Scientific Computing

Designing + Analyzing algorithms for solving computational problems involving continuous quantities

$\Rightarrow$ making approximation

$\Rightarrow$ errors.

Example: surface area of Earth

Radius : 6371 km. $\quad\quad 6371 \times 6371$

π : 3.14

$$\text{Surface area of sphere} = 4\pi r^2$$
$$= 4 \times 3.14 \times 6371 \times 6371$$
$$= 509.8 \times 10^6 \text{ km}^2.$$

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

What are the sources of error?

Earth not a sphere — modelling Error

Radius measured empirically — Empirical measure Truncation.

} Before Computation

Values of π truncated

" " radius truncated.

} Truncation Error } During Computation

Example of a computation problem.

Use mathematical model to understand the universe.

1. Developed a mathematical model. — $4\pi r^2$.
2. Developed an algorithm to solve the equation numerically
3. Implemented the algorithm
4. Run the algo. and interpret the result.

The focus of this course

We're going to focus on well-posed problem

① a solution exists.
② solution is unique
③ result depends continuously on the problem data

Opposite : ill-posed problems

~~ex~~ midterm avg for the class → midterm grade for each student.

image denoising : noisy img ⇒ clean img

finding the root of x^2+1

Typical Computation Problem:

Compute $f : \mathbb{R} \to \mathbb{R}$ (or $f : \mathbb{R}^n \to \mathbb{R}^m$)

Quantify error

Absolute Error = Approx Value − True Value

$(509.8 \times 10^6 \text{ km}^2 - 510.1 \times 10^6 \text{ km}^2)$

$= -0.3 \times 10^6 \text{ km}^2$

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

$$\left(\frac{-0.3 \times 10^6 \text{ km}^2}{510.1 \times 10^6 \text{ km}^2} = -0.06\% \right)$$

Data Error vs. Computation Error

② x — true input

$\hat{x}$ — approx input

$\hat{f}$ — approx function

want: $f(x)$ ①

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

$$= \underbrace{\left(\hat{f}(\hat{x}) - f(\hat{x})\right)}_{\text{① computational error}} + \underbrace{\left(f(\hat{x}) - f(x)\right)}_{\text{② propagated data error}}$$

Computational error:

- Truncation Error (true result) − (result of using exact arithmetic)
- Rounding Error (result using exact arithmetic) − (result from finite precision arithmetic)

eg// approximate $\cos(x) = 1 - \frac{x^2}{2}$

Truncation Error $\sum_{k=2}^{\infty} \frac{(-1)^k x^{2k}}{(2k!)}$

Forward and Backward Error

Want to compute $y = f(x)$ $f : \mathbb{R} \to \mathbb{R}$.

But $\hat{f}$ approximate $\Rightarrow$ $\hat{y} = \hat{f}(x)$ (abs. error $\hat{y} - y$, relative error $\frac{\hat{y} - y}{y}$)

Absolute Forward Error : $\Delta y = \hat{y} - y$.

Problem: difficult to estimate

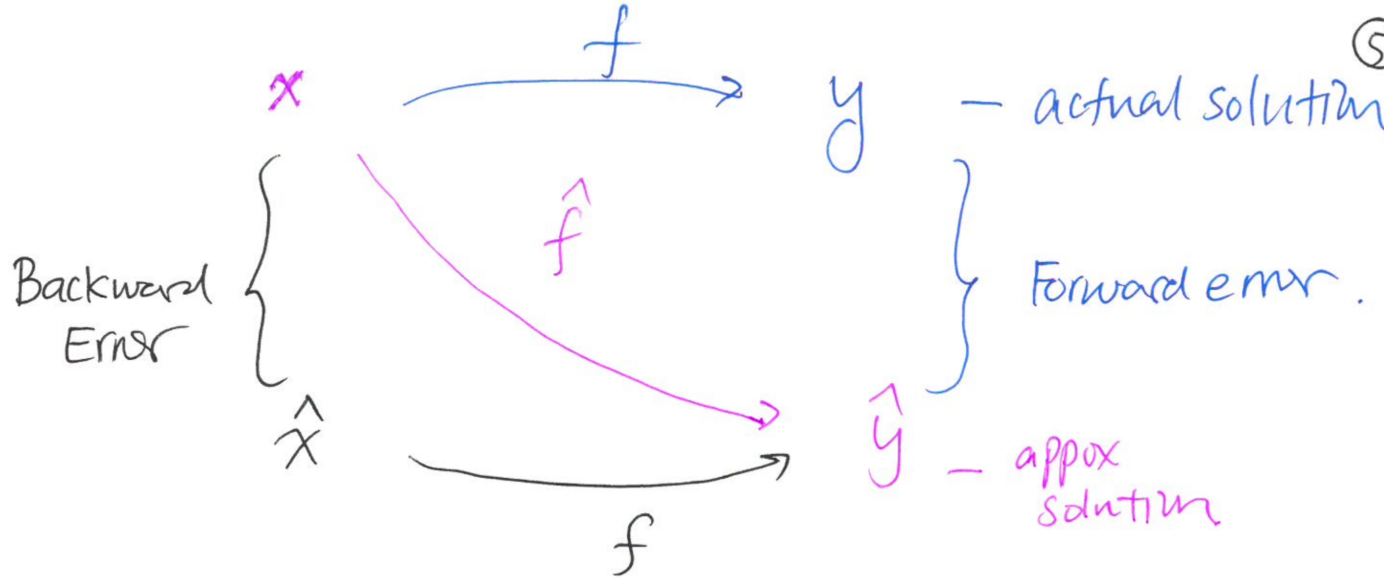
worse-case assumptions give pessimistic bounds.

Backward Error: $\Delta x = \hat{x} - x$. different $\hat{x}$ than last page

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

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

Approx. Solutions are "good" if it is the exact solution to a nearby problem.



Example $\quad f(x) = \cos(x)$

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

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

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

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

Sensitivity — describe a problem.

a problem is:

- insensitive or well-conditioned if

  a relative change in input cause similar relative change in solution.

- sensitive or ill-conditioned

  if relative change in solution is much larger than the change in input.

condition number (of a problem) $= \dfrac{|\Delta y / y|}{|\Delta x / x|}$ ← relative change in output; ← relative change in input.

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

If C.N. >> 1, the problem is ill-conditioned.

↳ represents an "amplification factor"

|Relative Forward Error| = C.N. * |Relative Backward Error|.

$$\left|\frac{\Delta y}{y}\right| = C.N. * \left|\frac{\Delta x}{x}\right|.$$

$\lesssim$ when C.N. is estimated by an upper bound.

For $f: \mathbb{R} \to \mathbb{R}$. — continuous, differentiable.

$\hat{x} = x + \Delta x$ approximate value:

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

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

$\Delta x \to 0$

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

$$C.N = \frac{|\text{Rel. Forward Error}|}{|\text{Rel. Backward Error}|}$$

$$= \left| \frac{f'(x)\,\frac{\Delta x}{f(x)}}{\frac{\Delta x}{x}} \right|$$

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

Stability of Algorithms

An algo. is stable if the result is relatively insensitive to perturbation during computation.

backward error: an algo is stable if result produced is the exact solution of nearby problem.

Accuracy: closeness of computed solution to actual solution:

Require 1. problem is well-conditioned

2. algorithm is stable