GMINRES or GLSQR?

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Matrix Computations – Foundation and Future
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Outline

1. Iterative matrix reductions

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2. CG-type iterative solvers

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3. Bi-tridiagonalization of general A

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4. Numerical results

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Abstract

Given a general matrix A and starting vectors (b, c), we can construct orthonormal matrices U_k and V_k that reduce A to tridiagonal form: $AV_k \approx U_k T_k$ and $A^T U_k \approx V_k T_k^T$. Saunders, Simon, and Yip (1988) proposed methods for solving square systems $Ax = b$ and $A^T y = c$ simultaneously. The solver USYMQR becomes equivalent to MINRES in the symmetric case with $b = c$.

The method was rediscovered by Reichel and Ye (2006) with emphasis on rectangular systems. For implementation reasons it was regarded as a generalization of LSQR (although it does not reduce to LSQR in any special case). The method has now been applied to two square systems by Golub, Stoll, and Wathen (2007) with focus on estimating $c^T x$ and $y^T b$.

Iterative matrix reductions

• Lanczos	1950	Symmetric
• Arnoldi	1951	Square
• Golub-Kahan	1965	Rectangular
• "New" tridiagonalization	1981–1988, 2006	Rectangular

We call them *processes*

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- Need starting vector $v_1 = b$ (Assume $\|b\| = 1$)

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$V_k^T V_k = I$ in theory, but at least $\|v_k\| = 1$

CG-type iterative solvers

for $Ax = b$

• MINRES	Lanczos	$AV_k = V_{k+1}H_k$
• GMRES	Arnoldi	$AV_k = V_{k+1}H_k$
• LSQR	Golub-Kahan bidiagonalization	$AV_k = U_{k+1}B_k$ $A^TU_{k+1} = V_kB_k^T + \cdots$
• GMINRES? GLSQR?	S-Simon-Yip bi-tridiagonalization	$AV_k = U_{k+1}H_k$ $A^TU_k = V_{k+1}\bar{H}_k$

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They all solve $\min \|X w_k - e_1\|$ and define $x_k = V_k w_k$

$(X = H_k$ or $B_k)$

MINRES

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Let $x_k = V_k w_k$, where we solve $\min \| H_k w_k - e_1 \|$

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- $Ax_k - b = V_{k+1}(H_k w_k - e_1)$
- Will be small if $H_k w_k \approx e_1$
- 3 subprobs make $H_k w_k \approx e_1$ $\longrightarrow$ CG, SYMMLQ, MINRES
- $v_1 = b \Rightarrow$ no need to assume V_k has orthogonal columns

Symmetric $\rightarrow$ Unsymmetric $Ax \approx b$

Lanczos on $\begin{pmatrix} I & A \\ A^T & -\delta^2 I \end{pmatrix} \begin{pmatrix} r \\ x \end{pmatrix} = \begin{pmatrix} b \\ 0 \end{pmatrix}$ (general A)
with CG-type subproblem gives Golub-Kahan and LSQR

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!)

Tridiagonalization of general A using orthogonal matrices

Bi-tridiagonalization

- 1988 Saunders, Simon, and Yip, SINUM 25

  "Two CG-type methods for unsymmetric linear equations"

  Focus on square A

  USYMLQ and USYMQR (GSYMMLQ and GMINRES)

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- 2007 Golub, Stoll, and Wathen

  "Approximation of the scattering amplitude"

  Focus on $Ax = b$, $A^T y = c$

  and estimation of $c^T x$, $b^T y$ (without x, y)

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- Bi-tridiagonalization of unsymmetric A is no more than twice the work and storage per iteration
- If A is symmetric, we get Lanczos and MINRES etc
- If A is nearly symmetric, total itns should be not much more

Elizabeth Yip'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.

Each iteration takes more work than the orthogonal bidiagonalization proposed by Golub-Kahan, Paige-Saunders for sparse least squares problems (LSQR).

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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))

Unsymmetric $Ax = b$, $A^T y = c$

Bi-tridiag process starting with (b, c)

$$\begin{aligned} AV_k &= U_{k+1} H_k \\ A^T U_k &= V_{k+1} \bar{H}_k \end{aligned}$$

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Similarly, let $y_k = U_k \bar{w}_k$ to solve $A^T y = c$

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Not much extra effort to get both x_k and y_k

Numerical results with unsymmetric tridiagonalization

Numerical results (SSY 1988)

$$A = \begin{pmatrix} B & -I & & & \\ -I & B & -I & & \\ & \ddots & \ddots & \ddots & \\ & & -I & B & -I \\ & & & -I & B \end{pmatrix}$$

400×400

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

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

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- Focused on rectangular A and least-squares
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  stopping early
  looking at $x_k = \begin{pmatrix} x_{k1} & x_{k2} & \dots & x_{kn} \end{pmatrix}$

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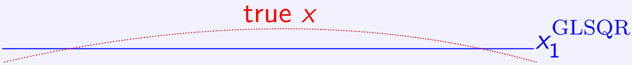
Example 1: We know $x \approx$ constant. Choose $c = \begin{pmatrix} 1 & 1 & \dots & 1 \end{pmatrix}^T$



Example 2 (Star cluster)

- 256×256 pixels ($n = 65536$), 470 stars

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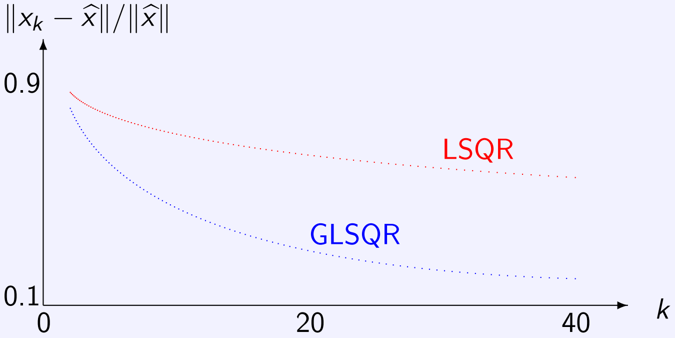

Conclusions

Subspaces

- Unsymmetric Lanczos generates two Krylov subspaces:

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

$$
\begin{aligned}
U_{2k} &\in \operatorname{span}\{b \;\; AA^T b \;\; \dots \;\; (AA^T)^{k-1} b \;\; Ac \;\; (AA^T)Ac \;\; \dots\} \\
V_{2k} &\in \operatorname{span}\{c \;\; A^T Ac \;\; \dots \;\; (A^T A)^{k-1} c \;\; A^T b \;\; (A^T A)A^T b \;\; \dots\}
\end{aligned}
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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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  - Matrices, moments, and quadrature
  - Golub, Minerbo, and Saylor
    Nine ways to compute the scattering cross-section
    (1): Estimating $c^T x$ iteratively

Block Lanczos

The Bi-tridiagonalization process is equivalent to

- Block Lanczos on $A^T A$ with starting block $\begin{pmatrix} c & A^T b \end{pmatrix}$
  Parlett 1987

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Messages from Marcus Grote (Switzerland) and Yong Sun (China)