt.subplot(2, 3, k+4)
    plt.plot(x, px0, '-b', x, np.zeros(100), '-r')
    plt.axis([1 - epsilon[k], 1 + epsilon[k], -max(abs(px0)),
                                  max(abs(px0))])

plt.show()
```

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



(very small) Project

Study the paper

Moler, C., Morisson, D., *Replacing square roots by Pythagorean sums*. IBM J. Res. Develop. 27(6), 1983

Then, implement the proposed method and compare it with the naive `sqrt()`-based approach.

In Python...

- basic (and not only) numerical functions are in `numpy` package
- ϵ_{mach} is returned by
  - single precision: `np.finfo(np.float32).eps` gives $1.1920929e-07 = 2^{-23}$
  - double precision: `np.finfo(np.float64).eps` gives $2.220446049250313e-16 = 2^{-52}$
- to obtain the smallest or largest single/double precision numbers, use `np.finfo(np.float32).min`, `np.finfo(np.float32).max`, `np.finfo(np.float64).min`, `np.finfo(np.float64).max`
- you have the special constants `np.Inf` and `np.NaN`

Questions?