Iterative methods for Linear System

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Outline

•Basics:

- Matrices and their properties
- Eigenvalues, Condition Number
- •Iterative Methods
 - Direct and Indirect Methods
- •Krylov Subspace Methods
 - Ritz Galerkin: CG
 - Minimum Residual Approach : GMRES/MINRES
 - Petrov-Gaelerkin Method: BiCG, QMR, CGS

Basics

•Linear system of equations

Ax = b

•A Hermitian matrix (or self-adjoint matrix) is a square matrix with complex entries which is equal to its own conjugate transpose, that is, the element in the *i*th row and *j*th column is equal to the complex conjugate of the element in the *j*th row and *i*th column, for all indices *i* and *j*

$$\mathbf{A} = \begin{bmatrix} 3 & 2+i \\ 2-i & 1 \end{bmatrix}$$

- *Symmetric* if $a_{ii} = a_{ii}$
- **Positive definite if, for every nonzero vector x**
- **Positive uspan X**¹**Ax** < 5 **Quadratic form: f**(**x**) = $\frac{1}{2}$ **x**^T**Ax b**^T**x** + **c Gradient of Quadratic form: f**'(**x**) = $\begin{bmatrix} \frac{\partial}{\partial x_1} f(\mathbf{x}) \\ \vdots \\ \frac{\partial}{\partial x_n} f(\mathbf{x}) \end{bmatrix} = \frac{1}{2}$ **A**^T**x** + $\frac{1}{2}$ **Ax b**

Various quadratic forms



Various quadratic forms





Eigenvalues and Eigenvectors

For any $n \times n$ matrix **A**, a scalar λ and a nonzero vector **v** that satisfy the equation

 $Av = \lambda v$

are said to be the eigenvalue and the eigenvector of A.

- •If the matrix is *symmetric*, then the following properties hold:
- (a) the eigenvalues of A are real
- (b) eigenvectors associated with distinct eigenvalues are orthogonal
- •The matrix **A** is *positive definite* (or positive semidefinite) if and only if all eigenvalues of **A** are positive (or nonnegative).

Eigenvalues and Eigenvectors

Why should we care about the eigenvalues? *Iterative methods often depend on applying A to a vector over and over again*:



Some more terms:

Spectral radius of a matrix is: $\rho(\mathbf{A}) = \max |\lambda_i|$ **Condition number** is : $K = \frac{\lambda_{max}}{\lambda_{min}}$

Error: $\mathbf{e} = \mathbf{x}_{\text{exact}} - \mathbf{x}_{\text{app}}$

Residual: $r = b-A.x_{app}$

Preconditioning

Preconditioning is a technique for improving the condition number of a matrix. Suppose that M is a symmetric, positive-definite matrix that approximates A, but is easier to invert. We can solve Ax = bindirectly by solving

$$M^{-1}Ax = M^{-1}b$$

Type of preconditioners:

•Perfect preconditioner M = A

Condition number =1 -> solution in one iteration

but Mx=b is not useful preconditioner •Diagonal preconditioner, trivial to invert but mediocre •Incomplete Cholesky: $A \rightarrow LL^{T}$

• Not always stable

Stationary and non-stationary methods

Stationary methods for Ax = b: $x^{(k+1)} = Rx^{(k)} + c$

neither R or c depend upon the iteration counter k.

•Splitting of A A = M - K with nonsingular M Ax = Mx - Kx = b $x = M^{-1}Kx - M^{-1}b = Rx + c$ Examples:

- Jacobi method
- Gauss-Seidel
- Successive Overrelaxation (SOR)

Jacobi Method

•Splitting for Jacobi Method, M=D and K=L+U $x^{(k+1)} = D^{-1}((L+U)x^{(k)}+b)$

solve for x_i from equation *i*, assuming other entries fixed

for i = 1 to n
for j = 1 to n
$$u_{i,j}^{(k+1)} = (u_{i-1,j}^{(k)} + u_{i+1,j}^{(k)} + u_{i,j-1}^{(k)} + u_{i,j+1}^{(k)})/4$$

Gauss-Siedel Method and SOR(Successive-Over-Relaxation)

Splitting for Jacobi Method, M=D-L and K=U $x^{(k+1)} = (D-L)^{-1}(Ux^{(k)}+b)$

While looping over the equations, use the most recent values x_i for i = 1 to n for j = 1 to n $u_{i,j}^{(k+1)} = (u_{i-1,j}^{(k+1)} + u_{i+1,j}^{(k)} + u_{i,j-1}^{(k+1)} + u_{i,j+1}^{(k)})/4$

Splitting for SOR:

$$x^{(k+1)} = \omega \underline{x}_{i}^{(k+1)} + (1-\omega) x_{i}^{(k)}$$
OR
$$(k+1) = (D - D) l(-D) + (1-\omega)$$

 $x^{(k+1)} = (D - \omega L)^{-1} (\omega U + (1 - \omega) D) x^{(k)} + \omega (D - \omega L)^{-1} b$

Stationary and non-stationary methods

•Non-stationary methods:

- The constant are computed by taking inner products of residual or other vectors arising from the iterative method
- Examples:
- Conjugate gradient (CG)
- Minimum Residual (MINRES)
- Generalized Minimal Residual (GMRES)
- BiConjugate Gradient (BiCG)
- Quasi Minimal Residual (QMR)
- Conjugate Gradient Squared (CGS)

Descent Algorithms

Fundamental underlying structure for almost all the descent algorithms:

- Start with an initial point
- Determine according to a fixed rule a direction of movement
- Move in that direction to a relative minimum of the objective function
- At the new point, a new direction is determined and the process is repeated.
- The difference between different algorithms depends upon the rule by which successive directions of movement are selected

- In the method of steepest descent, one starts with an arbitrary point $\mathbf{x}_{(0)}$ and takes a series of steps $\mathbf{x}_{(1)}$, $\mathbf{x}_{(2)}$, ... until we are satisfied that we are close enough to the solution.
- When taking the step, one chooses the direction in which f decreases most quickly, i.e.
- Definitions: $-f'(\mathbf{x}_{(i)}) = \mathbf{b} \mathbf{A}\mathbf{x}_{(i)}$ error vector: $\mathbf{e}_{(i)} = \mathbf{x}_{(i)} - \mathbf{x}$ residual: $\mathbf{r}_{(i)} = \mathbf{b} - \mathbf{A}\mathbf{x}_{(i)}$
- From **Ax=b**, it follows that

$$\mathbf{r}_{(i)} = -\mathbf{A}\mathbf{e}_{(i)} = -\mathbf{f}'(\mathbf{x}_{(i)})$$

Residual is direction of Steepest Descent



x2



• The algorithm



 $\mathbf{x}_{(i+1)} = \mathbf{x}_{(i)} + \alpha_{(i)}\mathbf{r}_{(i)} \implies \mathbf{e}_{(i+1)} = \mathbf{e}_{(i)} + \alpha_{(i)}\mathbf{r}_{(i)}$

• To avoid one matrix-vector multiplication, one uses

$$\mathbf{r}_{(i+1)} = \mathbf{r}_{(i)} - \alpha_{(i)} \mathbf{A} \mathbf{r}_{(i)}$$

The disadvantage of using this recurrence is that the residual sequence is determined without any feedback from the value of $\mathbf{x}_{(i)}$, so that round-off errors may cause $\mathbf{x}_{(i)}$ to converge to some point near \mathbf{x} .

Steepest Descent Problem



•The gradient at the minimum of a line search is orthogonal to the direction of that search \Rightarrow the steepest descent algorithm tends to make right angle turns, taking many steps down a long narrow potential well. Too many steps to get to a simple minimum.

Basic idea:

- Pick a set of orthogonal search directions d₍₀₎, d₍₁₎, ..., d_(n-1)
- Take exactly one step in each search direction to line up with x
- Solution will be reached in *n* steps

Mathematical formulation: 1. For each step we choose a point

$$\mathbf{x}_{(i+1)} = \mathbf{x}_{(i)} + \alpha_{(i)} \mathbf{d}_{(i)}$$

2. To find $\alpha_{(i)}$, we use the fact that $\mathbf{e}_{(i+1)}$ is orthogonal to $\mathbf{d}_{(i)}$

• To solve the problem of not knowing $\mathbf{e}_{(i)}$, one makes the search directions to be A-orthogonal rather then orthogonal to each other, i.e.: $\mathbf{d}_{(i)}^{T} A \mathbf{d}_{(i)} = 0$



• The new requirement is now that $\mathbf{e}_{(i+1)}$ is A-orthogonal to $\mathbf{d}_{(i)}$

$$\frac{d}{d\alpha} f(\mathbf{x}_{(i+1)}) = f'(\mathbf{x}_{(i+1)})^T \frac{d\mathbf{x}_{(i+1)}}{d\alpha} = 0$$

$$\mathbf{r}_{(i+1)}^T \mathbf{d}_{(i)} = 0$$

$$\mathbf{d}_{(i)}^T \mathbf{A} \mathbf{e}_{(i+1)} = 0$$

$$\mathbf{d}_{(i)}^T \mathbf{A} \left(\mathbf{e}_{(i)} + \alpha_{(i)} \mathbf{d}_{(i)} \right) = 0$$

$$\alpha_{(i)} = \frac{\mathbf{d}_{(i)}^T \mathbf{r}_{(i)}}{\mathbf{d}_{(i)}^T \mathbf{A} \mathbf{d}_{(i)}} \leftarrow$$

If the search vectors were the residuals, this formula would be identical to the method of steepest descent.

- Calculation of the A-orthogonal search directions by a **conjugate Gram-Schmidt process**
 - 1. Take a set of linearly independent vectors $\mathbf{u}_0, \mathbf{u}_1, \ldots, \mathbf{u}_{n-1}$
 - 2. Assume that $\mathbf{d}_{(0)} = \mathbf{u}_0$
 - 3. For i>0, take an \mathbf{u}_i and subtracts all the components from it that are not A-orthogonal to the previous search directions

$$\mathbf{d}_{(i)} = \mathbf{u}_{(i)} + \sum_{j=0}^{i-1} \beta_{ij} \mathbf{d}_{(j)} , \quad \beta_{ij} = -\frac{\mathbf{u}_{(i)}^{\mathrm{T}} \mathbf{A} \mathbf{d}_{(j)}}{\mathbf{d}_{(j)}^{\mathrm{T}} \mathbf{A} \mathbf{d}_{(j)}}$$

- The method of Conjugate Gradients is simply the method of conjugate directions where the search directions are constructed by conjugation of the residuals, i.e. $\mathbf{u}_i = \mathbf{r}_{(i)}$
- This allows us to simplify the calculation of the new search direction because

$$\beta_{ij} = \begin{cases} \frac{1}{\alpha_{(i-1)}} \frac{\mathbf{r}_{(i)}^{T} \mathbf{r}_{(i)}}{\mathbf{d}_{(i-1)}^{T} \mathbf{A} \mathbf{d}_{(i-1)}} = \frac{\mathbf{r}_{(i)}^{T} \mathbf{r}_{(i)}}{\mathbf{r}_{(i-1)}^{T} \mathbf{r}_{(i-1)}} & i = j+1 \\ 0 & i > j+1 \end{cases}$$

• The new search direction is determined as a linear combination of the previous search direction and the new residual

$$\mathbf{d}_{(i+1)} = \mathbf{r}_{(i+1)} + \beta_i \mathbf{d}_{(i)}$$

- One matrix-vector multiplication per iteration
- Two vector dot products per iteration
- Four n-vectors of working storage

Krylov subspace Krylov subspace K_j is the linear combinations of *b*, *Ab*,...,*A*^{*j*-1}*b*. **Krylov matrix** $Kj = [b Ab A^2b ... A^{j-1}b]$.

Methods to construct a basis for $\mathbf{K}_{\mathbf{j}}$: Arnoldi's method and Lanczos method

Approaches to choosing a good \mathbf{x}_i in \mathbf{K}_i :

- *Ritz-Galerkin approach*: r_j=b -Ax_j is orthogonal to K_j (Conjugate Gradient)
- Minimum Residual approach r, has minimum norm for x, in K;
 (GMRES and MINRES)
- *Petrov-Galerkin approach*: r_j is orthogonal to a different space K_i(A^T) (Biconjugate Gradient)

Arnoldi's Method

The best basis $q_1, ..., q_j$ for the Krylov subspace K_j is orthonormal. Each new q_j comes from orthogonalizing $t = Aq_{j-1}$ to the basis vectors $q_1, ..., q_j$ that are already chosen. The iteration to compute these orthonormal q's is Arnoldi's method.

 $\begin{array}{l} q_{1} = b \,/ \,||b|| \\ for \, j = 1, \dots, n_1 \\ t = A q_{j} \\ for \, i = 1, \dots, j \\ h_{ij} = q^{T}_{i} \\ t = t - h_{ij} q_{i} \\ end; \\ h_{j+1,j} = ||t|| \\ q_{j+1} = t \,/ \, h_{j+1,j} \\ end \end{array}$

 $AQ_{n-1} = Q_n H_{n,n-1}$

% Normalize b to $||q_{j}|| = 1$ % Start computation of q_{j+1} % one matrix multiplication % t is in the space K_{j+1} % $h_{ij}q^{T}_{i}$ =projection of t on q_{i} % Subtract that projection % t is orthogonal to $q_{1},...,q_{j}$ % Compute the length of t % Normalize t to $||q_{j+1}||=1$ % $q_{1},...,q_{n}$ are orthnormal

 $H_{n,n-1}$ is upper Hessenberg matrix

Lanczos Method

Lanczos method is specialized Arnoldi iteration, if A is symmetric (real) $H_{n-1,n-1} = Q_{n-1}^T A Q_{n-1}$

 $H_{n-1,n-1}$ is tridiagonal and this means that in the orthogonalization process, each new vector has to be orthogonalized with respect to the previous two vectors only, since the inner products vanish.

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\begin{array}{l} B_{0}=0, \ q_{0}=0, \ b= arbitrary, \ q_{1}=b \ / \ \|b\| \\ for \ i=1,...,n_{1} \\ v=Aq_{j} \\ a_{i}=q_{i}^{T}v \\ v=v-B_{i-1} \ q_{i-1} - a_{i}q \\ B_{i}=\|v\| \\ q_{j+1}=v \ / \ B_{i} \\ end \end{array}
```

Minimum Residual Methods

Problem: If **A** is **not symmetric positive definite**, CG is not guaranteed to solve Ax=b.

Solution: Minimum Residual Methods.

Choose x_i in the Krylov subspace K_i so that $||b - Ax_i||$ is minimal

The first orthonormal vectors q_1, \dots, q_j go in the columns Q_j so $Q_j^T Q_j = I$ Setting $x_j = Q_j y$ $||r_j|| = ||b - Ax_j|| = ||b - AQ_j y|| = ||b - Q_{j+1} H_{j+1,j} y||$

Using first *j* columns of Arnoldi's formula **AQ = QH**

First *j* columns of
$$\mathbf{QH} = \begin{bmatrix} q_1 & \cdots & q_{j+1} \end{bmatrix} \begin{bmatrix} h_{11} & \cdots & h_{1j} \\ h_{12} & \ddots & \vdots \\ & \ddots & h_{jj} \\ & & & h_{j+1,j} \end{bmatrix}$$

Minimum Residual Methods

The problem becomes: Choose **y** to minimize

$$||r_{j}|| = ||Q_{j+1}^{T}b - H_{j+,1,j}y||$$

This is least squares problem.

Using zeros in **H** and $Q_{i+1}^t b$ to find a fast algorithm that computes **y**.

GMRES (Generalised Minimal Residual Approach)A is *not symmetric* and the upper triangular part of *H* can be full.All previously computed vectors have to be stored.

MINRES: (Minimal Residual Approach)A is *symmetric* (likely indefinite) and *H* is tridiagonal. Avoids storageof all basis vectors for the Krylov subspace

Aim: to clear out the non-zero diagonal below the main diagonal of *H*. This is done by *Givens rotations*

GMRES

```
Algorithm: GMRES

q_1 = b / ||b||

for j = 1, 2, 3...

step j of Arnoldi iteration

Find y to minimize ||r_j|| = ||Q_{j+1}^T b - H_{j+,1,j}y||

x_j = Q_j y
```

Full-GMRES :

The upper triangle in H can be full and step j becomes expensive and possibly it is inaccurate as j increases.

GMRES(m):

Restarts the GMRES algorithm every *m* steps However tricky to choose *m*.

Petrov-Galerkin approach

- r_j is orthogonal to a different space K_j(A^T)
- BiCG (Bi-Conjugate Gradient)
- QMR (Quasi Minimum Residual)
- CGS (Conjugate Gradient Squared)

Lanczos Bi-Orthogonalization Procedure

•Extension of the symmetric Lanczos algorithm

•Builds a pair of bi-orthogonal bases for the two subspaces $K_m(A, v_1)$ and $K_m(A^T, w_1)$

Choose two vectors v_1, w_1 such that $(v_1, w_1) = 1$ Set $\beta_1 \equiv \delta_1 \equiv 0$. $w_0 \equiv v_0 \equiv 0$ For j = 1, 2, ..., m Do: $\alpha_i = (Av_i, w_i)$ $\hat{v}_{i+1} = Av_j - lpha_j v_j - eta_j v_{j-1}$ $\hat{w}_{i+1} = A^T w_i - lpha_i w_i - \delta_i w_{i-1}$ $\delta_{i+1} = |(\hat{v}_{i+1}, \hat{w}_{i+1})|^{1/2}$. If $\delta_{j+1} = 0$ Stop $eta_{i+1} = (\hat{v}_{i+1}, \hat{w}_{i+1}) / \delta_{i+1}$ $w_{j+1} = \hat{w}_{j+1}/eta_{j+1}$ $v_{j+1} = \hat{v}_{j+1}/\delta_{j+1}$ EndDo

Bi-Conjugate Gradient (BiCG)

Compute $r_0 := b - Ax_0$. Choose r_0^* such that $(r_0, r_0^*) \neq 0$. Set, $p_0 := r_0, p_0^* := r_0^*$ For j = 0, 1, ..., until convergence Do:, $lpha_j := (r_j, r_j^*)/(Ap_j, p_j^*)$ $x_{j+1} := x_j + \alpha_j p_j$ $r_{i+1} := r_i - \alpha_i A p_i$ $r_{i+1}^* := r_i^* - lpha_j A^T p_i^*$ $eta_j := (r_{j+1}, r^*_{j+1})/(r_j, r^*_j)$ $p_{i+1} := r_{i+1} + \beta_i p_i$ $p_{j+1}^* := r_{j+1}^* + eta_j p_j^*$ EndDo

Quasi Minimum Residual (QMR)

•QMR uses unsymmetric Lanczos algorithm to generate a basis for the Krylov subspaces

•The lookahead technique avoids breakdowns during Lanczos process and makes QMR robust.

Compute $r_0 = b - A x_0$ and $\gamma_0 := \|r_0\|_2$, $w_1 := v_1 := r_0/\gamma_1$

For $m = 1, 2, \ldots$, until convergence Do:

Compute α_m, δ_{m+1} and v_{m+1}, w_{m+1} as in Lanczos Algor.

Update the QR factorization of \bar{T}_m , i.e.,

Apply $\Omega_i, i = m-2, m-1$ to the m-th column of $ar{T}_m$

Compute the rotation coefficients c_m , s_m

Apply rotation Ω_m , to \overline{T}_m and \overline{g}_m , i.e., compute:

$$\gamma_{m+1}:=-s_m\gamma_m;\;\gamma_m:=c_m\gamma_m;$$
 and $lpha_m:=c_mlpha_m+s_m\delta_{m+1}$
 $p_m=\left(v_m- au_{i=m-2}^{m-1}t_{im}p_i
ight)/t_{mm}$
 $x_m=x_{m-1}+\gamma_mp_m$
If $|\gamma_{m+1}|$ is small enough Stop

EndDo

Conjugate Gradient Squared (CGS)

Compute
$$r_0 := b - Ax_0$$
; r_0^* arbitrary.
Set $p_0 := u_0 := r_0$.
For $j = 0, 1, 2...$, until convergence Do:
 $\alpha_j = (r_j, r_0^*)/(Ap_j, r_0^*)$
 $q_j = u_j - \alpha_j Ap_j$
 $x_{j+1} = x_j + \alpha_j(u_j + q_j)$
 $r_{j+1} = r_j - \alpha_j A(u_j + q_j)$
 $\beta_j = (r_{j+1}, r_0^*)/(r_j, r_0^*)$
 $u_{j+1} = r_{j+1} + \beta_j q_j$
 $p_{j+1} = u_{j+1} + \beta_j (q_j + \beta_j p_j)$
EndDo

Summary

•Stationary Iterative Solvers :

Jacobi, Gauss-Seidel, SORNon-Stationary Solvers:

- Krylov subspace methods
 - Conjugate Gradient
 - Symmetric postive definite systems
 - GMRES and MINRES
 - Non-symmetric matrices, but expensive
 - Bi-CG
 - Non-symmetric, two matrix-vector product
 - QMR
 - Non-symmetric, avoids irregular convergence of BiCG
 - CGS
 - Non-symmetric, faster than BICG, does not require transpose

References

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Thank You !