CS 450: Numerical Anlaysis[1]

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

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

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 $\boldsymbol{x} \in \mathbb{R}^n$, approximate output $\boldsymbol{y} = f(\boldsymbol{x})$
  - *Problem is well-posed if a unique solution exists and changes continuously with the initial conditions, i.e., f is a continuous function, $f(\hat{\boldsymbol{x}}) \to f(\boldsymbol{x})$ as $\hat{\boldsymbol{x}} \to \boldsymbol{x}$.*
  - *Otherwise, problem is ill-posed*
- **Error Analysis**:
  Quality of approximation is quantified by distance to the solution
  - *If solution $y = f(\boldsymbol{x})$ 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*

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

    the magnitude of which is measured by a given vector norm

Sources of Error

Demo: *Floating Point vs Program Logic*

- **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* $|fl(x) - x|/|x| \le \epsilon$
- **Propagated Data Error**: *error due approximations in the input,* $f(\hat{x}) - f(x)$
- **Computational Error =** $\hat{f}(x) - f(x)$ **= Truncation Error + 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**:

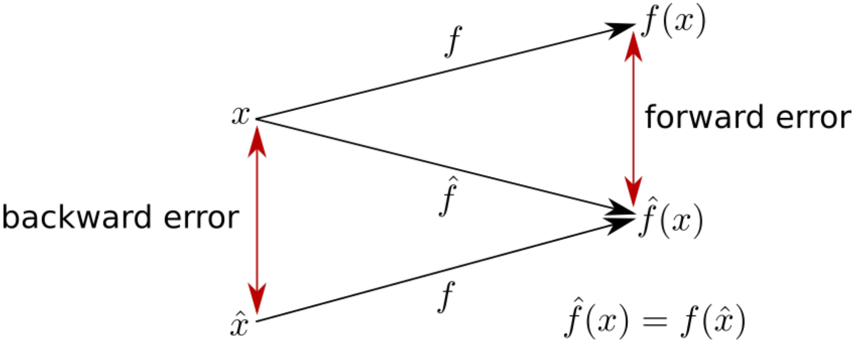
  It can be hard to tell what a 'good' forward error is, but backward error analysis enables us to measure computational error with respect to data propagation error

  - *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*

Visualization of Forward and Backward Error



Conditioning

- **Absolute Condition Number**:

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

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

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

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

  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

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

Posedness and Conditioning

- **What is the condition number of an ill-posed problem?**
  - *If the condition number is bounded and the solution is unique, we know the problem is well-posed (solution changes continously)*
  - *In fact, an alternative definition of an ill-posed problem is that f has a condition number of $\kappa_{abs}(f) = \infty$ (meaning f is not differentiable for some input)*
  - *This condition implies that the solutions to a well-posed problem f are continuous and differentiable in the given space of possible inputs to f*
  - *Geometrically, the condition number 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 and truncation 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

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

- 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*

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

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 $x_0, \ldots, x_{s-1}$

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

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

Rounding Error

- **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 $x_i \in \{0,1\}$)*

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

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

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

Demo: Catastrophic Cancellation

Rounding Error in Operations (I)

- **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 $x, y \neq 0$, $\kappa(f(x, y)) = \infty$. In general if $x + y$ is near 0 addition is ill-conditioned.*

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 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* $|x-y| \geq \epsilon 2^{-e}$

Floating Point Number Line