Lecture 2: Approximations and Errors

BT 2020 – Numerical Methods for Biology

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Strategies for Computational Solutions Problem Reduction

- ► Infinite-dimensional spaces ~> Finite-dimensional spaces
- ► Integrals ~→ Finite sums
- ▶ Derivatives → Finite differences
- ▶ Differential equations → Algebraic Equations
- Non-linear Problems → Linear Problems
- ► Complicated functions ~ Simple functions, e.g. polynomials
- **>** ...

Approximations in Scientific Computation

- Engineering is all about approximation!
- So is scientific computing
 - actually, we have no choice!
 - we need to use discrete computer systems and representations to work on continuous and *infinite* quantities!
- ► We need to compute accurately, using (limited) *finite precision* arithmetic!

Sources of Approximation

Before Computation

- ► The model itself!
- Measurement errors
 - e.g. arising out of instrument imprecision
- Previous computations

During Computation

- ► Truncation / discretisation
- Rounding
 - Finite precision computation

Approximation: An Example

▶ What is the surface area of the earth?

$$A=4\pi r^2$$

Can you list the approximations involved?

Approximation: An Example

▶ What is the surface area of the earth?

$$A=\pi r^2$$

Some approximations

- ► Shape of the earth!
- How do we measure the radius?
 - Empirically?
 - Based on other computations?
- ightharpoonup Value of π !
- Precision of the computers used
- **.**..

Absolute and Relative Errors

 Obviously, significance of an error is related to magnitude of measured quantity

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absolute error = approximate value - true value
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\frac{\text{relative error}}{\text{true value}}
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- Obviously, relative error is undefined if true value is zero
- ► Relative error can also be expressed in %

Precision vs. Accuracy

- Precision: Number of digits with which a number is expressed (recall significant figures?)
- Accuracy: Number of correct significant digits
- If an approximate value has an error of $\approx 10^{-p}$, then its decimal representation has $\approx p$ correct significant digits
- e.g. 3.6180339887498948482045868343656381177203 is a precise number, but not an accurate representation for π
- ► Often, we may not know the true value itself if we did, we may not need to approximate it!

Data Error and Computational Error

- ▶ Let's consider 1D problems to begin with, e.g. $f: \mathbb{R} \to \mathbb{R}$
- Let the true value of the input be $x \Rightarrow$ desired true result is f(x)
- ▶ But, our input may be inexact, say \hat{x}
- lacktriangle Also, our function computation may be approximate, say \hat{f}

Data Error and Computational Error

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

= $(\hat{f}(\hat{x}) - f(\hat{x})) + (f(\hat{x}) - f(x))$
= computational error + propagated data error

- ► Here, $\hat{f}(\hat{x}) f(\hat{x})$ is the difference between exact and approximate functions for the *same* input pure computational error
- ► $f(\hat{x}) f(x)$ denotes the difference between exact function values due to error in the input propagated data error
 - Choice of algorithm has no impact on this!

Data Error and Computational Error An Example

- Suppose we want a back-of-the-envelope calculation for $\sin(\pi/8)$
- ► How will you approximate it, without a calculator?
- ▶ What is the computational error? What is the data error?

- Suppose we want a back-of-the-envelope calculation for $\sin(\pi/8)$
- ► How will you approximate it, without a calculator?
- ▶ What is the computational error? What is the data error?
- $ightharpoonup \sin(\pi/8) \approx \sin(3/8) \approx 3/8 = 0.3750(!)$
- Using a calculator, $\sin(\pi/8) = 0.382683432... \approx 0.3827$
- ► Total error = $\hat{f}(\hat{x}) f(x) = 0.3750 0.3827 = -0.0077$
- Propagated data error, arising out of inexact input is $f(\hat{x}) f(x) = \sin(3/8) \sin(\pi/8) \approx 0.3663 0.3827 = -0.0164$
- Computational error, cause by truncating infinite series is $\hat{f}(\hat{x}) f(\hat{x}) = 3/8 \sin(3/8) \approx 0.3750 0.3663 = 0.0087$
- In this case, the errors are of opposing signs, offsetting one another!
- In other cases, they may reinforce one another!
- ► How to get more accurate??

Truncation Error vs. Rounding Error

Computational error can be further split into:

Truncation/Discretisation Error

- Difference between the true result (for actual input) and the result that would be produced by a given algorithm using exact / infinite-precision arithmetic
- The algorithm may truncate an infinite series (e.g. Taylor series), replace derivatives by finite differences etc.

Rounding Error

- Difference between the result produced by a given algorithm using exact arithmetic and the result produced by the same algorithm using finite-precision rounded arithmetic
- Arises out of the inexactness in representation of real numbers and arithmetic operations on these numbers

Truncation Error

Example — Finite Difference Approximation

For a differentiable function $f: \mathbb{R} \to \mathbb{R}$, consider the finite difference approximation to the first derivative,

$$f'(x) pprox rac{f(x+h) - f(x)}{h}$$

By Taylor's theorem,

$$f(x + h) = f(x) + hf'(x) + f''(\theta)h^2/2$$

for some $\theta \in [x, x+h]$. So, the truncation error of the finite difference approximation is bounded by Mh/2, where M is a bound on |f''(t)| for t near x.

Rounding Error

Example — Finite Difference Approximation

If the error in function values in bounded by ϵ , the rounding error in evaluating the finite difference formula is bounded by $2\epsilon/h$. The total computation errors is therefore:

$$\frac{Mh}{2} + \frac{2\epsilon}{h}$$

Clearly, as we decrease h, one term increases, while the other decreases \Rightarrow there's a trade-off.

The above function has its minimum at $h = 2\sqrt{\epsilon/M}$.

How to Reduce Error?

- ► *Truncation error* can be reduced by using better approximations, e.g. more terms in the expansion
- For instance, a more accurate finite difference formula can be used:

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}$$

► Rounding error can be reduced by working with higher-precision arithmetic (harder?)

Errors in Practice

- ► Although both truncation and rounding errors are important, in practice, one or the other tends to dominate
- Roughly speaking,
 - Rounding error dominates purely algebraic problems with finite solution algorithms, while
 - Truncation error dominates in problems involving integrals, derivatives, non-linearities etc. that require a theoretically infinite solution process
- ► The distinctions made among different types of errors are important for understanding the behaviour of numerical algorithms
- ► However, in practice, it is not necessary (or even possible!) to precisely delineate the different individual errors advantageous to lump them all together

Evaluating Complex Functions — Taylor Series

$$e^{x} = 1 + x + \frac{x^{2}}{2!} + \frac{x^{3}}{3!} + \dots = \sum_{n=0}^{\infty} \frac{x^{n}}{n!}$$

$$\sin(x) = x - \frac{x^{3}}{3!} + \frac{x^{5}}{5!} + \dots = \sum_{n=0}^{\infty} (-1)^{n} \frac{x^{(2n+1)}}{(2n+1)!}$$

$$\cos(x) = 1 - \frac{x^{2}}{2!} + \frac{x^{4}}{4!} + \dots = \sum_{n=0}^{\infty} (-1)^{n} \frac{x^{(2n)}}{(2n)!}$$

 N^{th} -order Taylor polynomial for y = f(x) at x_0 is:

$$p_N(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{f''(x_0)}{2!}(x - x_0)^2 + \dots + \frac{f^{(N)}(x_0)}{N!}(x - x_0)^N$$

$$\Rightarrow p_N(x) = \sum_{n=0}^{N} \frac{f^{(n)}(x_0)}{n!} (x - x_0)^n$$

Truncation Error — Exercise

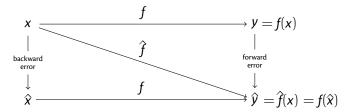
Use **Taylor Series** expansions with n = 0...6 to approximate f(x) = cos(x) at $x_{i+1} = \pi/3$ on the basis of the value of f(x) and its derivatives at $x_i = \pi/4$.

Forward Error and Backward Error

- ► Garbage in ~ Garbage out!
- ► If input data are accurate to only four significant digits, we can expect no more than four significant digits in computed result, no matter how accurate an algorithm we use!
- Suppose we want to compute y = f(x) (again $f : \mathbb{R} \to \mathbb{R}$) we obtain an approximate value \hat{y}
- The discrepancy between the computed and true values, $\Delta y = \hat{y} y$ is called *forward error*
- ► This is often difficult to compute ...

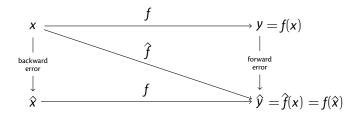
Forward Error and Backward Error

- Alternately, let's consider the approximate solution obtained to be the exact solution for a modified problem
- Now, "How large a modification to the original problem is required to give the result actually obtained?"
- Or, "How much data error in the initial input x would be required to explain all of the error in the output?"
- $\Delta x = \hat{x} x$, where $f(\hat{x}) = \hat{y}$ is the *backward error*



Note that the equality $f(\hat{x}) = \hat{f}(x)$ is due to the choice of \hat{x} — this requirement defines \hat{x}

Forward Error and Backward Error



Example

- As an approximation to $y = \sqrt{2}$, let us use $\hat{y} = 1.4$
- $|\Delta y| = |\hat{y} y| = |1.4 1.4142...| \approx 0.0142 (\approx 1\%)$
- ► What is the \hat{x} that would give the value of 1.4? 1.4² = 1.96
- ► Backward error = |1.96 2| = 0.04(2%)

Forward Error and Backward Error Another Example

Consider $y = \cos(x)$. What are the errors in computing $\cos(x)$ using the truncated Taylor expansion $1 - x^2/2$, for $x = \pi/3$

Sensitivity and Conditioning

- ▶ Difficulties in solving a problem accurately are not always due to an ill-conceived formula or algorithm, but may be inherent in the problem being solved
- Even with exact computation, the solution to the problem may be highly sensitive to perturbations in the input data
- ► A problem is said to be *insensitive*, or *well-conditioned*, if a given relative change in the input data causes a reasonably commensurate relative change in the solution
- ► A problem is said to be sensitive, or ill-conditioned, if the relative change in the solution can be much larger than that in the input data
- ▶ More formally, we define the condition number of a problem *f* at *x* as

$$Condition number = \frac{|relative change in solution|}{|relative change in input data|}$$

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

 $|Relative forward error| = |condition number| \times |Relative backward error|$

Thus, the condition number can be interpreted as an "amplification factor" that relates forward error to backward error. If a problem is *ill-conditioned* (large condition number), then the relative forward error (perturbation in solution) can be large even if the backward error (relative perturbation in input) is small.

Condition Number for a Differentiable Function

Absolute forward error = $f(x + \Delta x) - f(x) \approx f'(x)\Delta x$

Relative forward error
$$=\frac{f(x+\Delta x)-f(x)}{f(x)} \approx \frac{f'(x)\Delta x}{f(x)}$$

Condition number
$$\approx \frac{f'(x)\Delta x/f(x)}{\Delta x/x} = \left|\frac{xf'(x)}{f(x)}\right|$$

Stability and Accuracy

- ► The concept of *stability* of a computational algorithm is analogous to conditioning of a mathematical problem
- Both deal with the effects of perturbations
- Stability refers to the effects of computational error on the result computed by an algorithm
- Conditioning refers to the effects of data error on the solution to a problem
- An algorithm is stable if the result it produces is relatively insensitive to perturbations due to approximations made during the computation

Stability and Accuracy

- From the viewpoint of backward error analysis, an algorithm is stable if the result it produces is the exact solution to a nearby problem
- ▶ i.e. the effect of perturbations during the computation is no worse than the effect of a small amount of data error in the input
- A stable algorithm produces exactly the correct result for nearly the correct problem
- Accuracy refers to the closeness of a computed solution to the true solution
- Stability does not by itself guarantee accuracy accuracy depends on the conditioning of the problem as well as algorithm stability

Stability and Accuracy

- ➤ Stability tells us that the solution obtained is exact for a nearby problem but the solution to that nearby problem is not necessarily close to the solution to the original problem unless the problem is well-conditioned
- Inaccuracy can stem from applying
 - a stable algorithm to an ill-conditioned problem
 - an unstable algorithm to a well-conditioned problem
- ▶ Stable algorithm + well-conditioned problem \Rightarrow accurate solution!