Lecture 24
GMRES, Other Krylov Subspace Methods

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Introduction to Numerical Methods

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Minimizing Residuals

- *Generalized Minimal RESiduals* – iterative method for solving $Ax = b$
- Find $x_n \in \mathcal{K}_n$ that minimizes $\|r_n\| = \|b - Ax_n\|$
- This is a least squares problem: Find a vector c such that

$$\|AK_nc - b\| = \text{minimum}$$

  where K_n is the $m \times n$ Krylov matrix
- QR factorization could be used to solve for c, and $x_n = K_nc$
- In practice the columns of K_n are ill-conditioned and an orthogonal basis is used instead, produced by Arnoldi iteration

Minimal Residual with Orthogonal Basis

- Instead of $x_n = K_nc$ set $x_n = Q_ny$, where the orthogonal columns of Q_n span $\mathcal{K}_n$, and solve

$$\|AQ_ny - b\| = \text{minimum}$$

- For the Arnoldi iteration we showed that $AQ_n = Q_{n+1}\tilde{H}_n$:

$$\|Q_{n+1}\tilde{H}_ny - b\| = \text{minimum}$$

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

$$\|\tilde{H}_ny - Q_{n+1}^*b\| = \text{minimum}$$

- Finally, it is clear that $Q_{n+1}^*b = \|b\|e_1$:

$$\|\tilde{H}_ny - \|b\|e_1\| = \text{minimum}$$

The GMRES Algorithm

- High-level description of the algorithm:

Algorithm: GMRES

$q_1 = b/\|b\|$
for $n = 1, 2, 3, \dots$
  $\langle$ *step n of Arnoldi iteration* $\rangle$
  Find y to minimize $\|\tilde{H}_ny - \|b\|e_1\| = \|r_n\|$
  $x_n = Q_ny$

- The residual $\|r_n\|$ does not need to be computed explicitly from x_n
- Least squares problem has Hessenberg structure, solve with QR factorization of $\tilde{H}_n$ (computed by updating the factorization of $\tilde{H}_{n-1}$)
- Memory and cost grow with n – *restart* the algorithm by clearing accumulated data (might stagnate the method)

Convergence of GMRES

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

$$\|r_{n+1}\| \le \|r_n\| \quad \text{and} \quad \|r_m\| = 0$$

- The residual $r_n = p_n(A)b$, where $p_n \in P_n$ is a degree n polynomial with $p(0) = 1$, so GMRES also finds a minimizing polynomial:

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

- Based on this, diagonalizable $A = V\Lambda V^{-1}$ converges as:

$$\frac{\|r_n\|}{\|b\|} \le \kappa(V) \inf_{p_n \in P_n} \|p_n\|_{\Lambda(A)}$$

  or in words: If A has well-conditioned eigenvectors, the convergence is based on how small polynomials p_n can be on the spectrum

Other Krylov Subspace Methods

- CG on the Normal Equations (CGN)
  - Solve $A^*Ax = A^*b$ using conjugate gradients
  - Poor convergence, squared condition number $\kappa(A^*A) = \kappa(A)^2$
- 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