CSC 338 Numerical Methods. Lecture 1. Welcome!

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This course is about solving numerical problem involving continuous quantities using computational techniques.

↳ How do we represent continuous quantities using discrete hardware? (week 2)

↳ What kind of approximations do we need to make? How do we talk about "error" and "accuracy"? (week 1)

↳ How can we solve common computational problems efficiently with minimal error?

- Systems of Linear Equations. (week 3-4)
- Linear Least Squares (week 5-6)
- Non-linear Equations (week 8-9)
- Non-linear Optimization (week 10-11)

Example from hw1.

$$f(x) = \frac{x - \sin(x)}{x^3}$$

can show that $\lim_{x \to 0} f(x) = \frac{1}{6}$

But if we compute $f(0.00000001)$ in Python we get 0.

Example of a computational problem (scientific computing)

We want to compute the surface area of the earth.

Radius of earth : $r = 6371$ km

$\pi = 3.14$.

Surface area of sphere : $A = 4\pi r^2$ ← mathematical model

$\Rightarrow \quad A = 4 \times 3.14 \times 6371 \times 6371$

$= 509.8 \times 10^6 \text{ km}^2$

Actual $510.1 \times 10^6 \text{ km}^2$

} off by ~0.06%

What are the source of error?

- Earth is not a sphere — modeling error
- Radius measured empirically — empirical measurement error
- Value of π truncated
- Value of r truncated

} Before Computation

truncation error } During Computation

Process for solving a computational problem

1. Develop a mathematical model.
2. Develop an algorithm to solve the equation numerically
3. Implement the algorithm
4. Run the algo and interpret results.

focus of this course

We will focus on well-posed problem.

Def A problem is well-posed if

1. A solution exists
2. The solution is unique
3. The solution depends continuously on the problem data.

A problem is ill-posed if otherwise

Game: well-posed or ill-posed?

(a) Compute $f(x) = x^3 - x + 1$ ⇒ well-posed.

(b) Find x s.t. $x^3 - x + 1 = 0$ ⇒ well posed

(c) Find x s.t. $x^2 - 1 = 0$ ⇒ ill-posed

(d) Colour image → grayscale ⇒ well-posed

(e) grayscale image → colour ⇒ ill-posed

(f) final grade → exam grade. ⇒ ill-posed.

(Resume at 4:07 pm)

Def: Accuracy: the "closeness" of computed solution to the actual solution

Q: When can we obtain accurate solutions?

To answer this question, let's start by talking about 3 ways we can quantify error (closeness)

Absolute vs Relative Error

Absolute Error = Approx Val − True Value

$$\text{Relative Error} = \frac{\text{Absolute Error}}{\text{True Value}}$$

undefined when true value = 0.

earth eg//

$509.8 \times 10^6\ km^2$
$- 510.1 \times 10^6\ km^2$
$= -0.3 \times 10^6\ km^2$

$$\frac{-0.3\times 10^6\ km^2}{510.1 \times 10^6\ km^2} = -0.06\%$$

Data vs Computation Error

~~Does~~ Can we attribute error to input data vs. computational process

Computation problem: Compute $f: \mathbb{R} \to \mathbb{R}$

x — true input $\qquad \hat{x}$ — approx input

$f(x)$ — desired result $\qquad \hat{f}$ — approx ~~result~~ function

$$\text{Total (Absolute) Error} = \hat{f}(\hat{x}) - f(x)$$

$$= \underbrace{\left(\hat{f}(\hat{x}) - f(\hat{x})\right)}_{\text{Computational Error}} + \underbrace{\left(f(\hat{x}) - f(x)\right)}_{\text{Propagated Data Error}}$$

eg// Compute $f(x) = \cos(x)$ for $x = \frac{\pi}{6} \approx 0.523$.
Approximate x with $\hat{x} = 0.5$
Approximate $\cos(x)$ with $\hat{f}(x) = 1 - \frac{x^2}{2}$.

There are two components to the computational error

1. Truncation Error ~ comes from approximating f
2. Rounding Error ~ comes from using finite-precision arithmetics

eg// (from above) Truncation error $= \sum_{i=2}^{\infty} \frac{(-1)^i \hat{x}^{2i}}{(2i)!}$

Forward vs Backward Error

problem: Compute $y = f(x)$ $f: \mathbb{R} \to \mathbb{R}$
But $\hat{f}$ approximate, so we get $\hat{y} = \hat{f}(x)$

(Absolute) Forward Error: $\Delta y = \hat{y} - y$
Problem is that this quantity is difficult to estimate
worst-case assumptions give pessimistic bounds

(Absolute) Backward Error: $\Delta x = \hat{x} - x$
where $\hat{x}$ is chosen so that $\hat{y} = f(\hat{x})$
$\Rightarrow \hat{x} = f^{-1}(\hat{y})$

$\Rightarrow$ Backward Error is small when the approx solution is the exact solution to a nearby problem.

$$\begin{tikzcd} x \arrow[r, "f"] \arrow[dr, "\hat{f}"] & y \\ \boxed{\hat{x}} \arrow[r, "f"'] & \hat{y} \end{tikzcd}$$

Backward Error (x to $\hat{x}$)
y — actual sol'n
Forward Error (y to $\hat{y}$)
$\hat{y}$ — approx solution

eg// $f(x) = \cos(x)$

$\hat{f}(x) = 1 - \frac{x^2}{2}$

Forward Error : $\Delta y = \left(1 - \frac{x^2}{2}\right) - \cos(x)$

Backward Error: $\Delta x = \boxed{\arccos\left(1 - \frac{x^2}{2}\right)} - x$

$\hat{y} = \hat{f}(x) = 1 - \frac{x^2}{2}$

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

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

$= \arccos\left(1 - \frac{x^2}{2}\right)$

Sensitivity and Conditioning

Def A problem is insensitive or well-conditioned if a relative change in input causes similar relative change in the solution.

A problem is sensitive or ill-conditioned if a relative change in input causes much larger relative change in the solution

eg// (intuition) $f(x) = 0.7x$ $\quad g(x) = 1000x^6$

A small change Δx in $x = 10$ cause similar change in $f(x)$ but larger change $g(x)$.

Def The condition number (CN) of a problem is

$$CN = \frac{|\Delta y / y|}{|\Delta x / x|} \quad \begin{matrix} \text{relative change in output} \\ \text{relative change in input} \end{matrix}$$

$$= \frac{|(f(\hat{x}) - f(x)) / f(x)|}{|(\hat{x} - x) / x|}$$

The C.N. represents the "amplifization factor" of the error.

$$\left| \text{Relative Fwd Error} \right| = \text{C.N} \times \left| \text{Relative Backward Error} \right|.$$

$$\left| \frac{\Delta y}{y} \right| = \text{CN} \times \left| \frac{\Delta x}{x} \right|$$

If $\underbrace{\text{C.N.} \gg 1}_{\text{much larger than}}$, then the problem is ill-conditioned

For the problem of computing $f: \mathbb{R} \to \mathbb{R}$, continuous & differentiable

$$\text{Relative Forward Error} = \frac{f(x+\Delta x) - f(x)}{f(x)} \frac{\Delta x}{\Delta x}$$

$$\Delta x \to 0 \quad = \boxed{\frac{f(x+\Delta x) - f(x)}{\Delta x}} \frac{\Delta x}{f(x)}$$

$$= \boxed{f'(x) \frac{\Delta x}{f(x)}}$$

$$\text{C.N} = \frac{|\text{Rel Fwd Error}|}{|\text{Rel Back Error}|} = \frac{\left| f'(x) \frac{\cancel{\Delta x}}{f(x)} \right|}{|\cancel{\Delta x} / x|}$$

$$= \left| \frac{x f'(x)}{f(x)} \right| =: K_f(x)$$

eg// $f(x) = 0.7x \qquad g(x) = 1000x^6$

$$K_f(x) = \frac{x\,0.7}{0.7x} = 1$$

$$K_g(x) = \frac{x \, 6000 x^5}{1000 x^6} = 6$$

Stability ~~& Accuracy~~ of Algorithms

Def An algorithm is stable if the result is relatively insensitive to perturbations during computation.

Backward Error View: An algo is stable if result produced is the exact sol'n to a nearby problem.

Q: When can we obtain accurate solutions?

1. When the problem is well conditioned

and

2. When the algorithm is stable.