Brief Intro to Numerical Analysis

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Numerical Analysis

- Algorithms for solving numerical problems
  - Calculus, algebra, data analysis, etc.
  - Used even if answer is not simple/elegant: “math in the real world”
- Analyze/design algorithms based on:
  - Running time, memory usage (both asymptotic and constant factors)
  - Applicability, stability, and accuracy

Why Is This Hard / Interesting?

- Problems might not have an ideal solution (independent of algorithm)
- Algorithms might give wrong answer (even with perfect real numbers)
  - Iterative, randomized, approximate
- "Numbers" in computers ≠ numbers in math
  - Limited precision and range
- Tradeoffs in accuracy, stability, and running time

Catalog of Errors

- Inherent error in data or model
  - "Garbage in, garbage out"
  - Problem is ill-posed or ill-conditioned
- Approximation errors in algorithm
  - Discretization error – e.g., too-big steps for derivative
  - Truncation error – e.g., too few terms of Taylor series
  - Convergence error – stopping iteration too early
  - Statistical error – too few random samples
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Well-Posedness and Sensitivity

- Problem is well-posed if solution
  - exists
  - is unique
  - depends continuously on problem data

  Otherwise, problem is ill-posed

- Solution may still be sensitive to input data
  - Ill-conditioned: relative change in solution much larger than that in input data

Sensitivity & Conditioning

- Some problems propagate error in bad ways
  - e.g., $y = \tan(x)$ sensitive to small changes in x near $\pi/2$
- Small error in input → huge error in solution: ill-conditioned
- Well-conditioned problems may have ill-conditioned inverses, and vice versa
  - e.g., $y = \text{atan}(x)$

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Numbers in Computers

- "Integers"
  - Mostly sane, except for limited range
- Floating point
  - Most common approximation to real numbers (alternatives: fixed point, rational)
  - Much larger range
    (e.g. $-2^{31} \ldots 2^{31}$ for 32-bit integers, vs. $-2^{127} \ldots 2^{127}$ for 32-bit floating point)
  - Lower precision (e.g. 7 digits vs. 9)
  - *Relative* precision: actual accuracy depends on size

Floating Point Numbers

- Like scientific notation: e.g., *c* is

$$2.99792458 \times 10^{8} \text{ m/s}$$

- This has the form

$$(\text{multiplier}) \times (\text{base})^{(\text{power})}$$

- In the computer,
  - Multiplier is called mantissa
  - Base is almost always 2
  - Power is called exponent

IEEE Floating Point Representation (ISO/IEEE 754 Standard)

- Using 32 bits
  - Type **`float`** in C / Java,

    `np.single` or **`np.float32`** in NumPy
  - 1 bit: sign
    (0 ⇒ positive, 1 ⇒ negative)
  - 8 bits: exponent + 127
  - 23 bits: binary fraction of the form
    1.*bbbbbbbbbbbbbbbbbbbbbbb*

- Using 64 bits
  - Type **`double`** in C / Java,
    `float` in plain Python,
    `np.double` or **`np.float64`** in NumPy
  - 1 bit: sign
    (0 ⇒ positive, 1 ⇒ negative)
  - 11 bits: exponent + 1023
  - 52 bits: binary fraction of the form
    1.*bbbbbbbbbbbbbbbbbbbbbbbbbbbb*
    bbbbbbbbbbbbbbbbbbbbbbbb

Floating Point Example

- Sign (1 bit):
  - 1 ⇒ negative
- Exponent (8 bits):
  - 10000011_B = 131
  - 131 - 127 = 4
- Mantissa (23 bits):
  - $1.10110110000000000000000_B$
  - 1 + $(1*2^{-1})+(0*2^{-2})+(1*2^{-3})+(1*2^{-4})+(0*2^{-5})+(1*2^{-6})+(1*2^{-7})$ = 1.7109375
- Number:
  - $-1.7109375 * 2^4 = -27.375$

11000001110110110000000000000000

32-bit representation

Floating Point Consequences

- "Machine epsilon": smallest positive number you can add to 1.0 and get something other than 1.0
- For 32-bit: $\varepsilon \approx 10^{-7}$
  - No such number as 1.000000001
  - Rule of thumb: "almost 7 digits of precision"
- For double: $\varepsilon \approx 2 \times 10^{-16}$
  - Rule of thumb: "not quite 16 digits of precision"
- These are all *relative* numbers

Floating Point Consequences, cont.

- Just as decimal number system can represent only certain rational numbers with finite digit count…
  - Example: 1/3 *cannot* be represented
- Binary number system can represent only certain rational numbers with finite digit count
  - Example: 1/5 *cannot* be represented
- Beware of *roundoff error*
  - Error resulting from inexact representation
  - Can accumulate

Decimal Approx	Rational Value
.3	3/10
.33	33/100
.333	333/1000
...	

Binary Approx	Rational Value
0.0	0/2
0.01	1/4
0.010	2/8
0.0011	3/16
0.00110	6/32
0.001101	13/64
0.0011010	26/128
0.00110011	51/256
...	

So What?

- Simple example: add $^1/_{10}$ to itself 10 times

```
sum = 0.0
for i in range(10):
     sum += 0.1
if sum == 1.0:
     print("All is well")
else:
     print("Yikes!")
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```
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```

Yikes!

- Result: ${}^{1}/_{10} + {}^{1}/_{10} + \ldots \neq 1$
- Reason: 0.1 can't be represented exactly in binary floating point
  - Like ${}^{1}/_{3}$ in decimal

- Rule of thumb: comparing floating point numbers for equality is "always" wrong

More Subtle Problem

- Using quadratic formula

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

  to solve $x^2 - 9999x + 1 = 0$

  – Only 4 digits: single precision should be OK, right?

- Correct answers: 0.0001… and 9998.999…
- Actual answers in single precision: 0 and 9999
  – First answer is 100% off!
  – Total cancellation in numerator because $b^2 \gg -4ac$

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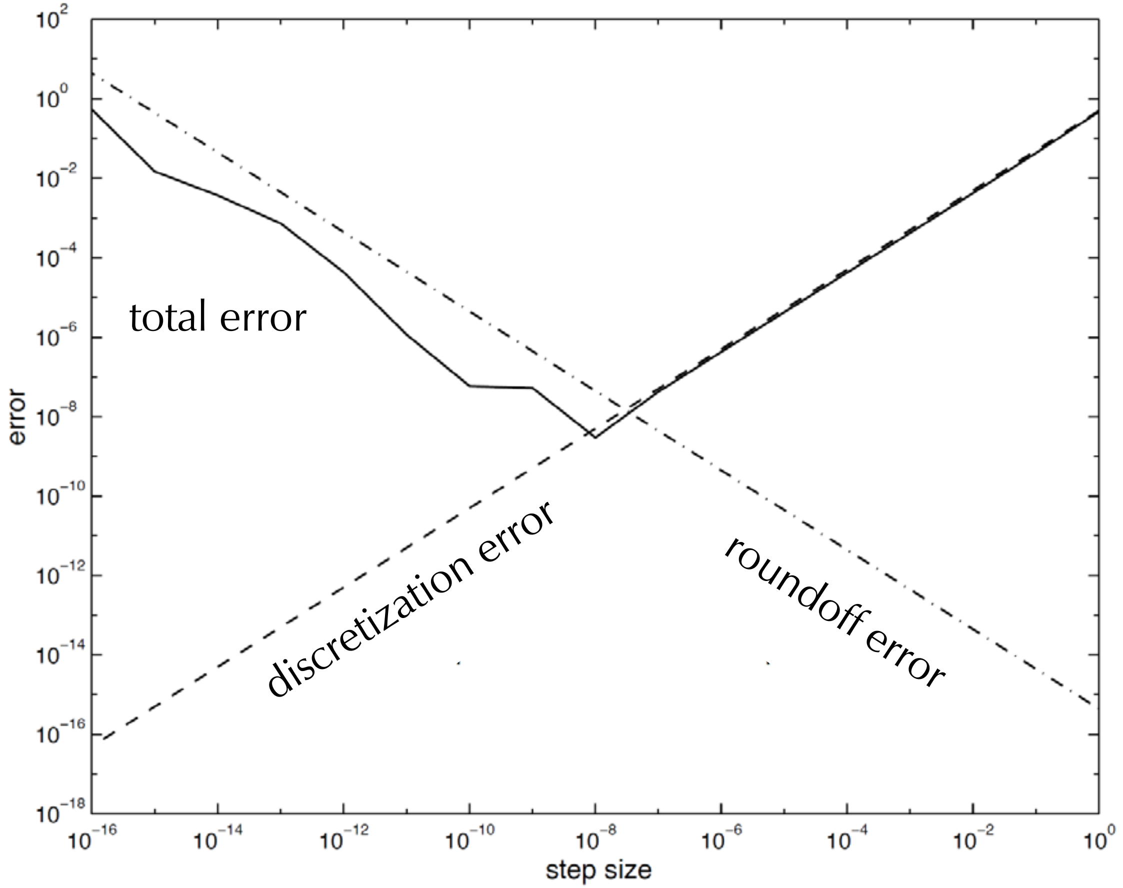
Error Tradeoff Example – Computing Derivative

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



[Heath]