Iterative Methods

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11:28

Ways to think about optimal solution

1) minimize "energy"

2) Galerkin condition

To choose "optimal" solution from V

Make residual $r = Ax - b$ orthogonal to test space W

- $W = V$ Bubnov-Galerkin (Galerkin)
- $W \neq V$ Petrov-Galerkin

3) Minimize error (or residual) in some norm

- CG minimize $\|e\|_A$ where $e = x_k - x$ ★
  or $\|r\|_{A^{-1}}$ when $r = Ax_k - b$ †

CG high Level

- Form Krylov subspace $K_k(A, b)$
- Minimize

$$\varphi(x) = \tfrac{1}{2} x^T A x - x^T b \quad \text{over subspace}$$

Q_k = Lanczos basis for $K_k(A, b)$

pick $x_k = Q_k z$ minimizing φ

$$\varphi(Q_k z) = \tfrac{1}{2} z^T \underbrace{Q_k A Q_k}_{T_k} z - z^T \underbrace{Q_k^T b}_{\|b\| e_1}$$

$$\delta\varphi = Q_k^T (\underbrace{AQ_k z - b}_{r})$$

★ $e = x_k - x \qquad x_k = x + e$

$$\varphi(x_k) - \varphi(x) = \left(\tfrac{1}{2}(x+e)^T A (x+e) - (x+e) b\right) - \left(\tfrac{1}{2} x^T A x - x^T b\right)$$

$$= \tfrac{1}{2} e^T A e + e^T A x - e^T b$$

$$= \frac{1}{2} e^T A e + e^T A x - e^T b$$

$$= \frac{1}{2} \|e\|_A^2 + \cancel{e^T (Ax - b)} \to 0$$

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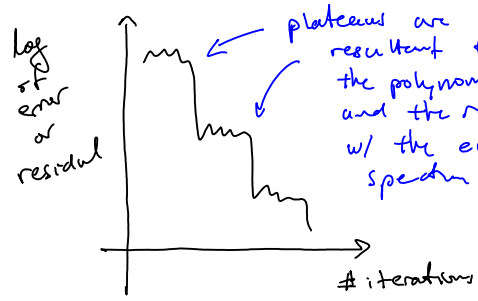
† $Ae = r$ $\quad e = A^{-1} r$ $\quad \|e\|_A^2 = e^T A e$

$$= r^T A^{-1} A A^{-1} r$$

$$= r^T A^{-1} r = \|r\|_{A^{-1}}^2$$

Properties of CG

- minimize energy norm error / A^{-1} norm residual per step $\Rightarrow$ monotone convergence in those norms (this is not true in the 2-norm! because you're not minimizing the 2-norm)
- It's a three-term recurrence $\Rightarrow$ limited storage requirements
- CG is an iterative method (though it looks exact in exact arith)
- Convergence bounds related to $\sqrt{K(A)}$ ← condition #



plateaus are resultant from the polynomials and the relationship w/ the eigenvalue spectrum

wigglyness a factor of the norm. 2-norms wiggle, energy norms are monotonic

- Rarely used alone! Use a preconditioner!

Common Theme: Krylov subspace and "optimal" approximation recipe.

→ symmetric, positive definite $\Rightarrow$ use CG

→ symmetric, indefinite $\Rightarrow$ use MINRES (minimal residual)

- turns out you can do this w/ a three-term recurrence w/o too much more complication

→ non-symmetric (bifurcation in methods)

- GMRES - generalized minimal residual

- (minimize residual over subspace)
  - not a three-term recurrence
  - have to restart periodically (5-10 steps, then restart because housekeeping is expensive)
- Force three term
  - minimize squared residual?
    - CGNE - gets you a symmetric posidef system, but now you've also squared your condition #; so you converge more slowly
    - Galerkin style things
      - BiCG
      - QMR

If you're going to do this stuff for real, look @ Templates for the Solution of Linear Systems by Barrett et al. free on Netlib or cheap via SIAM

packages that implement these methods:

- PETSc, Trilinos } big C/C++ } parallel + nice design space exploration stuff, i.e. turning solver knobs.
- Itpack } FORTRAN

CG = Lanczos + Energy Minimization.

GMRES = Arnoldi + Residual Minimization

Arnoldi: generate orthonormal basis for $K_k(A, b)$

$$q_1 = \frac{b}{\|b\|}$$

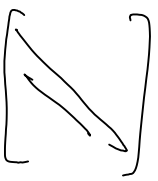
for $k = 2 \ldots$

$$w = A q_{k-1}$$

$$\tilde{q}_k = w - \sum_{j=1}^{k-1} q_j q_j^T w \quad \text{(Gram-Schmidt)}$$

$$q_k = \tilde{q}_k / \|q_k\|$$

$$A Q_k = Q_{k+1} H_k$$

$H_k =$ 

reduces to Hess.

end

/ reduces to Upper Hessenberg

minimize $\|H_k z - \|b\| e_1\|^2$ ⇒ equivalent to minimizing residual over subspace