

CS 450: Numerical Analysis¹

Introduction to Scientific Computing

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¹*These slides have been drafted by Edgar Solomonik as lecture templates and supplementary material for the book “Scientific Computing: An Introductory Survey” by Michael T. Heath ([slides](#)).*

Scientific Computing Applications and Context

- ▶ **Mathematical modelling for computational science** *Typical scientific computing problems are numerical solutions to PDEs*
 - ▶ *Newtonian dynamics: simulating particle systems in time*
 - ▶ *Fluid and air flow models for engineering*
 - ▶ *PDE-constrained numerical optimization: finding optimal configurations (used in engineering of control systems)*
 - ▶ *Quantum chemistry (electronic structure calculations): many-electron Schrödinger equation*
- ▶ **Linear algebra and computation**
 - ▶ *Linear algebra and numerical optimization are building blocks for machine learning methods and data analysis*
 - ▶ *Computer architecture, compilers, and parallel computing use numerical algorithms (matrix multiplication, Gaussian elimination) as benchmarks*

Example: Mechanics²

- ▶ Newton's laws provide incomplete particle-centric picture
- ▶ Physical systems can be described in terms of *degrees of freedom* (DoFs)
 - ▶ A piston moving up and down requires 1 DoFs
 - ▶ 1-particle system requires 3 DoFs
 - ▶ 2-particle system requires 6 DoFs
 - ▶ 2-particles at a fixed distance require 5 DoFs
- ▶ N -particle system *configuration* described by $3N$ DoFs
 - ▶ Trajectories in *configuration space* (\mathbb{R}^{3N}) describe free energy configuration
 - ▶ Various choice of *basis functions* (i.e. coordinate system) for configuration space are possible

²*Variational Principles of Mechanics*, Cornelius Lanczos, Dover Books on Physics, 1949.

Course Structure

- ▶ **Complex numerical problems are generally reduced to simpler problems**
 - ▶ *Discretization* corresponds to representing a continuous function/model by a discrete set of points
 - ▶ *Nonlinear problems are mapped to linear problems*
 - ▶ *Complicated functions are mapped to polynomials*
 - ▶ *Differential equations are mapped to algebraic equations*
- ▶ **The course topics will follow this hierarchical structure**
 - ▶ *Error, conditioning, and floating point are the starting point for representation and evaluation of algorithms for any numerical problem*
 - ▶ *Linear systems provide the simplest and most important building block for solving linear algebra problems*
 - ▶ *Least squares and eigenvalue problems provide basic technology for matrices*
 - ▶ *Nonlinear equations and optimization make use of matrix algebra to solve more general modelling problems*
 - ▶ *Numerical interpolation, differentiation, and quadrature provide the building blocks to reduce numerical PDE problems to matrix algebra*

Numerical Analysis

▶ Numerical Problems involving Continuous Phenomena:

Given input $x \in \mathbb{R}^n$, approximate output $y = f(x)$

- ▶ Problem is *well-posed* if f is a smoothly varying function, $f(\hat{x}) \rightarrow f(x)$ as $\hat{x} \rightarrow x$.
- ▶ Otherwise, problem is *ill-posed*

▶ Error Analysis:

Quality of approximation is quantified by distance to the solution

- ▶ If solution $y = f(x)$ is a scalar, distance from computed solution \hat{y} to correct answer is the *absolute error*

$$\Delta y = \hat{y} - y,$$

while the normalized distance is the *relative error*

$$\Delta y / y = \frac{\hat{y} - y}{y}$$

- ▶ More generally, we are interested in the error

$$\Delta \mathbf{y} = \hat{\mathbf{y}} - \mathbf{y}$$

the magnitude of which is measured by a given *vector norm*

Sources of Error

▶ Representation of Numbers:

- ▶ *We cannot represent arbitrary real numbers in a finite amount of space, e.g. a computer cannot exactly represent π*
- ▶ *Moreover, hardware architectures are only well-fit to work with fixed-length (32-bit or 64-bit) representations*
- ▶ *As we will see, the best we can do is represent a wide range of numbers with a relatively uniform **precision**, which corresponds to **scientific notation***
- ▶ *With scientific notation, we seek to store the most significant digits of each number, so that the magnitude of the relative error in the floating point representation $fl(x)$ for most real numbers x will be $|fl(x) - x|/|x| \leq \epsilon$*

▶ Propagated Data Error: *error due approximations in the input, $f(\hat{x}) - f(x)$*

▶ Computational Error = $\hat{f}(x) - f(x) = \text{Truncation Error} + \text{Rounding Error}$

- ▶ ***Truncation error** is the error made due to approximations made by the algorithm (simplified models used in our approximation)*
- ▶ ***Rounding error** is the error made due to inexact representation of quantities computed by the algorithm*

Error Analysis

▶ Forward Error:

Forward error is the computational error of an algorithm

- ▶ Absolute: $\hat{f}(x) - f(x)$
- ▶ Relative: $(\hat{f}(x) - f(x))/f(x)$
- ▶ Usually, we care about the **magnitude** of the final error, but carrying through signs is important when analyzing error

▶ Backward Error:

It can be hard to tell what a 'good' forward error is, but **backward error analysis** enables us to measure computational error with respect to data propagation error

- ▶ An algorithm is **backward stable** if its a solution to a nearby problem
- ▶ If the computed solution $\hat{f}(x) = f(\hat{x})$ then

$$\text{backward error} = \hat{x} - x$$

- ▶ More precisely, we want the nearest \hat{x} to x with $\hat{f}(x) = f(\hat{x})$
- ▶ If the backward error is smaller than the propagated data error, the solution computed by the algorithm is as good as possible

Conditioning

► **Absolute Condition Number:**

The *absolute condition number is a property of the problem*, which measures its sensitivity to perturbations in input

$$\kappa_{abs}(f) = \lim_{\text{size of input perturbation} \rightarrow 0} \max_{\text{inputs}} \max_{\text{perturbations in input}} \left| \frac{\text{perturbation in output}}{\text{perturbation in input}} \right|$$

For problem f at input x it is simply the derivative of f at x ,

$$\kappa_{abs}(f) = \lim_{\Delta x \rightarrow 0} \left| \frac{f(x + \Delta x) - f(x)}{\Delta x} \right| = \left| \frac{df}{dx}(x) \right|$$

When considering a space of inputs \mathcal{X} it is $\kappa_{abs} = \max_{x \in \mathcal{X}} \left| \frac{df}{dx}(x) \right|$

► **(Relative) Condition Number:**

The relative condition number considers relative perturbations in input and output, so that

$$\kappa(f) = \kappa_{rel}(f) = \max_{x \in \mathcal{X}} \lim_{\Delta x \rightarrow 0} \left| \frac{(f(x + \Delta x) - f(x))/f(x)}{\Delta x/x} \right| = \frac{\kappa_{abs}(f)|x|}{|f(x)|}$$

Posedness and Conditioning

- ▶ **What is the condition number of an ill-posed problem?**
 - ▶ *If the condition number is bounded and the solution is unique, the problem is **well-posed***
 - ▶ *An **ill-posed** problem f either has no unique solution or has a (relative) condition number of $\kappa(f) = \infty$*
 - ▶ *This condition implies that the solutions to problem f are continuous and differentiable in the given space of possible inputs to f*
 - ▶ *Sometimes well-posedness is defined to only require continuity*
 - ▶ *Generally, $\kappa(f)$ can be thought of as the reciprocal of the **distance** (in an appropriate geometric embedding of problem configurations) from f **to the nearest ill-posed problem***

Stability and Accuracy

- ▶ **Accuracy:**

*An algorithm is **accurate** if $\hat{f}(x) = f(x)$ for all inputs x when $\hat{f}(x)$ is computed in infinite precision*

- ▶ *In other words, the truncation error is zero (rounding error is ignored)*
- ▶ *More generally, an algorithm is accurate if its truncation error is negligible in the desired context*
- ▶ *Yet more generally, the **accuracy** of an algorithm is expressed in terms of bounds on the magnitude of its truncation error*

- ▶ **Stability:**

*An algorithm is **stable** if its output in finite precision (floating point arithmetic) is always near its output in exact precision*

- ▶ ***Stability** measures the sensitivity of an algorithm to **roundoff error***
- ▶ *In some cases, such as the approximation of a derivative using a finite difference formula, there is a trade-off between stability and accuracy*

Error and Conditioning

- ▶ Two major sources of error: *roundoff* and *truncation* error.
 - ▶ roundoff error concerns floating point error due to finite precision
 - ▶ truncation error concerns error incurred due to algorithmic approximation, e.g. the representation of a function by a finite Taylor series

$$f(x+h) \approx g(h) = \sum_{i=0}^k \frac{f^{(i)}(x)}{i!} h^i$$

The absolute truncation error of this approximation is

$$f(x+h) - g(h) = \sum_{i=k+1}^{\infty} \frac{f^{(i)}(x)}{i!} h^i = O(h^{k+1}) \text{ as } h \rightarrow 0$$

- ▶ To study the propagation of roundoff error in arithmetic we can use the notion of conditioning. *The condition number tells use the worst-case amplification of output error with respect to input error*

$$\kappa(f) = \max_{x \in \mathcal{X}} \lim_{\Delta x \rightarrow 0} \left| \frac{(f(x + \Delta x) - f(x))/f(x)}{\Delta x/x} \right| = \frac{|f'(x)x|}{|f(x)|}$$

Floating Point Numbers

Demo: Picking apart a floating point number

Demo: Density of Floating Point Numbers

▶ Scientific Notation

Floating-point numbers are a computational realization of scientific notation,

$$4.12165 \times 10^6, 2.145 \times 10^{-3}$$

- ▶ *Scientific-notation provides a unique representation of any real number for a given amount of 'precision' (number of significant digits)*
- ▶ *Normalized floating-point numbers are just a binary form of scientific notation,*

$$1.01001 \times 2^5, 1.0110 \times 2^{-3}$$

▶ Significand (Mantissa) and Exponent Given x with s leading bits x_0, \dots, x_{s-1}

$$fl(x) = \sum_{i=0}^{s-1} x_i 2^{k-i} = \underbrace{x_0.x_1 \dots x_{s-1}}_{\text{significand/mantissa}} \times 2^{\overbrace{\text{exponent}}^k}$$

A floating point number's binary representation has $s - 1$ significand bits (excluding $x_0 = 1$), some bits to represent the exponent, and a sign bit

▶ Maximum Relative Representation Error (Machine Epsilon)

- ▶ *If we have s significant digits in scientific notation, our error is bounded to variations of 1 in least significant digit, whose magnitude relative to the number we are trying to represent is 10^{1-s} in decimal and 2^{1-s} in binary*
- ▶ *Formally, with s significant binary digits the **relative representation error** of positive real number x is (with $k = \lfloor \log_2(|x|) \rfloor$ and each $x_i \in \{0, 1\}$)*

$$x = \sum_{i=0}^{\infty} x_i 2^{k-i} = x_{rem} + \sum_{i=0}^{s-1} x_i 2^{k-i}, \quad \text{where } |x_{rem}/x| \leq 2^{1-s}$$

- ▶ *The maximum such error, 2^{1-s} , is called **machine epsilon**,*

$$\epsilon = \operatorname{argmin}_{\epsilon > 0} (fl(1 + \epsilon) - 1)$$

Rounding Error in Operations (I) *Activity: Cancellation in Standard Deviation Computation*

▶ Addition and Subtraction

- ▶ Subtraction is just negation of a sign bit followed by addition
- ▶ *Catastrophic cancellation* occurs when the magnitude of the result is much smaller than the magnitude of both operands
- ▶ Cancellation corresponds to losing significant digits, e.g.

$$3.1423 \times 10^5 - 3.1403 \times 10^5 = 2.0 \times 10^2$$

- ▶ Generally, we can bound the error incurred during addition of two real numbers x, y in floating point (ignoring final rounding, which has relative error ϵ) as

$$\frac{|(x + y) - (fl(x) + fl(y))|}{|x + y|} \leq \frac{\epsilon(|x| + |y|)}{|x + y|}$$

by this we can also observe that the condition number of addition of x, y i.e. $f(x, y) = x + y$, is $\kappa(f(x, y)) = (|x| + |y|)/|x + y|$

- ▶ Consequently, when $x + y = 0$ and $x, y \neq 0$ addition is *ill-posed*

Rounding Error in Operations (II)

► Multiplication and Division

- *Multiplication is a lot safer than addition in floating point*
- *To analyze its error, we use a 2-term **Taylor series approximation** typical in relative error analysis*

$$f(\epsilon) = (1 + n\epsilon)^k \approx f(0) + \frac{df}{d\epsilon}(0)\epsilon = 1 + kn\epsilon$$

since ϵ is small, this linear approximation is accurate (to within $O(\epsilon^2)$)

- *Aside from final rounding, we can bound the error in multiplication as*

$$\frac{|xy - fl(fl(x)fl(y))|}{|xy|} \leq \frac{|xy - (x(1 + \epsilon)y(1 + \epsilon))(1 + \epsilon)|}{|xy|} \approx 3\epsilon$$

- *Consequently, multiplication $f(x, y) = xy$ is always **well-conditioned**, $\kappa(f) \approx 3$*
- *Division is multiplication by the reciprocal, and reciprocation is also well-conditioned*

Exceptional and Subnormal Numbers

▶ Exceptional Numbers

We had mentioned that the leading bit in normalized floating point numbers is assumed to be 1, but how do represent 0?

- ▶ *Exceptional* floating point numbers are $0, -0, \infty, -\infty$, and $\text{NaN} = 0/0 = \infty - \infty$

▶ Subnormal (Denormal) Number Range

- ▶ *The range of magnitudes of normalized floating point numbers with an exponent range $[-e, e]$ is $[2^{-e}, 2^{e+1}(1 - \epsilon/2)]$*
- ▶ *For numbers of magnitude $< 2^{-e}$, the relative representation error is unbounded*
- ▶ *Subnormal numbers* are evenly spaced in $[-2^{-e}, 2^{-e}]$ with gaps of $\epsilon 2^{-e}$
- ▶ *Consequently, the absolute representation error in $[-2^{-e}, 2^{-e}]$ is at most $\epsilon 2^{-e}$*

▶ Gradual Underflow: Avoiding underflow in addition

The main benefit of subnormal numbers is that for any machine numbers (floating-point numbers) x and y , $fl(x - y) = 0$ if and only if $x = y$, since the gap between any two representable numbers is $|x - y| \geq \epsilon 2^{-e}$