Lecture 3

Arnoldi and GMRES

New Directions in Mathematics

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Krylov Subspace Methods

- Problem: Find $x \in \mathbb{R}^n$, such that $Ax = b$, with $A \in \mathbb{R}^{n \times n}$
- Consider the Krylov subspace of order k,

$$\mathcal{K}_k = K_k(A; b) \quad = \quad \langle b, Ab, \ldots, A^{k-1} b \rangle$$

- Goal: Search for approximate solutions of the form

$$x^{(k)} \in \mathcal{K}_k, \quad k \leqslant n,$$

such that $x^{(k)}$ be the best approximation of x in $\mathcal{K}_k$

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 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 $AQ_k = Q_{k+1}\hat{H}_k$

$$A \left[\begin{array}{c|c|c} & & \\ q_1 & \cdots & q_k \\ & & \end{array}\right] = \left[\begin{array}{c|c|c} & & \\ q_1 & \cdots & q_{k+1} \\ & & \end{array}\right] \begin{bmatrix} h_{11} & h_{12} & \cdots & h_{1k} \\ h_{21} & h_{22} & & \\ & \ddots & \ddots & \vdots \\ & & h_{k,k-1} & h_{kk} \\ & & & h_{k+1,k} \end{bmatrix}$$

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 3.1: 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.

Arnoldi Iteration Breakdown

- Exercise 3.2 ($*$): 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 $h_{k+1,k} = 0$ is called a breakdown of the Arnoldi interation

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 $r^{(k)} \perp \mathcal{K}_k$

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

- 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 $H_k = Q_k^T AQ_k$, we have

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

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

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

FOM / Arnoldi Method for Linear Systems

Theorem 3.1

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 3.3: 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.

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 3.2

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 3.4: 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 3.5: 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 3.6: Repeat Exercise 3.3 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 3.3

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

HW Exercises

- Exercise 3.7: Consider $K_n = [b \mid Ab \mid ... \mid A^{n-1}b]$ (Krylov matrix) for a given matrix $A \in \mathbb{R}^{n\times n}$ and a vector $b \in \mathbb{R}^n$.
  In Matlab: `Kn = gallery('krylov',A,b,n)`
  1. Varying n between 2 and 20, choose a random matrix A and b and determine the condition number
  $$\text{cond}(K_n) = \|K_n\|_2 \|K_n^{-1}\|_2$$
  of matrix K_n and plot the data in logarithmic scale.
  2. Let us suppose that we want to solve the system $K_n x = c$, where c is determined such that $x = [1, 1, ..., 1]^T$ is the exact solution of the system. Plot the evolution of the relative error with respect the calculated approximation $\bar{x}$,
  $$r(\bar{x}) = \|x - \bar{x}\|_2 / \|x\|_2,$$
  as a function of n (make the range from 2 to 20).
  3. Prove that, if $K_n \bar{x} = \bar{c}$,
  $$r(\bar{x}) \leqslant \text{cond}(K_n) r(\bar{c})$$
  and plot the evolution of this upper bond for the relative error as a function of n (make the range from 2 to 20).

HW Exercises (cont.)

- Exercise 3.8: In the last lectures we considered the Conjugate Gradient (CG) method, the Krylov subspace methods and Richardson iteration method.
  1. Explain the relationship between these three methods.
  2. How does the CG method fit into the broader framework of Krylov subspace methods? Furthermore, discuss how Richardson iteration can be viewed as a special case of both the CG method and Krylov methods.
  3. Provide insights into the similarities and differences between these iterative techniques, and discuss the implications of understanding this relationship for solving linear systems efficiently.
  4. Prove that, for SPD matrices, solving $Ax = b$ is equivalent to finding the minimizer $x \in \mathbb{R}^n$ of the quadratic form
  $$\phi(y) = \frac{1}{2} y^T A y - y^T b$$
  and explain how this can be used to develop an interactive method for solving a system of linear equations.