

Lecture 14: CMSC 878R/AMSC698R

Iterative Methods and the FMM

Outline

- Direct Solution of Linear Systems
 - Inverse, LU decomposition, Cholesky, SVD, etc.
- Iterative methods for linear systems
 - Why?
- Matrix splittings and fixed-point schemes
 - SOR, Jacobi, Gauss Seidel, etc.
- Krylov Methods
 - Conjugate Gradient, GMRES
- Convergence and Preconditioning
- Eigenvalue Problems
- Iterative methods for eigenvalue problems

Preliminary Comments

- FMM accelerates matrix-vector multiplication
- However, most problems require solution of linear systems
- Goal: See how linear systems can be solved using FMM
- Take home message
 - Iterative methods require matrix vector products
 - Can be written as FMM
 - Some methods can be guaranteed to converge in N steps
 - With good guess and clever algorithms may converge much faster
- Philosophy:
 - In general it is better to be a “consumer” of linear algebra
 - Use canned software which asks you to provide a product routine
 - However, with FMM there may not be “canned” or “tuned” software available and we may have to develop our own

Direct Solution of linear systems

$$\mathbf{Ax}=\mathbf{b} \rightarrow \mathbf{x}=\mathbf{A}^{-1}\mathbf{b}$$

- Almost never a good idea to construct inverse to solve
- Computing inverse is more expensive than solving system
 - Computing inverse leads to loss of precision
- Exceptions
 - Analytical expression for inverse can be obtained, e.g.,

Sherman Morrison Woodbury

$$(\mathbf{A} + \mathbf{u} \otimes \mathbf{v})^{-1} = \mathbf{A}^{-1} - \frac{(\mathbf{A}^{-1}\mathbf{u}) \otimes (\mathbf{v} \cdot \mathbf{A}^{-1})}{1 + \lambda}, \quad \lambda \equiv \mathbf{v} \cdot \mathbf{A}^{-1}\mathbf{u}.$$

Woodbury Formula

$$(\mathbf{A} + \mathbf{UV}^T)^{-1} = \mathbf{A}^{-1} - [\mathbf{A}^{-1}\mathbf{U}(1 + \mathbf{V}^T\mathbf{A}^{-1}\mathbf{U})^{-1}\mathbf{V}^T\mathbf{A}^{-1}].$$

Direct solutions (2)

- Consumer level – Use LAPACK or MATLAB,
– (vectorized, cache-optimized, etc.) -- ATLAS
- For non symmetric matrices use LU decomposition
- LU decomposition $\simeq N^3/3$ operations
- Backsubstitution $O(N^2)$
- For symmetric matrices use Cholesky decomposition $\simeq N^3/6$ operations
- All these methods require storage of the matrix and for dense matrices have memory complexity $O(N^2)$

References

- C.T. Kelley, “Iterative methods for Linear and Nonlinear Equations, SIAM, 1995)
- J. Shewchuck, “An Introduction to the Conjugate Gradient Method Without the Agonizing Pain”
(downloadable from <http://www-2.cs.cmu.edu/~jrs/jrspapers.html>)
- “Templates for the solution of linear systems: Building Blocks and Iterative Methods,” Barrett et al, SIAM
(downloadable at http://www.netlib.org/linalg/html_templates/Templates.html)
- Yousef Saad has two good books online
Numerical Methods for Large Eigenvalue Problems
Iterative methods for sparse linear systems.
(downloadable at <http://www-users.cs.umn.edu/~saad/books.html>)

Iterative Methods: Notation

$$Ax = b$$

- A is a nonsingular $N \times N$ matrix, $x, b \in \mathbb{R}^N$
- Ax can be calculated using FMM
- x^* is the solution to be found. $x^* = A^{-1}b \in \mathbb{R}^N$
- Definitions

Norm of A

$$\|A\| = \max_{\|x\|=1} \|Ax\|$$

Condition number of A

$$\kappa(A) = \|A\| \|A^{-1}\|$$

Residual

$$r = b - Ax$$

Error

$$e = x - x^*$$

Fixed point iteration

- In fixed point iteration we write $x=Mx$
- If M is a contraction ($\|M\| < 1$) then following converges
 - Start with guess x_0
 - Generate successive estimates $x_k=M x_{k-1}$

- How to write our equation as a fixed point scheme?

$$Ax=Ix + (A-I)x =b$$

- So, $I x = (I-A)x +b$
- (Richardson iteration) $x_{k+1} = (I-A)x_k +b$
- For convergence we require $\|I-A\| < 1$
- Iteration Matrix M here is $\|I-A\|$

Left Preconditioning

- What if $\|I-A\| = \text{or} > 1$?
- Let B be another matrix.
- Then $BAx = Ix + (BA-I)x = Bb$
- So,
$$Ix = (I-BA)x + Bb$$
- (Richardson iteration)
$$x_{k+1} = (I-BA)x_k + Bb$$
- For convergence we require $\|I-BA\| < 1$
- If B is simple (e.g., diagonal) this is easy to compute
- Iteration matrix $M = \|I-BA\|$
- This is left preconditioning
- Can also device right preconditioning

Right Preconditioning

- Let B be another matrix.
- Let $AB^{-1}u=b$ and $u=Bx$
- Then $AB^{-1}(Bx)=b$
- So,
$$x_{k+1} = x_k - AB^{-1}u_k + b$$
- Compute
$$u_k = Bx_k$$

Classical fixed point methods

- Write $A=A_1+A_2$
- Then iteration becomes $x_{k+1} = A_1^{-1}(b - A_2x_k)$
 - For convergence $\|A_1^{-1}A_2\| < 1$
 - A_1^{-1} should be easy to compute
 - In addition the FMM should be used to compute A_2x_k
- Jacobi iteration $A_1=D$ $A_2=L+U$
 - A_1^{-1} is easy to compute (1/ entries along diagonal)
 - This is easy to compute with the FMM
 - At element level $(x_{k+1})_i = a_{ii}^{-1} \left(b_i - \sum_{j \neq i} a_{ij} (x_k)_j \right)$
- Other classical iterations (Gauss-Seidel, SOR, etc. are harder to write in a way that FMM can be used).

Krylov methods

- Different class of methods
- Do not involve an iteration matrix
- Motivation: Say in functional space we are at a point x_0 and we want to reach the solution x^*
- Can do it by taking steps along some directions
- Method of steepest descent
- Define function $f(x)$ $f(x) = \frac{1}{2}x^t Ax - b^t x$
- So minimum of $f(x)$ is attained at $\nabla f(x)=0$

$$\nabla f = \frac{1}{2} (A + A^t) x - b = 0$$

$$\frac{1}{2} (A + A^t) x = b \quad \text{or} \quad Ax = b$$

for symmetric A

Steepest descent

- So finding minimizer of the quadratic form gives a solution
- Start at guess x_0 , take a step along $-\nabla f(x_0)$

$$\nabla f(x_0) = Ax_0 - b = -r_0$$

$$x_1 = x_0 + \alpha r_0$$

- How big should the step α be?
- We can find α that minimizes $f(x_0 + \alpha r_0)$

$$\frac{d}{d\alpha} f(x_0 + \alpha r_0) = r_0 \cdot \nabla f|_{x=x_0 + \alpha r_0}$$

- So if α should be chosen so that r_0 is orthogonal to ∇f

- Can show
$$\alpha = \frac{r_0^t r_0}{r_0^t A r_0}$$

Steepest Descent method

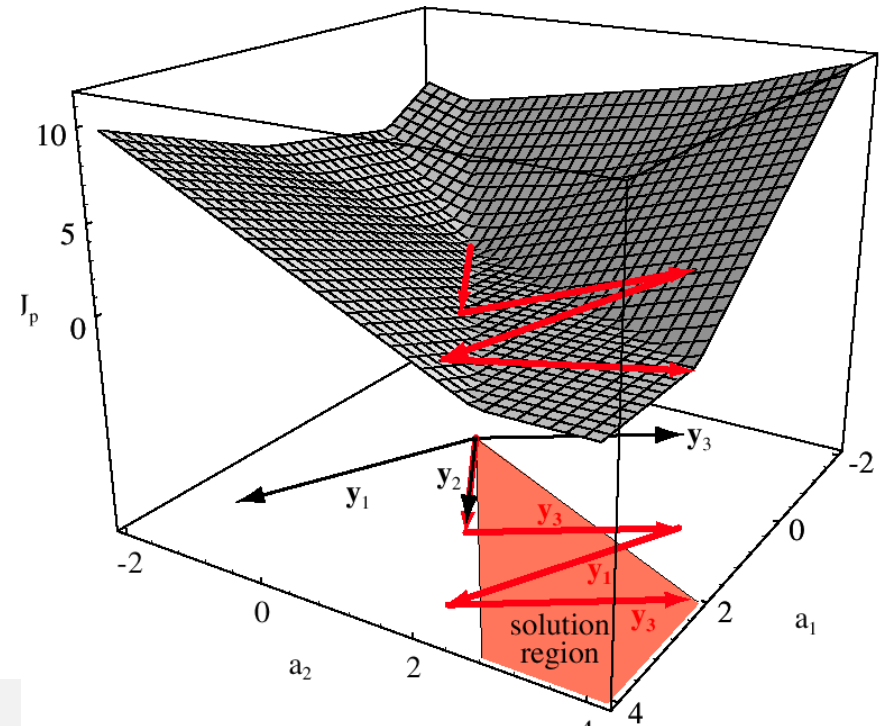
- Putting things together
- Requires two matrix vector products with A per iteration
- Can reduce one
- Can convert last equation to
- only need calculate Ar_i
- What about convergence?
- Can show at k th iteration

$$\|e_k\|_A \leq \left(\frac{\kappa(A) - 1}{\kappa(A) + 1} \right)^k \|e_0\|_A \quad \text{where} \quad \kappa(A) = \lambda_{max} / \lambda_{min}$$

$$r(i) = b - Ax(i),$$

$$\alpha(i) = \frac{r(i)^T r(i)}{r(i)^T A r(i)},$$

$$x(i+1) = x(i) + \alpha(i) r(i).$$



Conjugate Gradient

- Instead of minimizing each time along gradient, choose a set of basis directions to minimize along
- Choose these directions to be from the Krylov subspace
- Definition: Krylov subspace $\mathcal{K}_k = \text{span}(r_0, Ar_0, \dots, A^{k-1}r_0)$
- Definition: Energy or A -norm of a vector $\|x\|_A = (x^t Ax)^{1/2}$
- Idea of conjugate gradient method
 - Generate Krylov subspace directions, and take a step that minimizes the A norm of the residual along this direction
- Let search direction be at step $k+1$ be d_{k+1}
- We require $f(x_k + \alpha_{k+1} d_{k+1})$ is minimized along direction
- Conjugacy property $d_{k+1}^t A K^k = 0$

CG Algorithm

- Each iteration requires computation of one matrix vector product Ad_i
- Guaranteed to converge after N iterations (for exact arithmetic)
- So FMM guaranteed to solve equations in $O(N^2)$ time
- Method does not require storage of any of the Krylov basis vectors
- Trivial to add preconditioning
- Implemented in Matlab as **pcg**

$$d_{(0)} = r_{(0)} = b - Ax_{(0)},$$

$$\alpha_{(i)} = \frac{r_{(i)}^T r_{(i)}}{d_{(i)}^T Ad_{(i)}} \quad (1)$$

$$x_{(i+1)} = x_{(i)} + \alpha_{(i)} d_{(i)},$$

$$r_{(i+1)} = r_{(i)} - \alpha_{(i)} Ad_{(i)},$$

$$\beta_{(i+1)} = \frac{r_{(i+1)}^T r_{(i+1)}}{r_{(i)}^T r_{(i)}},$$

$$d_{(i+1)} = r_{(i+1)} + \beta_{(i+1)} d_{(i)}.$$

Convergence of CG

- If there are k distinct eigenvalues of A , then CG converges in at most k iterations to the exact solution (in exact arithmetic)
- Usually we go to $\|b - Ax_k\|_2 \leq \eta \|b\|_2$

$$\|x_* - x_m\|_A \leq 2 \left[\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right]^m \|x_* - x_0\|_A.$$

- Converges quickly

Non symmetric matrices

- Can't apply CG to nonsymmetric matrices
- One simple solution – CGNR j
 - convert system to a symmetric system

$$A^tAx=A^tb$$

- However we will need two matrix vector multiplies per iteration
- Also, if A is poorly conditioned then A^tA is even more poorly conditioned (condition number is squared)
- However the method requires no storage of Krylov basis.

GMRES

- Instead of requiring minimization along conjugate direction, minimize residual in a subspace
- Krylov subspace $\mathcal{K}_k = \text{span}(r_0, Ar_0, \dots, A^{k-1}r_0)$
- Require x to minimize $\|b - Ax\|_2 \quad \forall x \text{ in } x_0 + \mathcal{K}^k$
- Construct basis


```

w(i) = Av(i)
for k = 1, ..., i
    w(i) = w(i) - (w(i), v(k))v(k)
end
v(i+1) = w(i) / ||w(i)||
      
```
- Then require that each $x^{(i)} = x^{(0)} + y_1 v^{(1)} + \dots + y_i v^{(i)}$, satisfies minimum $\|b - Ax^{(i)}\|$
- Can be done by simple minimization
- Implemented as a black-box in Matlab

Bi Conjugate methods

- Since A is non symmetric, A^t and A have different eigenvalues and eigenvectors
- Form the Krylov basis of A^t for some vector g (usually equal to r_0) $\bar{\mathcal{K}}_k = \text{span}(r_0, A^t r_0, \dots, (A^t)^{k-1} r_0)$
- Minimize successively along directions so that $p_k A d_l = 0$
- Storage cost is lower ... Bi-CGSTAB

Eigenvalue problems: Power Iteration

- Computes the dominant eigen value and eigen vector of a given matrix A .
- $x_k = Ax_{k-1}$ converges to the dominant eigen vector v_1
- Ratio of values of given component of x_k from one iteration to next converges to the dominant eigen value λ_1 .
- If two eigen values are equal may converge to a linear combination of the corresponding eigen vectors.
- To prevent overflow or underflow use Normalized power iteration. $x_k = Ax_{k-1}$ $x_k = x_k / \|x_k\|_\infty$.
- Can do power iteration with shift to increase convergence rate.

Research: Preconditioning for the FMM

- In all these methods (especially at the large sizes where the FMM is used), iterative methods are slowly convergent
- Unless iteration converges relatively quickly (less than 100 iterations), it may not be practically useful
- Condition number is important in quantifying convergence
 - Project for estimating condition number
- Most preconditioners were invented to speed up sparse matrix computations
- Take $O(N^2)$ time for dense matrices (or too slow)
- Goal: Fashion good preconditioners for the FMM

Preconditioner cost

- To be effective with the FMM the preconditioner cost should be $O(N \log N)$ or less
- Otherwise we negate the advantage of the FMM
- We present results for two preconditioners we have used
 - First, for highly oscillatory kernel --- multiple scattering with the Helmholtz equation
 - Second, we accelerate a highly successful preconditioner developed by Faul, Powell and Goodsell (2005), but which has a complexity of $O(N^2)$ to $O(N \log N)$.