Generalized MINRES and LSQR

Orthogonal tridiagonalization of general matrices

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Outline

1. History

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2. Tridiagonalization of symmetric A

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3. Bidiagonalization of rectangular A

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7. Unsymmetric $Ax = b$
8. Elizabeth Yip's aim

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History of iterative solvers

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- 1982 Paige-Saunders LSQR
  Golub-Kahan bidiagonalization for general $Ax = b$, $\min \|Ax - b\|$

History (contd)

- 1981 Saunders, 2 months in Sweden
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  "The Lanczos algorithm for ... nonsymmetric linear systems"
  (?? Seems to be LSQR with partial reorthogonalization)
- 1988 Saunders, Simon, and Yip, SINUM 25
  "Two CG-type methods for unsymmetric linear equations"
  (USYMLQ and USYMQR $\equiv$ GMINRES)

History (contd)

- 2006 Reichel and Ye

  "A generalized LSQR algorithm" (GLSQR)

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  "A generalized LSQR algorithm" (GLSQR)
  Unsymmetric tridiagonalization, focused on rectangular A
- 2007 Golub, Stoll, and Wathen (draft)
  "Approximation of outputs"
  Unsymmetric tridiagonalization, focused on $Ax = b$, $A^T y = c$
  and estimation of $c^T x$ and $b^T y$

Tridiagonalization of symmetric A using orthogonal matrices

Symmetric A

- Tridiagonalization for dense EVD (eigenvalues)

$$V_1^T A = \begin{pmatrix} * & * & * & * \\ * & * & * & * \\ & * & * & * \\ & * & * & * \end{pmatrix}, \quad V_1^T A V_1 = \begin{pmatrix} * & * & & \\ * & * & * & * \\ & * & * & * \\ & * & * & * \end{pmatrix} \quad \cdots \rightarrow \begin{pmatrix} * & * & & \\ * & * & * & \\ & * & * & * \\ & & * & * \end{pmatrix}$$

$$V^T A V = T \quad \Rightarrow \quad AV = VT$$

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- Symmetric Lanczos process on A, b

$$\beta_1 v_1 = b$$

$$p_1 = Av_1 \qquad \alpha_1 = v_1^T p_1$$
$$\beta_2 v_2 = p_1 - \alpha_1 v_1$$

$$p_2 = Av_2 \qquad \alpha_2 = v_2^T p_2$$
$$\beta_3 v_3 = p_2 - \alpha_2 v_2 - \beta_1 v_1$$

$$T_k = \begin{pmatrix} \alpha_1 & \beta_2 & & \\ \beta_2 & \alpha_2 & \beta_3 & \\ & * & * & * \\ & & \beta_k & \alpha_k \end{pmatrix}$$

$$V_k = \begin{pmatrix} v_1 & v_2 & \ldots & v_k \end{pmatrix}$$

$$AV_k = V_k T_k + \beta_{k+1} v_{k+1} e_k^T$$

Bidiagonalization of rectangular A

Rectangular A

- Bidiagonalization for dense SVD (Golub and Kahan 1965)

$$U_1^T A = \begin{pmatrix} * & * & * & * \\ & * & * & * \\ & * & * & * \\ & * & * & * \\ & * & * & * \end{pmatrix}, \quad U_1^T A V_1 = \begin{pmatrix} * & * & & \\ & * & * & * \\ & * & * & * \\ & * & * & * \\ & * & * & * \end{pmatrix} \quad \cdots \longrightarrow \begin{pmatrix} * & * & & \\ & * & * & \\ & & * & * \\ & & & * \\ & & & \end{pmatrix}$$

$$U^T A V = B \quad \Rightarrow \quad AV = UB, \quad A^T U = V B^T$$

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$$U^T AV = B \quad \Rightarrow \quad AV = UB, \quad A^T U = VB^T$$

- Golub-Kahan process on A, b

$$\beta_1 u_1 = b, \quad \alpha_1 v_1 = A^T u_1$$

$$\beta_2 u_2 = Av_1 - \alpha_1 v_1$$
$$\alpha_2 v_2 = A^T u_2 - \beta_2 v_1$$

$$B_k = \begin{pmatrix} \alpha_1 & & & \\ \beta_2 & \alpha_2 & & \\ & * & * & \\ & & \beta_k & \alpha_k \\ & & & \beta_{k+1} \end{pmatrix}$$

$$U_k = \begin{pmatrix} u_1 & u_2 & \dots & u_k \end{pmatrix}$$
$$V_k = \begin{pmatrix} v_1 & v_2 & \dots & v_k \end{pmatrix}$$

$$AV_k = U_{k+1} B_k, \quad A^T U_k = V_k L_k^T$$

Upper or lower bidiagonal?

- Dense A

$$AV = UB \quad = \quad U \begin{pmatrix} * & * & & \\ & * & * & \\ & & * & * \\ & & & * \\ & & & \end{pmatrix}$$

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$$AV = UB = U \begin{pmatrix} * & * & & \\ & * & * & \\ & & * & * \\ & & & * \\ & & & \end{pmatrix}$$

- Sparse A with $b = \beta_1 u_1$

$$AV_k = U_{k+1} B_k \quad \Rightarrow \quad \begin{pmatrix} b & AV_k \end{pmatrix} = U_{k+1} \begin{pmatrix} \beta_1 e_1 & B_k \end{pmatrix}$$

$$\Rightarrow \quad \begin{pmatrix} b & A \end{pmatrix} \begin{pmatrix} 1 & \\ & V_k \end{pmatrix} = U_{k+1} \begin{pmatrix} * & * & & \\ & * & * & \\ & & * & * \\ & & & * \end{pmatrix}$$

Tridiagonalization of unsymmetric or rectangular A (the "new method")

Rectangular A

- Tridiagonalization for dense EVD (eigenvalues)

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$$U^T A V = T \quad \Rightarrow \quad AV = UT, \quad A^T U = VT^T$$

- Bi-tridiagonalization process on A, b, c

$$\beta_1 u_1 = b \qquad \gamma_1 v_1 = c$$

$$p_1 = A v_1 \qquad \alpha_1 = u_1^T p_1$$

$$\beta_2 u_2 = p_1 - \alpha_1 u_1 - \gamma_1 u_0$$

$$q_1 = A^T u_2$$

$$\gamma_2 v_2 = q_1 - \alpha_1 v_1 - \beta_1 v_0$$

$$T_k = \begin{pmatrix} \alpha_1 & \gamma_2 & & \\ \beta_2 & \alpha_2 & \gamma_3 & \\ & * & * & * \\ & & \beta_k & \alpha_k \end{pmatrix}$$

$$U_k = \begin{pmatrix} u_1 & u_2 & \ldots & u_k \end{pmatrix}$$

$$V_k = \begin{pmatrix} v_1 & v_2 & \ldots & v_k \end{pmatrix}$$

$$\begin{aligned} AV_k &= U_k T_k + \beta_{k+1} u_{k+1} e_k^T \\ A^T U_k &= V_k T_k^T + \gamma_{k+1} v_{k+1} e_k^T \end{aligned}$$

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- CG, SYMMLQ, MINRES work well for symmetric $Ax = b$
- Bi-tridiagonalization of unsymmetric A is no more than twice the work and storage per iteration
- If A is symmetric, we get Lanczos
- If A is nearly symmetric, total itns should be not much more

Solving symmetric $Ax = b$ via Lanczos

Symmetric $Ax = b$

Lanzcos process:

$$AV_k = V_{k+1}H_k, \qquad H_k = \begin{pmatrix} \alpha_1 & \beta_2 & & \\ \beta_2 & \alpha_2 & \beta_3 & \\ & * & * & * \\ & & \beta_k & \alpha_k \\ & & & \beta_{k+1} \end{pmatrix}$$

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Suppose $x_k = V_k w_k$ for some w_k

- $r_k = b - Ax_k$
- $r_k = V_{k+1}(\beta_1 e_1 - H_k w_k)$

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- $\|r_k\|$ will be small if $H_k w_k \approx \beta_1 e_1$

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Three subproblems make $H_k w_k \approx \beta_1 e_1 \quad \Rightarrow \quad$ CG, SYMMLQ, MINRES
(e.g. $T_k w_k = \beta_1 e_1$ for CG)

Symmetric → Unsymmetric

Lanczos on $\begin{pmatrix} I & A \\ A^T & \end{pmatrix} \begin{pmatrix} r \\ x \end{pmatrix} = \begin{pmatrix} b \\ 0 \end{pmatrix}$ (general A)

leads to Golub-Kahan and LSQR

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Lanczos on $\begin{pmatrix} & A \\ A^T & \end{pmatrix} \begin{pmatrix} y \\ x \end{pmatrix} = \begin{pmatrix} b \\ c \end{pmatrix}$ (square A)

is not equivalent to bi-tridiagonalization (but seems worth trying!)

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Lanczos on $\begin{pmatrix} I & A \\ A^T & \end{pmatrix} \begin{pmatrix} r \\ x \end{pmatrix} = \begin{pmatrix} b \\ c \end{pmatrix}$ (general A)

is not equivalent either (Who would like to try?)

Solving unsymmetric $Ax = b$
via bi-tridiagonalization

Unsymmetric $Ax = b$

Bi-tridiag process:

$$\begin{aligned} AV_k &= U_k T_k + \beta_{k+1} u_{k+1} e_k^T &\equiv& \quad U_{k+1} H_k^{\beta} \\ A^T U_k &= V_k T_k^T + \gamma_{k+1} v_{k+1} e_k^T &\equiv& \quad V_{k+1} H_k^{\gamma} \end{aligned}$$

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Suppose $x_k = V_k w_k$ for some w_k
Three subproblems make $H_k^{\beta} w_k \approx \beta_1 e_1 \quad \Rightarrow \quad$ UCG, USYMLQ, USYMQR

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Similarly, let $y_k = U_k \bar{w}_k$ to solve $A^T y = c$
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Similarly, let $y_k = U_k \bar{w}_k$ to solve $A^T y = c$
Three subproblems make $H_k^{\gamma} y_k \approx \gamma_1 e_1$

Not much extra effort to get both x_k and y_k

Elizabeth Yip's motivation (1982)

(Boeing Computer Services Co.)

Elizabeth's SIAM conference abstract (1982)

CG method for unsymmetric matrices applied to PDE problems

We present a CG-type method to solve $Ax = b$, where A is an arbitrary nonsingular unsymmetric matrix. The algorithm is equivalent to an orthogonal tridiagonalization of A.

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We apply a preconditioned version (Fast Poisson) to the difference equation of unsteady transonic flow with small disturbances. (Compared with ORTHOMIN(5))

Numerical results with unsymmetric tridiagonalization

Numerical results (SSY 1988)

$$A = \begin{pmatrix} B & -I & & & \\ -I & B & -I & & \\ & \ddots & \ddots & \ddots & \\ & & -I & B & -I \\ & & & -I & B \end{pmatrix} \qquad B = \text{tridiag}\begin{pmatrix} -1-\delta & 4 & -1+\delta \end{pmatrix}$$

400×400 $\qquad$ 20×20

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Megaflops to reach $\|r\| \le 10^{-6}\|b\|$:

δ	0.0	0.01	0.1	1.0	10.0	100.0
ORTHOMIN(5)	0.31	0.57	0.75	0.83	2.55	2.11
LSQR	0.28	1.38	1.48	0.80	0.57	0.27
USYMQR	0.30	1.88	1.98	1.41	0.99	0.64

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$$B = \text{tridiag}\begin{pmatrix} -1-\delta & 4 & -1+\delta \end{pmatrix}$$

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ORTHOMIN(5)	0.31	0.57	0.75	0.83	2.55	2.11
LSQR	0.28	1.38	1.48	0.80	0.57	0.27
USYMQR	0.30	1.88	1.98	1.41	0.99	0.64

Bottom line:
ORTHOMIN sometimes good, can fail. LSQR always better than USYMQR

Numerical results (Reichel and Ye 2006)

- Focused on rectangular A and least-squares
  (Forgot about SSY88 and USYMQR — hence GLSQR)

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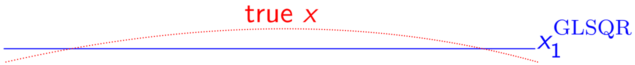
Example 1: We know $x \approx$ constant. Choose $c = \begin{pmatrix} 1 & 1 & \dots & 1 \end{pmatrix}^T$



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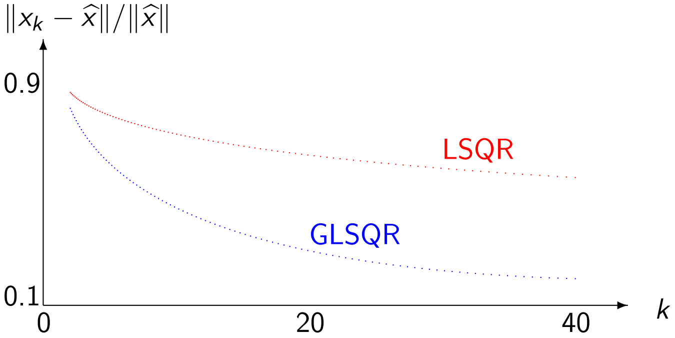

Conclusions

Subspaces

- Unsymmetric Lanczos generates two Krylov subspaces:

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\begin{aligned}
U_k &\in \operatorname{span}\{b \quad Ab \quad A^2 b \quad \ldots \quad A^{k-1} b\} \\
V_k &\in \operatorname{span}\{c \quad A^T c \quad (A^T)^2 c \quad \ldots \quad (A^T)^{k-1} c\}
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- Bi-tridiagonalization generates

$$\begin{array}{lll} U_{2k} & \in & \text{span}\{b \;\; AA^T b \;\; \ldots \;\; (AA^T)^{k-1} b \;\; Ac \;\; (AA^T)Ac \;\; \ldots\} \\ V_{2k} & \in & \text{span}\{c \;\; A^T Ac \;\; \ldots \;\; (A^T A)^{k-1} c \;\; A^T b \;\; (A^T A) A^T b \;\; \ldots\} \end{array}$$

Functionals $c^T x$, $b^T y$

- Lu and Darmofal (SISC 2003) use unsymmetric Lanczos with QMR to solve $Ax = b$ and $A^T y = c$ *simultaneously* and to estimate $c^T x$ and $b^T y$ at a *superconvergent rate*:

$$|c^T x_k - c^T x| \approx |b^T y_k - b^T y| \approx \frac{\|b - Ax_k\| \|c - A^T y_k\|}{\sigma_{\min}(A)}$$

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Thanks for your patience!!