Fundamental Concepts in Computational and Applied Mathematics

Juan Meza

School of Natural Sciences

University of California, Merced

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

- Basic Linear Algebra
  - dot products, matvec, sappy
  - Solve $Ax = b$
  - Solve $Ax = \lambda x$

Rule of Thumb

We cannot solve anything except linear systems

- Almost all discretization methods you will encounter will have a special structure

- Sparse methods take advantage of special structure in matrices to improve computational efficiency

Stationary Iterative Methods

- Based on splitting techniques
- Widely used in engineering, but have been superseded by more modern techniques
- Still useful in certain contexts, e.g. preconditioners

Basic Method

Consider $Ax = b$

Let $A = L + D + U$ and then "split" the matrix A such that

$$(L + D)x^{k+1} = b - Ux^k, k = 0, \ldots$$

or

$$
\begin{aligned}
Mx^{k+1} &= b + Nx^k, k = 0, \ldots & (1) \\
x^{k+1} &= M^{-1}b + M^{-1}Nx^k, & (2) \\
x^{k+1} &= Gx^k + c & (3)
\end{aligned}
$$

where $G = M^{-1}N, c = M^{-1}b$

Useful Facts

Fact 1: If we use the SIM in equation (3) $x^k \to \hat{x} \iff \rho(G) < 1$

Fact 2: $e^{k+1} = Ge^k$

Fact 3: Many matrices resulting from problems in S&E satisfy $\rho(G) < 1$

Finite Precision

- In exact arithmetic the CG method will converge to the solution of $Ax = b$

- Sadly, in finite precision, roundoff error will contaminate the solution

- And even in the exact case, what does this mean for a system with dimension 1M or 1B

Krylov subspace methods

CG is an example of what we now call a Krylov space method

- Definition: A *Krylov* space is defined by:

$$\mathcal{K}_k(A, b) = span\{b, Ab, A^2 b, A^3 b, \ldots, A^{k-1} b\}$$

  Idea: Choose your iterate, x^k, such that it belongs to the Krylov space and it minimizes the distance between it and $\hat{x}$

CG Convergence Rate

Can show that

$$||x^k - \hat{x}||_A \leq 2 \left(\frac{\sqrt{\kappa(A)} - 1}{\sqrt{\kappa(A)} + 1} \right)^k ||x^0 - \hat{x}||_A \qquad (4)$$

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

Preconditioning Idea

Discussion

- Why precondition?
- What should the general idea be?
- How would you go about doing that?

Summary

- Sparse methods can be used to take advantage of special structure
- Iterative methods are the dominant form of solving systems of linear equations in modern day applications
- Most iterative methods must be preconditioned to be effective

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.

- **Matrix Computations, 3rd Ed.**, Gene H. Golub and Charles F. Van Loan, Johns Hopkins, 1996.

- **Iterative Methods for Linear and Nonlinear Equations**, C.T. Kelley, SIAM, 1995.