COS 323: Computing for the Physical and Social Sciences

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COS 323

- Course webpage

  http://www.cs.princeton.edu/~cos323/

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What’s This Course About?

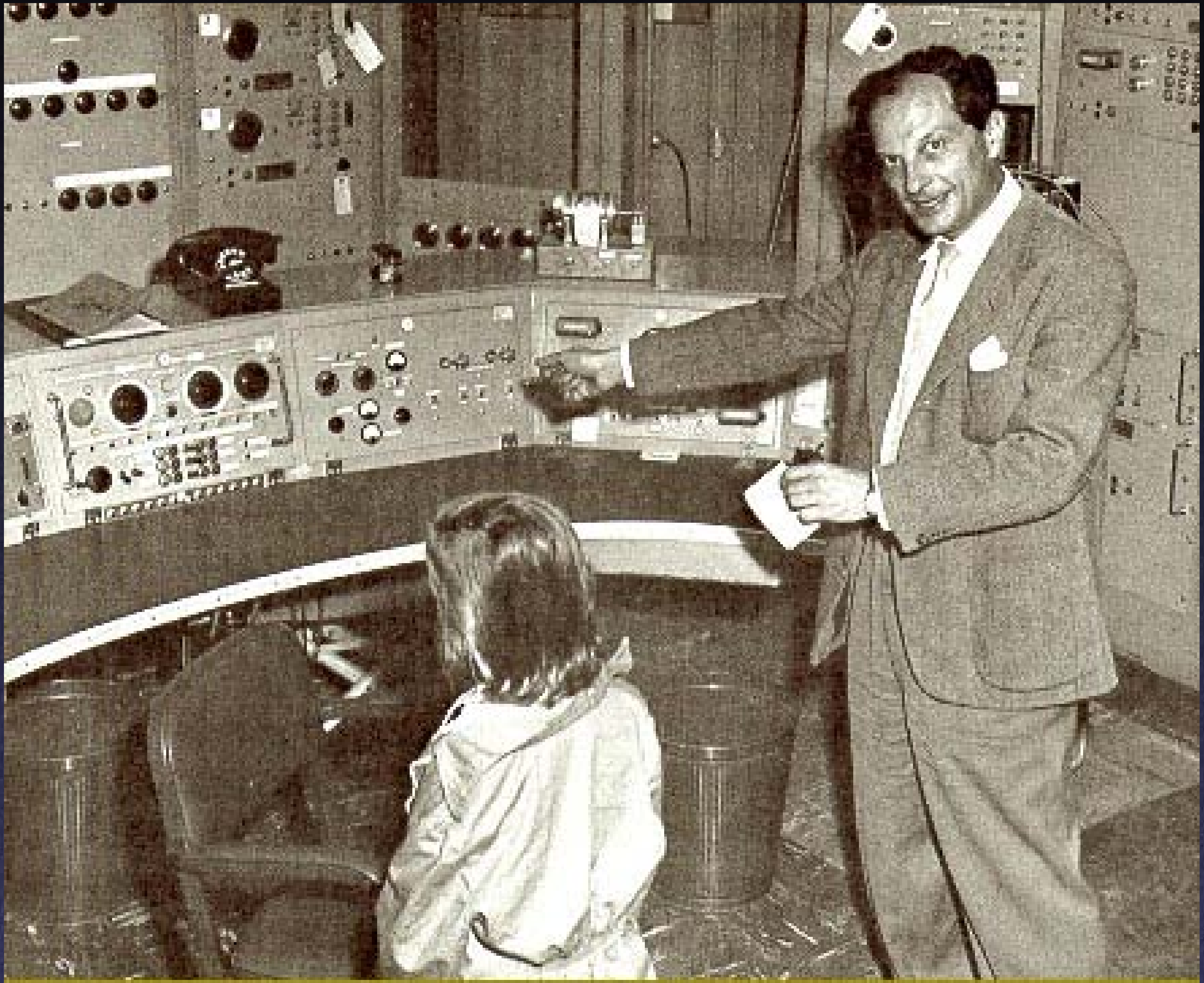
- Numerical Algorithms
- Analysis of Data
- Simulation

  - Learn through applications

Scientific Computing

Computers through the 70s/80s were used mostly to solve problems

- Before "personal" computers (!)
- Users were scientists: producers of numerical "codes" rather than consumers of "applications"



Ojciec demonstruje córce komputer MANIAC,
Los Alamos Scientific Laboratory, 1955

Stanisław Ulam with MANIAC I --- about 10^4 ops/sec

Numerical Analysis

- Algorithms for solving numerical problems
  - Calculus, algebra, data analysis, etc.
  - Applications in all scientific and engineering fields
- Analyze/design algorithms based on:
  - Running time, memory usage
    (both asymptotic and constant factors)
  - Applicability, stability, and accuracy
    for different classes of problems

Why Is This Hard/Interesting?

- "Numbers" in computers ≠ numbers in math
  - Limited precision and range
- Algorithms sometimes don't give right answer
  - Iterative, randomized, approximate
  - Unstable
- Running time / accuracy / stability tradeoffs

Numbers in Computers

- "Integers"
  - Implemented in hardware: fast
  - Mostly sane, except for limited range
- Floating point
  - Implemented in most hardware
  - Much larger range
    (e.g. -2^{31}.. 2^{31} for integers, vs. -2^{127}.. 2^{127} for FP)
  - 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

Modern Floating Point Formats

- Almost all computers use IEEE 754 standard
- "Single precision":
  - 24-bit mantissa, base = 2, 8-bit exponent, 1 bit sign
  - All fits into 32 bits (!)
- "Double precision":
  - 53-bit mantissa, base = 2, 11-bit exponent, 1 bit sign
  - All fits into 64 bits
- Sometimes also have "extended formats"

Other Number Representations

- Fixed point
  - *Absolute* accuracy doesn't vary with magnitude
  - Represent fractions to a fixed precision
  - Not supported directly in hardware, but can hack it
- "Infinite precision"
  - Integers or rationals allocated dynamically
  - Can grow up to available memory
  - No direct support in hardware, but libraries available

Consequences of Floating Point

- "Machine epsilon": smallest positive number you can add to 1.0 and get something other than 1.0
- For single precision: $\varepsilon \approx 10^{-7}$
  - 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

So What?

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

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

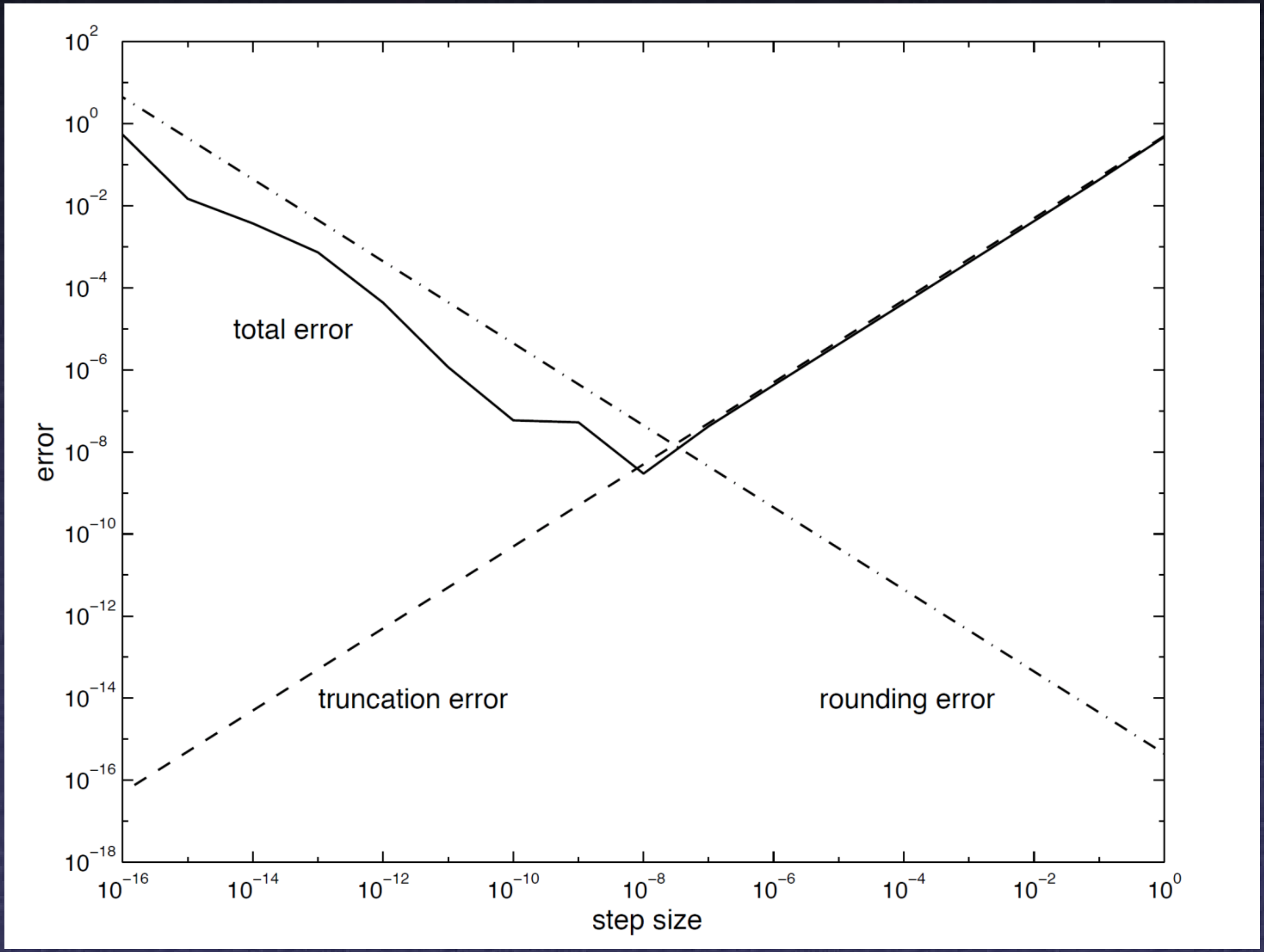
$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

  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 $b^2 >> 4ac$

Catalog of Errors

- Roundoff error – caused by limitations of floating-pointb “numbers”
- Truncation error – caused by stopping an approximate technique early
  - e.g., too few terms of Taylor series for sin(θ)
- Inherent error – limitation on data available
  - GIGO
- Statistical error – too few random samples

Error Tradeoff



[Heath]

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

[Heath]

Running Time

- Depending on algorithm, we'll look at:
  - Asymptotic analysis for noniterative algorithms (e.g., inverting an $n \times n$ matrix requires time proportional to n^3)
  - Convergence order for iterative approximate algorithms (e.g., an answer to precision δ might require iterations proportional to $1/\delta$ or $1/\delta^2$)

Simulation and Modeling

- Purposes: quantitative or qualitative prediction, development of intuition, theory testing
- Often requires changing the problem (modeling)
  - Continuous → discrete
  - Infinite → finite
  - Omitting effects, variables, dimensions
  - Q: how accurate is the resulting approximation?

Example Applications

- Population genetics
- Digital signal processing (including images/audio)
- Simulation of markets
- Classical mechanics
- Weather prediction

This Course

- Basic techniques: root finding, optimization, linear systems
- Data analysis and modeling: least squares, dimensionality reduction, visualization, statistics
- Signal processing: sampling, filtering
- Integration and differential equations
- Data analysis, fitting, and modeling
- Simulation

Mechanics

- Programming assignments
  - Typically more thought than coding
  - Some in MATLAB, some in Java
  - Analysis, writeup counts a lot!
- Final project