MA633L-Numerical Analysis

Lecture 29 : Numerical Linear Algebra - Conjugate Gradient Method

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Recap

Iterative Methods

$$Qx^{(k)} = (Q - A)x^{(k-1)} + b, \quad k = 1, 2, 3, \cdots$$

- Richardson $Q = I$
- Jacobi $Q = D(A)$
- G-S $Q = D - L$
- SOR $Q = \frac{1}{\omega}(D - \omega L)$

Relaxation Methods

$$Qz^{(k)} = (Q - A)x^{(k-1)} + b$$
$$x^{(k)} = \omega z^{(k)} + (1 - \omega)x^{(k-1)}$$

or

$$x^{(k)} = \omega[(I - Q^{-1}A)x^{(k-1)} + Q^{-1}b] + (1 - \omega)x^{(k-1)}$$

Convergence

$$x^{(k)} = Gx^{(k-1)} + c, \quad k = 1, 2, 3, \cdots \tag{1}$$

Theorem 1

The iteration (1) converges to $(I - G)^{-1}c$ if and only if $\rho(G) < 1$.

SOR

Theorem 2
The SOR method fails to converge if $\omega \leq 0$ or $\omega \geq 2$.

Proof: As per SOR method,

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

$$\implies x^{(k)} = (D - \omega L)^{-1}\left[((1-\omega)D + \omega U)x^{(k-1)} + \omega b\right]$$

Hence

$$G = (D - \omega L)^{-1}((1-\omega)D + \omega U)$$

SOR

Let $\{\lambda_i\}$ denote the eigenvalues of the SOR iteration matrix, then

$$\begin{aligned}\left|\prod_{i=1}^{n}\lambda_i\right| &= |\det[(D-\omega L)^{-1}((1-\omega)D+\omega U)]| \\ &= |\det[(D-\omega L)^{-1}||\det((1-\omega)D+\omega U)]| \\ &= |\det(D^{-1})||1-\omega|^n|\det(D)| \\ &= |1-\omega|^n\end{aligned}$$

Hence, at least one eigenvalue λ_i must exist such that $|\lambda_i| \geq |1-\omega|$ and thus in order for convergence to hold. Therefore, we must have

$$|1-\omega| < 1 \implies 0 < \omega < 2$$

Exercise

Exercise 1: Easy

Assume that $A = (a_{ij})$ is symmetric and positive definite

1. Prove that A can be written as $A = D - L - L^T$
2. Prove that $a_{ii} > 0$ for all i
3. Prove that L is lower triangular and $(D - \omega L)$ is nonsingular
4. Let $G = (D - \omega L)^{-1}[(1 - \omega)D + \omega L^T]$ and $P = A - G^T AG$. Prove that P is symmetric.
5. Show that $G = I - \omega(D - \omega L)^{-1}A$
6. Let $S = \omega(D - \omega L)^{-1}A$ then $G = I - S$ and $P = S^T[AS^{-1} - A + S^{-T}A]S$
7. Show that $P = \left(\frac{2}{\omega} - 1\right) S^T DS$ and P is positive definite if $0 < \omega < 2$.

Hint for Exercise

- For symmetric, we have $A = D - L - L^T$
- If A is positive definite, then all its diagonal entries are positive. For, take $x = e_i$, $x^T A x = a_{ii} > 0$. Therefore, D is positive definite.
- It is obvious that $D - \omega L$ is lower triangular and nonsingular.
- $P^T = (A - G^T A G)^T = A^T - (G^T A G)^T = A - G^T A^T (G^T)^T = A - G^T A G = P$
- $G = (D - \omega L)^{-1}[D - \omega D + \omega L - \omega L + \omega L^T] = (D - \omega L)^{-1}[(D - \omega L) + \omega A]$ $= I - \omega(D - \omega L)^{-1} A$
- $G = I - S$ is obvious. Now
  $G^T A G = (I - S)^T A (I - S) = (A - S^T A)(I - S) = A - AS - S^T A + S^T A S$
  $S^T[AS^{-1} - A + S^{-T} A]S = [S^T A S^{-1} - S^T A + S^T S^{-T} A]S$
  $= S^T A S^{-1} S - S^T A S + AS = S^T A - S^T A S + AS = A - G^T A G = P$

Hint for Exercise

- For $P = S^T D S$, it is sufficient to prove that
  $AS^{-1} - A + S^{-T}A = \left(\frac{2}{\omega} - 1\right) D$.
  $S^{-1} = \frac{1}{\omega} A^{-1}(D - \omega L) \implies AS^{-1} = \frac{1}{\omega}(D - \omega L)$
  $S^{-T} = \frac{1}{\omega}(D - \omega L)^T A^{-T} = \frac{1}{\omega}(D - \omega L^T)A^{-1} \implies S^{-T}A = \frac{1}{\omega}(D - \omega L^T)$
  $AS^{-1} - A + S^{-T}A = \frac{1}{\omega}(D - \omega L) - D + L + L^T + \frac{1}{\omega}(D - \omega L^T) = \left(\frac{2}{\omega} - 1\right) D$
- We have already proved that D is positive definite, the proof of P follows.

Exercise

Exercise 2: Easy

Assume that $A = (a_{ij})$ is symmetric and positive definite

1. Prove that L is lower triangular and $(D - L)$ is nonsingular
2. Let $G = (D - L)^{-1}L^T$ and $P = A - G^T AG$. Prove that P is symmetric.
3. Show that $G = I - (D - L)^{-1}A$
4. Let $S = (D - L)^{-1}A$ then $G = I - S$ and $P = S^T[AS^{-1} - A + S^{-T}A]S$
5. Show that $P = S^T DS$ and P is positive definite.

Hint: Use $\omega = 1$ in previous exercises.

SOR

Theorem 3
If A is symmetric, positive definite matrix and $0 < \omega < 2$, then the SOR method converges for any starting vector $x^{(0)}$.

Proof: Let

$$Q = \frac{1}{\omega}(D - \omega L) \implies G = I - Q^{-1}A$$

<u>**Claim:**</u> $\rho(G) = \rho(I - Q^{-1}A) < 1.$

$$\begin{aligned}
A - G^T A G &= A - (I - Q^{-1}A)^T A (I - Q^{-1}A) \\
&= A - (I - Q^{-1}A)^T (A - AQ^{-1}A) \\
&= A - A + (Q^{-1}A)^T A + AQ^{-1}A - (Q^{-1}A)^T AQ^{-1}A \\
&= (Q^{-1}A)^T Q^T Q^{-1}A + A^T Q^{-T} Q Q^{-1}A - (Q^{-1}A)^T AQ^{-1}A \\
&= (Q^{-1}A)^T [Q^T + Q - A] Q^{-1}A
\end{aligned}$$

SOR

Now,

$$
\begin{aligned}
Q^T + Q - A &= \frac{1}{\omega}(D - \omega L)^T + \frac{1}{\omega}(D - \omega L) - A \\
&= \frac{2}{\omega}D - L^T - L - D + L + L^T = \frac{1}{\omega}(2 - \omega)D
\end{aligned}
$$

Since $0 < \omega < 2$, this proves that $Q^T + Q - A$ is symmetric positive definite. Therefore, $P = A - G^T AG$ is symmetric positive definite (SPD). Let $\lambda \in \mathbb{C}$ be any eigenvalue of $I - Q^{-1}A$ and $x \in \mathbb{C}^n$ and $x \neq 0$ be corresponding eigenvector. Then

$$
x^* Ax > x^*(I - Q^{-1}A)^T A(I - Q^{-1}A) = (\lambda x)^* A(\lambda x) = |\lambda|^2 x^* Ax
$$

$$
\implies |\lambda|^2 < 1
$$

Therefore, $\rho(I - Q^{-1}A) < 1$. Hence the proof.

SOR

Theorem 4
If A is symmetric, positive definite matrix, then the Gauss-Seidel method converges for any starting vector $x^{(0)}$.

Proof: Use $\omega = 1$ and proceed as above.

Krylov Subspace Methods

Krylov Subspace Methods

Our aim is to solve $Ax = b$

- Krylov Subspace methods are a family of algorithm to solve the linear system.
- We need to search for an approximate solution from a Krylov subspace.
- Krylov subspace methods are again iterative methods which involves mostly matrix-vector product.

Krylov Subspace Methods

- Most popular Krylov subspace methods are
    1. Arnoldi
    2. Lanczos
    3. Conjugate Gradient
    4. BiCGSTAB
    5. GMRES
    6. MINRES
    7. SYMMLQ

Krylov Subspace Methods

Let A be an invertible matrix. Let us consider the sequence of vectors

$$b, Ab, A^2b, \cdots, A^{n-1}b, A^nb, \cdots,$$

Consider the first $n+1$, **Krylov matrix**

$$b, Ab, A^2b, \cdots, A^{n-1}b, A^nb$$

then these set become $n+1$ linearly dependent vectors of a n-dimensional space. Therefore, there exist coefficients $\alpha_0, \alpha_1, \cdots, \alpha_n$ such that

$$\sum_{j=0}^{n} \alpha_j A^j b = 0$$

All combinations of the Krylov matrix form a subspace which is called **Krylov subspace** $(\mathcal{K}_j)$.

Krylov Subspace Methods

Let k be the least integer such that $\alpha_k \neq 0$. Since A^{-1} exists

$$\implies A^{-1}b = -\frac{1}{\alpha_k}\sum_{j=k+1}^{n} \alpha_j A^{(j-k-1)}$$

We need to choose the best linear combinations as our improved x_j. Four different approaches to choose a good x_j leads to important decision

1. $r_j = b - Ax_j$ is orthogonal to $\mathcal{K}_j$: Conjugate Gradient
2. $r_j = b - Ax_j$ is orthogonal to $\mathcal{K}_j(A^T)$: BiCGSTAB
3. $r_j = b - Ax_j$ has minimum norm for x_j in $\mathcal{K}_j$: GMRES and MINRES
4. The error e_j has minimum norm: SYMMLQ

Conjugate Gradient Method

Conjugate Gradient Method

- One of most popular iterative methods for solving sparse system of linear equations
- Applicable for symmetric matrices A.

Definition 5 (Inner Product)
The inner product of two vectors

$$u = (u_1, u_2, \cdots, u_n), v = (v_1, v_2, \cdots, v_n)$$

is defined as

$$\langle u, v \rangle = u^T v = \sum_{i=0}^{n} u_i v_i$$

Conjugate Gradient Method

Definition 6 (Orthogonal)
If u and v are mutually orthogonal, then

$$\langle u, v \rangle = 0$$

Definition 7 (A-Inner Product)
The A-inner product of two vectors

$$u = (u_1, u_2, \cdots, u_n), v = (v_1, v_2, \cdots, v_n)$$

is defined as

$$\langle u, v \rangle_A = \langle Au, v \rangle = u^T A^T v$$

Conjugate Gradient Method

Definition 8 (A-Conjugate)
Two nonzero vectors u and v are A-conjugate if

$$\langle u, v \rangle_A = 0$$

Definition 9 (Positive Definite)
A square matrix is positive definite if

$$\langle x, x \rangle_A > 0$$

for all nonzero vector $x \in \mathbb{R}^n$.

Conjugate Gradient Method

Definition 10 (Quadratic Form)
A quadratic form is a scalar quadratic function of a vector of the form

$$f(x) = \frac{1}{2}\langle x, x\rangle_A - \langle b, x\rangle + c$$

Definition 11 (Gradient)
The gradient of a quadratic form is

$$f'(x) = \left[\frac{\partial f(x)}{\partial x_1}, \frac{\partial f(x)}{\partial x_2}, \cdots, \frac{\partial f(x)}{\partial x_n}\right]^T$$

Conjugate Gradient Method

From the gradient, we can observe that

$$f'(x) = \frac{1}{2}A^T x + \frac{1}{2}Ax - b$$

If A is symmetric, then we obtain that

$$f'(x) = Ax - b$$

If we set $f'(x) = 0$, and solve for x, then we can obtain the solution for our problem.

Conjugate Gradient Method

Suppose that $\mathcal{B} = \{p^{(1)}, p^{(2)}, p^{(3)}, \cdots, p^{(n)}\}$ is a set containing a sequence of n mutually conjugate director vectors. Then, $\mathcal{B}$ forms a basis for $\mathbb{R}^n$. If A is symmetric and positive definite, then $f(x)$ is minimized by the true solution vector x_r of $Ax = b$ into a linear combination of these basis vectors

$$x_r = \sum_{i=1}^{n} \alpha_i p^{(i)}$$

where

$$\alpha_i = \frac{\langle p^{(k)}, b\rangle}{\langle p^{(k)}, p^{(k)}\rangle_A}$$

Conjugate Gradient Method

This method was introduced by Hestenes and Stiefel in 1952, but it was not popular as it was viewed as direct method. However, when Reid viewed it as an iterative process in 1971, this became popular and many variants of CG methods are available.

In the iterative method, it takes less computation time and less storage and much more useful for large sparse linear systems.

Conjugate Gradient Method

Assume that A is symmetric and positive definite (SPD)

- Start with initial guess $x^{(0)} = 0$
- Let x_r be the unique minimizer of $f(x)$, that is

$$f(x) = \frac{1}{2}x^T Ax - x^T x$$

- Take the first basis vector of $p^{(1)}$ to be the gradient of f at $x = x^{(0)}$

$$f'(x) = -b$$

- The other vectors in the basis are now conjugate to the gradient. Hence the name conjugate gradient method.

Conjugate Gradient Method

- The kth residual is given by

$$r^{(k)} = b - Ax^{(k)}$$

- The CG method moves in the direction $r^{(k)}$.
- Take the direction closest to the gradient vector $r^{(k)}$ by insisting that the direction vector $p^{(k)}$ be conjugate to each other.

$$p^{(k+1)} = r^{(k)} - \frac{\langle p^{(k)}, r^{(k)} \rangle_A}{\langle p^{(k)}, p^{(k)} \rangle_A} p^{(k)}$$

- CG method solves the system $Ax = b$ in at most n steps.

Conjugate Gradient Method

Observations

- Start with initial guess $x^{(0)} = 0$
- The kth residual is given by

$$r^{(k)} = b - Ax^{(k)}$$

- $r^{(k)}$ is the negative gradient of f at $x = x^{(k)}$
- The gradient descent method would require to move in the direction $r^{(k)}$.
- As we insist that to be in the direction $p^{(k)}$ be conjugate to each other That is,

$$p^{(k)} = r^{(k)} - \sum_{i<k} \frac{p^{(i)T} A r^{(k)}}{p^{(i)T} A p^{(i)}} p^{(i)}$$

Conjugate Gradient Method

Observations

- The next optimal location is given by

$$x^{(k+1)} = x^{(k)} + \alpha_k p^{(k)}$$

  where

$$\alpha_k = \frac{p^{(k)T}(b - Ax^{(k)})}{p^{(k)T}Ap^{(k)}} = \frac{p^{(k)T}(r^{(k)})}{p^{(k)T}Ap^{(k)}}$$

- It is obtained by minimizing f w.r.t. α_k

$$g(\alpha_k) := f(x^{(k+1)}) = f(x^{(k)} + \alpha_k p^{(k)})$$

$$g'(\alpha_k) = 0 \implies \alpha_k = \frac{p^{(k)T}(b - Ax^{(k)})}{p^{(k)T}Ap^{(k)}}$$

Conjugate Gradient Method

Theorem 12

If A is SPD, then CG method converges to the true solution within n iterations.

Theorem 13

If A has only n distinct eigenvalues, then the CG method converges in at most n steps.

Theorem 14

If A is SPD and the error between the true solution and CG approximation is $e_k = x_k - x_*$, then

$$\|e_k\|_A \leq 2 \left(\frac{\sqrt{\kappa(A)_2} - 1}{\sqrt{\kappa(A)_2} + 1} \right)^k \|e_0\|_A$$

BiCGStab

BiConjugate Gradient Method

- For Conjugate gradient method, we need A to be symmetric or self-adjoint.
- CG method is one of the fastest solver if A is SPD.
- For non-SPD matrices, this could fail.
- To overcome this another Krylov subspace $\mathcal{K}^{\mathcal{T}}$ is introduced.

$$b, A^T b, A^{2T} b, \cdots, A^{(n-1)T} b, A^{nT} b, \cdots,$$

- In BiCGStab, we look for orthogonality properties as in CG, however, there is no stability issues of solving $A^T A x = A^T b$.
- Note that BiCGStab has worse efficiency compared to CG when applied to SPD matrices as it requires more matrix vector multiplications

Thanks

Doubts and Suggestions

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