COS 323: Computing for the Physical and Social Sciences
COS 323

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• Course webpage:
  http://www.cs.princeton.edu/cos323
What’s This Course About?

• Numerical Algorithms
• Analysis of Data
• Simulation

  – Learn through applications
Scientific Computing

Computers, from their invention until the 70s/80s, were used mostly to solve problems

– Before “personal” computers (!)
– Users were scientists: producers of numerical “codes” rather than consumers of “applications”
Betty Jean Jennings and Fran Bilas with ENIAC I – first general-purpose electronic computer
Stanisław Ulam with MANIAC I – about $10^4$ ops/sec
The Best of the 20th Century: Editors Name Top 10 Algorithms

By Barry A. Cipra

Algós is the Greek word for pain. Algorit is Latin, to be cold. Neither is the root for algorithm, which stems instead from al-Khwārizmī, the name of the ninth-century Arab scholar whose book al-jabr wa’l-muqabalah devoted into today’s high school algebra textbooks. Al-Khwārizmī stressed the importance of methodical procedures for solving problems. Were he around today, he’d no doubt be impressed by the advances in his eponymous approach.

Some of the very best algorithms of the computer age are highlighted in the January/February 2000 issue of Computing in Science & Engineering, a joint publication of the American Institute of Physics and the IEEE Computer Society. Guest editors Jack Dongarra of the University of Tennessee and Oak Ridge National Laboratory and Francis Sullivan of the Center for Computing Sciences at the Institute for Defense Analyses put together a list they call the “Top Ten Algorithms of the Century.”

“We tried to assemble the 10 algorithms with the greatest influence on the development and practice of science and engineering in the 20th century,” Dongarra and Sullivan write. As with any top-10 list, their selections—and non-selections—are bound to be controversial; they acknowledge. When it comes to picking the algorithmic best, there seems to be no best algorithm.

Without further ado, here’s the USEN top-10 list, in chronological order. (Dates and names associated with the algorithms should be read as first-order approximations. Most algorithms take shape over time, with many contributors.)

1946: John von Neumann, Stan Ulam, and Nick Metropolis, all at the Los Alamos Scientific Laboratory, cook up the Metropolis algorithm, also known as the Monte Carlo method.

The Metropolis algorithm aims to obtain approximate solutions to numerical problems with unmanageably many degrees of freedom and to combinatorial problems of factorial size, by mimicking a random process. Given the digital computer’s reputation for deterministic calculation, it’s fitting that one of its earliest applications was the generation of random numbers.

1947: George Danzig, at the RAND Corporation, creates the simplex method for linear programming.

In terms of widespread application, Danzig’s algorithm is one of the most successful of all time: Linear programming dominates the world of industry, where economic survival depends on the ability to optimize within budgetary and other constraints. Of course the “real” problems of industry are often nonlinear; the use of linear programming is sometimes dictated by the computational budget. The simplex method is an elegant way of arriving at optimal answers. Although theoretically susceptible to exponential delays, the algorithm in practice is highly efficient—which in itself says something interesting about the nature of computation.

1950: Magnus Hestenes, Eduard Stiefel, and Cornelius Lanczos, all from the Institute for Numerical Analysis at the National Bureau of Standards, initiate the development of Krylov subspace iteration methods.

These algorithms address the seemingly simple task of solving equations of the form $Ax = b$. The catch, of course, is that $A$ is a huge $n \times n$ matrix, so that the algebraic answer $x = b/A$ is too easy to compute.

(Indeed, matrix “division” is not a particularly useful concept.) Iterative methods—such as solving equations of the form $K_{n-1}x = K_n + b - A_0 x$ with a simpler matrix $A$ that’s ideally “close” to $A$—lead to the study of Krylov subspaces. Named for the Russian mathematician Nikolai Krylov, Krylov subspaces are spanned by powers of a matrix applied to an initial “remainder” vector $r_0 = b - A_0 x$. Lanczos found a nifty way to generate an orthogonal basis for such a subspace when the matrix is symmetric. Hestenes and Stiefel proposed an even niftier method, known as the conjugate gradient method, for systems that are both symmetric and positive definite. Over the last 50 years, numerous researchers have improved and extended these algorithms. The current suit includes techniques for non-symmetric systems, with acronyms like GMRES and Bi-CGSTAB, (GMRES and Bi-CGSTAB premiered in SIAM Journal on Scientific and Statistical Computing, in 1986 and 1992, respectively.)

1951: Alston Householder of Oak Ridge National Laboratory formalizes the decompositional approach to matrix computations.

The ability to factor matrices into triangular, diagonal, orthogonal, and other special forms has turned out to be extremely useful. The decompositional approach has enabled software developers to produce flexible and efficient matrix packages. It also facilitates the analysis of rounding errors, one of the big bogeys of numerical linear algebra. (In 1951, James Wilkinson of the National Physical Laboratory in London published a seminal paper in the Journal of the ACM, titled “Error Analysis of Direct Methods of Matrix Inversion,” based on the LU decomposition of a matrix as a product of lower and upper triangular factors.)

1957: John Backus leads a team at IBM in developing the Fortran optimizing compiler.

The creation of Fortran may rank as the single most important event in the history of computer programming. Finally, scientists
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Some challenging but important & common problems…
Root finding

E.g., estimate molal volume of a gas at a given pressure & temperature using van der Waals:

\[(p + a/v^2)(v-b) = RT\]
Solving systems of linear equations

e.g., determine the current at each point in an electrical circuit, using Kirchoff’s rule and Ohm’s law.
Optimization

E.g., design the cheapest wastewater treatment given geography, pollution patterns, and environmental regulations.
Integration

E.g., compute the work performed in a mechanical system given a variable force
How do we solve these problems?
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?

• “Numbers” in computers ≠ numbers in math
  – Limited precision and range

• Algorithms sometimes don’t give right answer
  – Iterative, randomized, approximate
  – Unstable

• Tradeoffs in accuracy, stability, and running time
Numbers in Computers

and their consequences
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. $-2^{31} \ldots 2^{31}$ for integers, vs. $-2^{127} \ldots 2^{127}$ 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 (!) – mantissa has implicit leading 1
- “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: $\epsilon \approx 10^{-7}$
    – No such number as 1.000000001
    – Rule of thumb: “almost 7 digits of precision”
  • For double: $\epsilon \approx 2 \times 10^{-16}$
    – Rule of thumb: “not quite 16 digits of precision”
• These are all relative numbers
So What?

- Simple example: add $\frac{1}{10}$ to itself 10 times
Yikes!

- **Result:** $\frac{1}{10} + \frac{1}{10} + \ldots \neq 1$
- **Reason:** 0.1 can’t be represented exactly in binary floating point
  - Like $\frac{1}{3}$ 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 \( b^2 >> 4ac \)
Accuracy

error is inevitable
Catalog of Errors

• **Inherent error** in data or model
  – “Garbage in, garbage out”

• **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

• **Roundoff error** due to floating-point “numbers”
Error Tradeoff Example – Computing Derivative

\[ f'(x) \approx \frac{f(x + h) - f(x)}{h} \]
Other Considerations of Problem Formulation & Algorithm

Sensitivity & conditioning, stability & accuracy
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 $\rightarrow$ huge error in solution: ill-conditioned

• Well-conditioned problems may have ill-conditioned inverses, and vice versa
  – e.g., $y = \arctan(x)$
Stability & Accuracy

• A **stable** algorithm introduces “only a little” computational error
  – Solution is an exact to solution to a “nearby” problem
  – Computational error is indistinguishable from a small data error

• An **accurate** algorithm produces a solution that is close to the true solution

  stable algorithm + well-conditioned problem → accurate solution
Running time
Running Time

• Depending on algorithm, we’ll look at:
  – **Asymptotic analysis** for noniterative algorithms (e.g., most methods for inverting an $n \times n$ matrix require time proportional to $n^3$)
  – **Convergence order** for iterative approximate algorithms (e.g., an answer to precision $\delta$ might require iterations proportional to $1/\delta$ or $1/\delta^2$)
Course Overview
Basic Techniques

- root finding
- optimization
- linear systems
- integration
- ODEs, PDEs
- Plus…
Signal Analysis & Signal Processing
Data Analysis and Model Fitting

Note: 1972 to 2006. Sample size: 41,795. Each circle represents an income range of $2,000 (e.g., $10,001 to $12,000), in 2006$. Its diameter is proportional to the number of people in that range.

Source: My calculations from General Social Survey data.
Simulation

Zombie Infection Simulation v2.3 - The Original

Simulation Rules
Zombies are grey, move very slowly and change direction randomly and frequently unless they can see something moving in front of them, in which case they start walking towards it. After a while they get bored and wander randomly again.

If a zombie finds a survivor standing directly in front of it, it bites and infects them; the survivor immediately joins the ranks of the undead.

Survivors are pink and run five times as fast as zombies, occasionally changing direction at random. If they see a zombie directly in front of them, they turn around and panic.

Panicked survivors are bright pink and run twice as fast as other survivors. If a survivor sees another panicked survivor, it starts panicking as well. A panicked survivor who has seen nothing to panic about for a while will calm down again.

Controls
- Press g to toggle between grey and green zombies.
- Press s to alter the simulation speed.
- Press space to uninfest all but one zombie.
- Press z or reload the page to reset to a new city.
- Press x and z to adjust population (this also resets the city).
- Press p to toggle complete panic (as in v1).

(You'll need to click on the Java window before it'll accept keypresses.)

Links
The Zombie Infection Simulation was built with Processing (for which you can download and play here:
- Matt Carder's modified version
- Alan Gordon's 3D version
- Harding's miku-dropping game variant
- Pretty Little Incredible Zombie Machine

500
450
400
350
300
250
200
150
100
50
0

Population Values (1000%)

0 2 4 6 8 10
Time

Susceptibles
Zombies
Simulation

“ In summary, a zombie outbreak is likely to lead to the collapse of civilization, unless it is dealt with quickly. […] As seen in the movies, it is imperative that zombies are dealt with quickly, or else we are all in a great deal of trouble.”

– Munz et al., Infectious Disease Modelling Research Progress, 2009
Visualization
Course Information
Mechanics

• 5 programming assignments: 50%
  – Typically more thought than coding
  – MATLAB
  – Analysis, writeup counts a lot!

• 2 in-class exams: 25%
  – Short-answer, focusing on topics not covered in programming assignments

• Final project (in groups): 25%
To Do

- Course webpage:
  
  http://www.cs.princeton.edu/cos323

- MATLAB:
  - Install it now – instructions on webpage
  - Engineering school tutorial, or we’ll do our own

- Assignment 0:
  - Available on course web page, due Tuesday Sep 24

- Sign up for Piazza