Lecture 4

Arnoldi and GMRES

Computational Mathematics

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Krylov Subspace

- Consider the Krylov subspace of order k,

$$\mathcal{K}_k(A; v) = \langle v, Av, \ldots, A^{k-1}v \rangle$$

Theorem 4.1

Let $A \in \mathbb{R}^{n\times n}$ and $v \in \mathbb{R}^n$. The Krylov subspace $\mathcal{K}_k(A; b)$ has dimension equal to k iff the degree of v with respect to A is not less than k.

- The degree of v is defined as the minimum degree of a monic non null polynomial p in A, for which $p(A)v = 0$

Richardson Method ($P = I$)

- Algorithm: Richardson Method ($P = I$)

  $x^{(0)} = 0$; $r^{(0)} = b - Ax^{(0)} = b$
  for $k = 0, 1, \ldots$
  solve $Iz^{(k)} = r^{(k)}$
  compute α_k
  $x^{(k+1)} = x^{(k)} + \alpha_k z^{(k)}$
  $r^{(k+1)} = r^{(k)} - \alpha_k A z^{(k)}$
  until convergence
- Residual at the k-th step

$$r^{(k)} = \prod_{j=0}^{k-1} (I - \alpha_j A) b \quad \Rightarrow \quad r^{(k)} = p_k(A) b \in \mathcal{K}_{k+1},$$

  where $p_k(A)$ is a polynomial in A of degree k
- The iterate $x^{(k)}$

$$x^{(k)} = 0 + \sum_{j=0}^{k-1} \alpha_j r^{(j)} = \sum_{j=0}^{k-1} \alpha_j r^{(j)} = q_{k-1}(A) b \in \mathcal{K}_k$$

Krylov Subspace Methods

- Goal: Search for approximate solutions of the form

$$x^{(k)} = q_{k-1}(A) b,$$

  such that $x^{(k)}$ be the best approximation of x (exact solution of $Ax = b$) in $\mathcal{K}_k$
- Two alternative strategies
  - FOM (Full Orthogonalization Method) or Arnoldi method

    Compute $x^{(k)} \in \mathcal{K}_k$ such that the residual $r^{(k)} \perp \mathcal{K}_k$, i.e.,

$$v^T (b - Ax^{(k)}) = 0, \quad \forall v \in \mathcal{K}_k$$

  - GMRES method (Generalized Minimum RESidual method)

    Compute $x^{(k)} \in \mathcal{K}_k$ minimizing $\|r^{(k)}\|_2$, i.e.,

$$\|b - Ax^{(k)}\|_2 = \min_{v \in \mathcal{K}_k} \|b - Av\|_2$$

- (Preliminary) Goal: Compute an orthogonal basis of $\mathcal{K}_k$

Arnoldi Iteration

The Arnoldi Iteration

- For a fixed k it is possible to compute an orthogonal basis for $\mathcal{K}_k$ using the so-called Arnoldi algorithm.
- The Arnoldi process reduces a general, nonsymmetric A to Hessenberg form by similarity transforms: $A = QHQ^T$
- Allows for reduced factorizations by a Gram-Schmidt-style iteration instead of Householder reflections
- Let Q_n be the $n \times k$ matrix with the first k columns of Q, and consider the first m columns of $AQ = QH$, or $AQ_k = Q_{k+1}\hat{H}_k$

$$A \left[\begin{array}{c|c|c} q_1 & \cdots & q_k \end{array} \right] = \left[\begin{array}{c|c|c} q_1 & \cdots & q_{k+1} \end{array} \right] \begin{bmatrix} h_{11} & \cdots & h_{1k} \\ h_{21} & & \\ & \ddots & \vdots \\ & & h_{k+1,k} \end{bmatrix}$$

Hessenberg Matrix

- $H_k \in \mathbb{R}^{k\times k}$ is an upper Hessenberg matrix if

$$H_k = \begin{bmatrix} h_{11} & h_{12} & \cdots & h_{1k} \\ h_{21} & h_{22} & & \\ & \ddots & \ddots & \vdots \\ & & h_{k,k-1} & h_{kk} \end{bmatrix},$$

- The matrix $\hat{H}_k \in \mathbb{R}^{(k+1)\times k}$ is such that

$$\hat{H}_k = \begin{bmatrix} h_{11} & h_{12} & \cdots & h_{1k} \\ h_{21} & h_{22} & & \\ & \ddots & \ddots & \vdots \\ & & h_{k,k-1} & h_{kk} \\ & & & h_{k+1,k} \end{bmatrix}, \quad h_{ij} = q_i^T A q_j$$

- Note that $H_k = Q_k^T A Q_k = \hat{H}_{1:k,1:k}$

The Arnoldi Algorithm

- The k-th column of $AQ_k = Q_{k+1}\hat{H}_k$ gives

$$Aq_k = h_{1k}q_1 + \cdots + h_{kk}q_k + h_{k+1,k}q_{k+1}$$

which can be used to compute q_{k+1} similarly to modified GS

- Algorithm: Arnoldi Iteration

b arbitrary; $q_1 = b/\|b\|$
for $k = 1, 2, \ldots$
  $v = Aq_k$
  for $i = 1$ to k do
    $h_{ik} = q_i^T v$
    $v = v - h_{ik}q_i$
  end for
  $h_{k+1,k} = \|v\|_2$
  $q_{k+1} = v/h_{k+1,k}$
end for

- Algorithm: Gram-Schmidt

% For orthonormalize $\{a_1, \ldots, a_n\}$
for $k = 1$ to n do
  $v = a_k$
  for $i = 1$ to $k-1$ do
    $\begin{cases} r_{ik} = q_i^T a_k \text{ (CGS)} \\ r_{ik} = q_i^T v \text{ (MGS)} \end{cases}$
    $v = v - r_{ik}q_i$
  end for
  $r_{kk} = \|v\|_2$
  $q_k = v/r_{kk}$
end for

- Exercise 1: What if q_1 happens to be an eigenvector of A?

QR Factorization of Krylov Matrix

- The vectors q_j from Arnoldi are orthonormal bases of the successive Krylov subspaces

$$\mathcal{K}_k = \mathcal{K}_k(A; b) = \langle b, Ab, \ldots, A^{k-1}b \rangle = \langle q_1, q_2, \ldots, q_k \rangle \subseteq \mathbb{R}^n$$

- $Q_k \in \mathbb{R}^{n \times k}$ is the reduced QR factorization $K_k = Q_k R_k$ of the Krylov matrix

$$K_k = \left[\begin{array}{c|c|c|c} b & Ab & \cdots & A^{k+1}b \end{array} \right]$$

- The projection of A onto this space gives $k \times k$ Hessenberg matrix $H_k = Q_k^T A Q_k$, whose eigenvalues may be good approximations of A's

Symmetric Matrices and the Lanczos Iteration (*)

- For symmetric A, H_k reduces to tridiagonal T_k, and q_{k+1} can be computed by a three-term recurrence:

$$Aq_k = \beta_{k-1} q_{k-1} + \alpha_k q_k + \beta_k q_{k+1}$$

- Algorithm: Lanczos Iteration

$\beta_0 = 0$; $q_0 = 0$; b arbitrary; $q_1 = b/\|b\|$
for $k = 1, 2, \ldots$
    $v = Aq_k$
    $\alpha_k = q_k^T v$
    $v = v - \beta_{k-1} q_{k-1} - \alpha_k q_k$
    $\beta_k = \|v\|_2$
    $q_{k+1} = v/\beta_k$
end for

Properties of Arnoldi and Lanczos Iterations (*)

- Eigenvalues of H_k (or T_k in Lanczos iterations) are called Ritz values
- When $k = n$, Ritz values are eigenvalues
- Even for $k \ll n$, Ritz values are often accurate approximations to eigenvalues of A
- For symmetric matrices with evenly spaced eigenvalues, Ritz values tend to first convert to extreme eigenvalue
- With rounding errors, Lanczos iteration can suffer from loss of orthogonality and can in turn lead to spurious "ghost" eigenvalues.

FOM or Arnoldi for Linear Systems

FOM / Arnoldi Method for Linear Systems

- Full Orthogonalization Method: iterative method for $Ax = b$
- Compute $x^{(k)} \in \mathcal{K}_k$ such that $r^{(k)} \perp \mathcal{K}_k$, i.e.,

$$v^T r^{(k)} = v^T (b - Ax^{(k)}) = 0, \quad \forall v \in \mathcal{K}_k$$

- Considering $x^{(k)} \in \mathcal{K}_k$, we may write $x^{(k)} = Q_k y$ where y is such that $r^{(k)} \perp \mathcal{K}_k$

$$Q_k^T r^{(k)} = Q_k^T (b - AQ_k y) = Q_k^T b - Q_k^T A Q_k y = 0$$

- Due to the orthonormality of the basis we have

$$Q_k^T b = \|b\|_2 e_1, \quad (e_1 \text{ is the first unit vector in } \mathbb{R}^k)$$

and $H_k = Q_k^T A Q_k$, we have

$$Q_k^T b - Q_k^T A Q_k y = 0 \quad \Leftrightarrow \quad H_k y = \|b\|_2 e_1$$

- The system can be easily solved (H_k is upper Hessenberg)

$$x^{(k)} = Q_k y$$

FOM / Arnoldi Method for Linear Systems

Theorem 4.2

In exact arithmetic, the Arnoldi method yields the solution of $Ax = b$ after at most n iterations. Moreover, if a breakdown occurs after $k < n$ iterations, $x^{(k)} = x$.

- Proof: Since $\mathcal{K}_n = \mathbb{R}^n$, if the method terminates at the n-th iteration, then $x^{(n)} = x$.
  Conversely, from the relations

$$Q_k^T A Q_k = H_k, \quad Q_k^T A Q_k y = Q_k^T b \quad \text{and} \quad x^{(k)} = Q_k y,$$

if a breakdown occurs after $k < n$ iterations, we get

$$x^{(k)} = Q_k H_k^{-1} Q_k^T b = A^{-1} b = x. \ \square$$

FOM Algorithm

- Algorithm: FOM

  b arbitrary; $q_1 = b/\|b\|$
  for $k = 1, 2, \ldots$
  $\langle$ step k of Arnoldi iteration $\rangle$
  Solve $H_k y = \|b\|_2 e_1$
  $x^{(k)} = Q_k y$
  until convergence

- The residual is available by

$$\|b - Ax^{(k)}\|_2 = h_{k+1,k}|e_k^T y|$$

- Stopping criteria: for a fixed tolerance ϵ

$$h_{k+1,k}|e_k^T y|/\|b\|_2 \leqslant \epsilon$$

- Exercise 2: Implement the previous algorithm to solve the linear system $Ax = b$ with $A = \text{tridiag}_{100}(-1, 2, -1)$ and b such that the solution is $x = 1$. The initial vector is $x^{(0)} = 0$ and $\epsilon = 1e-10$. Plot $\|r^{(k)}\|_2/\|b\|_2$ as a function of k.

Arnoldi Iteration Breakdown

- Exercise 3: Suppose that the Arnoldi algorithm is executed for a particular A and b until at some step k, an entry $h_{k+1,k} = 0$ is encountred.
  (a) Show that $AQ_k = Q_{k+1}\hat{H}_k$ can be symplified in this case. What does it imply about the structure of a full $n \times n$ Hessembeg reduction $A = QHQ^T$ of A?
  (b) Show that $\mathcal{K}_k$ is an invariant subspace of A, i.e., $A\mathcal{K}_k \subseteq \mathcal{K}_k$.
  (c) Show that $\mathcal{K}_k = \mathcal{K}_{k+1} = \mathcal{K}_{k+2} = \cdots$.
  (d) Show that each eigenvalue of H_k is an eigenvalue of A.
  (e) Show that if A is nonsingular, then the solution x of $Ax = b$ lies in $\mathcal{K}_k$.
- The appearence of any entry $h_{k+1,k}$ is called a breakdown of the Arnoldi interation

GMRES

Minimizing Residuals

- Generalized Minimal RESiduals: iterative method for $Ax = b$
- Find $x^{(k)} = K_k y \in \mathcal{K}_k$ that minimizes $\|r^{(k)}\|_2 = \|b - Ax^{(k)}\|_2$
- This is a least squares problem: Find a vector y such that

$$\|AK_k y - b\|_2 = \text{minimum}$$

  where K_k is the $n \times k$ Krylov matrix
- QR factorization can us to solve for y, and $x^{(k)} = K_k y$
- In practice the columns of K_k are ill-conditioned and an orthogonal basis is used instead, produced by Arnoldi iteration

Minimal Residual with Orthogonal Basis

- Set $x^{(k)} = Q_k y$ (orthogonal columns of Q_k span K_k) and solve

$$\|AQ_k y - b\|_2 = \text{minimum}$$

- Find $x^{(k)} \in \mathcal{K}_k$ that minimizes $\|r^{(k)}\|_2 = \|b - Ax^{(k)}\|_2$
- Since for the Arnoldi iteration $AQ_k = Q_{k+1}\hat{H}_k$

$$\|Q_{k+1}\hat{H}_k y - b\|_2 = \text{minimum}$$

- Left multiplication by Q_{k+1}^T does not change the norm (since both vectors are in the column space of Q_{k+1})

$$\|\hat{H}_k y - Q_{k+1}^T b\|_2 = \text{minimum}$$

- Finally, it is clear that $Q_{k+1}^T b = \|b\|_2 e_1$

$$\|\hat{H}_k y - \|b\|_2 e_1\|_2 = \text{minimum}$$

The GMRES Method

- Algorithm: GMRES

  b arbitrary; $q_1 = b/\|b\|$
  for $k = 1, 2, \ldots$
      $\langle$ step k of Arnoldi iteration $\rangle$
      Find y to minimize $\|\hat{H}_k y - \|b\|_2 e_1\|_2$
      $x^{(k)} = Q_k y$
  until convergence

- The residual $\|r^{(k)}\|_2$ does not need to be computed explicitly from $x^{(k)}$
- Least squares problem has Hessenberg structure, solve with QR factorization of $\hat{H}_k$ (computed by updating the factorization of $\hat{H}_{k-1}$)
- Memory and cost grow with k: restart the algorithm by clearing accumulated data (might stagnate the method)

Convergence of GMRES

Theorem 4.3

A breakdown occurs for the GMRES method at a step k (with $k < n$) iff the computed solution $x^{(k)}$ coincides with the exact solution to the system.

- Exercise 4: The recurrence

$$x^{(k+1)} = x^{(k)} + \alpha r^{(k)} = x^{(k)} + \alpha(b - Ax^{(k)}),$$

where α is a scalar constant is the Richardson iteration. What polynomial $p(A)$ at step k does this correspond to?

- Exercise 5: Our statement of the GMRES begins with the initial guest $x^{(0)} = 0$, $r^{(0)} = b$. Show that if one wishes to start an arbitrary initial guess $x^{(0)}$, this can be accomplished by an easy modification of the right-hand side b.

GMRES and Polynomial Approximation

- GMRES can be interpreted as the related approximation problem: find $p_k \in P_k$, where

$$P_k = \{\text{polynomial } p \text{ of degree } \leqslant k \text{ with } p(0) = 1\},$$

to minimize $\|p_k(A)b\|_2$.

- The iterate $x^{(k)}$ can be written as

$$x^{(k)} = q_{k-1}(A)b,$$

where q is a polynomial of degree $k - 1$

- The corresponding residual $r^{(k)} = b - Ax^{(k)}$ is

$$r^{(k)} = (I - Aq_{k-1}(A))b = p_k(A)b$$

Convergence of GMRES

- Two obvious observations based on the minimization in $\mathcal{K}_k$: GMRES converges monotonically and it converges after at most n steps,

$$\|r^{(k+1)}\|_2 \leqslant \|r^{(k)}\|_2 \quad \text{and} \quad \|r^{(n)}\|_2 = 0.$$

This will happen because $\mathcal{K}_n = \mathbb{R}^n$.
- The residual $\|r^{(k)}\|_2 = \|p_k(A)b\|_2$, where $p_k \in P_k$ is a degree k polynomial with $p(0) = 1$, so GMRES also finds a minimizing polynomial

$$\|p_k(A)b\|_2 = \text{minimum}$$

- The factor that determines the size of this quantity is usually $\|p_k(A)\|_2$, that is

$$\frac{\|r^{(k)}\|_2}{\|b\|_2} \leqslant \inf_{p_k \in P_k} \|p_k(A)\|_2.$$

- Exercise 6: Repeat Exercise 2 for the GMRES method.

Convergence of GMRES

- How small can $\|p_k(A)\|_2$ be?
- If A is diagonalizable $A = V\Lambda V^{-1}$ for some nonsingular matrix Λ

$$\|p(A)\|_2 \leqslant \|V\|_2 \|p(\Lambda)\|_2 \|V^{-1}\|_2 = K_2(V)\|p\|_{\Lambda(A)},$$

being $\|p\|_{\Lambda(A)} = \sup_{\lambda \in \Lambda(A)} |p(\lambda)|$

Theorem 4.4

At the step k of the GMRES iteration, the residual $r^{(k)}$ satisfies

$$\frac{\|r^{(k)}\|_2}{\|b\|_2} \leqslant \inf_{p_k \in P_k} \|p_k(A)\|_2 \leqslant k(V) \inf_{p_k \in P_k} \|p_k\|_{\Lambda(A)}.$$

- In other words: If A has well-conditioned eigenvectors, the convergence is based on how small polynomials p_k can be on the spectrum

Other Krylov Subspace Methods

Other Krylov Subspace Methods

- CG on the Normal Equations (CGN)
  - Solve $A^*Ax = A^*b$ using CG
  - Poor convergence, squared condition number $K(A^*A) = K(A)^2$
- BiConjugate Gradients (BiCG)
  - Makes residuals orthogonal to another Krylov subspace, based on A^*
  - Memory requirements only constant number of vectors
  - Convergence sometimes comparable to GMRES, but unpredictable
- Conjugate Gradients Squared (CGS)
  - Avoids multiplication by A^*, sometimes twice as fast convergence
- Quasi-Minimal Residuals (QMR) and Stabilized BiCG (Bi-CGSTAB)
  - Variants of BiCG with more regular convergence