Fundamental Concepts in Computational and Applied Mathematics

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Fall 2014

Recap

- Beware catastrophic cancellation – know the limits of precision
- Learn about the conditioning of your problem
- Choose algorithms known to be stable so as to not introduce any more loss of precision than necessary
    - Conditioning is fundamentally a characteristic of the problem while
    - Stability is related to algorithms

Dense Linear Algebra methods

Let $x, y \in R^N$ and $A \in R^{N \times N}$

- Basic Linear Algebra
  - dot products: $x^T y$
  - matvec: Ax
  - saxpy: $ax + y$
  - Solve $Ax = b$
  - Solve $Ax = \lambda x$

Rule of Thumb

We cannot solve anything except linear systems

Warning

Never (EVER) solve a linear system by calculating the inverse of the matrix and multiplying!

Linear Algebra methods

- Various standard methods
  - LU
  - Cholesky
  - QR
  - SVD
- All have advantages and disadvantages – learn about them!
- Your choice will depend on the application, software availability, and time constraints

Some Useful Definitions

Definition (Condition Number)

The condition number of a matrix A is given by: $\kappa(A) = ||A|| \cdot ||A^{-1}||$

Definition (Residual)

The residual of linear system is given by $b - Ax$

Definition (Machine Precisions)

The machine precision is denoted by μ

Definition

A problem is said to be ill-conditioned if $\mu\kappa_\infty(A) \approx 1$

Fun Facts

- Gaussian elimination always produces solutions with relatively small residuals (minor caveats)
- Best possible error bound for solving a system of linear equations can be given by

$$\frac{||x - \hat{x}||_\infty}{||x||_\infty} \leq 4\mu\kappa_\infty(A) \tag{1}$$

where μ is machine precision of the computer.

Stable or Unstable? Well conditioned or ill-conditioned?

Consider $Ax = b$ where

$$A = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

Comparison of algorithms

Table: Number of iterations to reduce error by 10^{-3}.

$\kappa(A)$	Value	iter
1	0.0	1
10^2	0.82	15
10^4	0.98	150
10^8	0.9998	15,000

LU with Partial Pivoting

- Can show that LU/PP generates the exact solution to a perturbed problem $(A + E)x = b$, such that

$$||E||_\infty \leq 8n^3 \rho ||A||_\infty \mu \tag{2}$$

- The growth factor ρ can grow exponentially, but in practice is usually of order 10
- Consider the residual, $b - Ax$:

Summary

- A
- B
- C

References

- **Methods of Conjugate Gradients for Solving Linear Systems**, Magnus R. Hestenes and Eduard Stiefel, J. Res. of NBS, Vol. 49, No. 6, Dec. 1952.
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