Generalized MINRES or Generalized LSQR?

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New Frontiers in Numerical Analysis and Scientific Computing
on the occasion of Lothar Reichel's 60th birthday
and the 20th anniversary of ETNA

Department of Mathematical Sciences
Kent State University

Motivation

The Golub-Kahan orthogonal bidiagonalization of $A \in \mathbb{R}^{m \times n}$ gives us freedom to choose 1 starting vector $b \in \mathbb{R}^m$ and solve sparse systems $Ax \approx b$ (as in LSQR)

But orthogonal tridiagonalization gives us freedom to choose 2 starting vectors $b \in \mathbb{R}^m$ and $c \in \mathbb{R}^n$ and solve two sparse systems systems $Ax \approx b$ and $A^T y \approx c$ (as in USYMQR $\equiv$ GMINRES)

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Reichel and Ye (2008) chose c to speed up the computation of x

Golub, Stoll and Wathen (2008) wanted $c^T x = b^T y$

Abstract

Given a general matrix A, we can construct orthogonal matrices U, V that reduce A to tridiagonal form: $U^TAV = T$. We can also arrange that the first columns of U and V are proportional to given vectors b and c. For square A, an iterative form of this orthogonal tridiagonalization was given by Saunders, Simon, and Yip (SINUM 1988) and used to solve square systems $Ax = b$ and $A^Ty = c$ simultaneously. (One of the resulting solvers becomes MINRES when A is symmetric and $b = c$.)

The approach was rediscovered by Reichel and Ye (NLAA 2008) with emphasis on rectangular A and least-squares problems $Ax \approx b$. The resulting solver was regarded as a generalization of LSQR (although it doesn't become LSQR in any special case). Careful choice of c was shown to improve convergence.

In his last year of life, Gene Golub became interested in "GLSQR" for estimating $c^Tx = b^Ty$ without computing x or y (Golub, Stoll, and Wathen (ETNA 2008)). We review the tridiagonalization process and Gene et al.'s insight into its true identity.

Orthogonal matrix reductions

Direct: $V =$ **product of Householder transformations** $n \times n$

Iterative: $V_k = \begin{pmatrix} v_1 & v_2 & \ldots & v_k \end{pmatrix}$ $n \times k$

Mostly short-term recurrences

Tridiagonalization of symmetric A

Direct:

$$\begin{pmatrix} 1 & \\ & V^T \end{pmatrix} \begin{pmatrix} 0 & b^T \\ b & A \end{pmatrix} \begin{pmatrix} 1 & \\ & V \end{pmatrix} = \begin{pmatrix} 0 & x & & & \\ x & x & x & & \\ & x & x & x & \\ & & x & x & x \\ & & & x & x \end{pmatrix}$$

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Iterative: Lanczos process

$$\begin{pmatrix} b & AV_k \end{pmatrix} = V_{k+1} \begin{pmatrix} \beta e_1 & T_{k+1,k} \end{pmatrix}$$

Bidiagonalization of rectangular A

Direct:

$$U^T \begin{pmatrix} b & A \end{pmatrix} \begin{pmatrix} 1 & \\ & V \end{pmatrix} = \begin{pmatrix} x & x & & & \\ & x & x & & \\ & & x & x & \\ & & & x & x \\ & & & & x \\ & & & & \\ & & & & \end{pmatrix}$$

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Iterative: Golub-Kahan process

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Tridiagonalization of rectangular A

Direct:

$$\begin{pmatrix} 1 & \\ & U^T \end{pmatrix} \begin{pmatrix} 0 & c^T \\ b & A \end{pmatrix} \begin{pmatrix} 1 & \\ & V \end{pmatrix} = \begin{pmatrix} 0 & x & & & \\ x & x & x & & \\ & x & x & x & \\ & & x & x & x \\ & & & x & x \\ & & & & x \\ & & & & \end{pmatrix}$$

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Iterative: S-Simon-Yip (1988), Reichel-Ye (2008)

$$\begin{pmatrix} b & AV_k \end{pmatrix} = U_{k+1} \begin{pmatrix} \beta e_1 & T_{k+1,k} \end{pmatrix}$$
$$\begin{pmatrix} c & A^T U_k \end{pmatrix} = V_{k+1} \begin{pmatrix} \gamma e_1 & T_{k,k+1}^T \end{pmatrix}$$

MINRES-type solvers

based on

Lanczos, Arnoldi, Golub-Kahan, orth-tridiag

MINRES-type solvers for $Ax \approx b$

A	Process			Solver
symmetric	Lanczos	Paige-S	1975	MINRES
		Choi-Paige-S	2011	MINRES-QLP
rectangular	Golub-Kahan	Paige-S	1982	LSQR
		Fong-S	2011	LSMR
unsymmetric	Arnoldi	Saad-Schultz	1986	GMRES
unsymmetric	orth-tridiag	S-Simon-Yip	1988	USYMQR
rectangular	orth-tridiag	Reichel-Ye	2008	GLSQR

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All these processes produce similar outputs:

$$\text{Lanczos} \qquad \begin{pmatrix} b & AV_k \end{pmatrix} = V_{k+1} \begin{pmatrix} \beta e_1 & T_{k+1,k} \end{pmatrix}$$

$$\text{Golub-Kahan} \qquad \begin{pmatrix} b & AV_k \end{pmatrix} = U_{k+1} \begin{pmatrix} \beta e_1 & B_{k+1,k} \end{pmatrix}$$

$$\text{orth-tridiag} \qquad \begin{pmatrix} b & AV_k \end{pmatrix} = U_{k+1} \begin{pmatrix} \beta e_1 & T_{k+1,k} \end{pmatrix}$$

$$\text{and} \qquad \begin{pmatrix} c & A^T U_k \end{pmatrix} = V_{k+1} \begin{pmatrix} \gamma e_1 & T_{k,k+1}^T \end{pmatrix}$$

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All methods:

$$\begin{pmatrix} b & AV_k \end{pmatrix} = U_{k+1} \begin{pmatrix} \beta e_1 & H_k \end{pmatrix}$$

$$b - AV_k w_k = U_{k+1}(\beta e_1 - H_k w_k)$$

$$\|b - AV_k w_k\| \le \|U_{k+1}\| \, \|\beta e_1 - H_k w_k\|$$

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$$\|b - AV_k w_k\| \le \|U_{k+1}\| \, \|\beta e_1 - H_k w_k\|$$

$\Rightarrow \; x_k = V_k w_k$ where we choose w_k from $\min \|\beta e_1 - H_k w_k\|$

Symmetric methods for unsymmetric $Ax \approx b$

Lanczos on $\begin{pmatrix} I & A \\ A^T & -\delta^2 I \end{pmatrix} \begin{pmatrix} r \\ x \end{pmatrix} = \begin{pmatrix} b \\ 0 \end{pmatrix}$ gives Golub-Kahan

CG-type subproblem gives LSQR

MINRES-type subproblem gives LSMR

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CG-type subproblem gives LSQR
MINRES-type subproblem gives LSMR

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 orthogonal tridiagonalization
(but seems worth a try!)

Tridiagonalization of general A using **orthogonal** matrices

Some history

Orthogonal 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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  "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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- 2012 Patrick Küschner, Max Planck Institute, Magdeburg

  Eigenvalues

  Need to solve $Ax = b$ and $A^T y = c$

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- 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.

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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 orthogonal 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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400×400 $\qquad$ 20×20

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
GMINRES	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 GMINRES

Numerical results (Reichel and Ye 2008)

- Focused on rectangular A and least-squares
  (Forgot about SSY 1988 and USYMQR — hence GLSQR)
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- Remember $x_1 \propto v_1 \propto c$ (since $x_k = V_k w_k$ and $c = \gamma v_1$)
- Focused on
  - choice of c
  - stopping early
  - looking at $x_k = \begin{pmatrix} x_{k1} & x_{k2} & \dots & x_{kn} \end{pmatrix}$

Numerical results (Reichel and Ye 2008)

Example 1 (Fredholm equation)

$$\int_0^\pi \kappa(s,t)x(t)dt = b(s), \qquad 0 \le s \le \frac{\pi}{2}$$

- Discretize to get $A\hat{x} = \hat{b}$, $n = 400$ Solve $Ax = b$, $\|b - \hat{b}\| = 10^{-3}\,\|\hat{b}\|$

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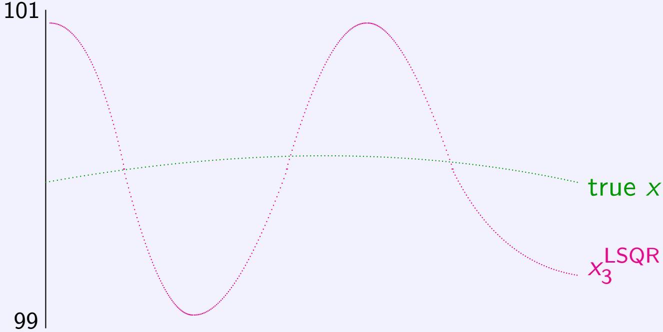
- Among $\{x_k^{\text{LSQR}}\}$, x_3^{LSQR} is closest to $\hat{x}$



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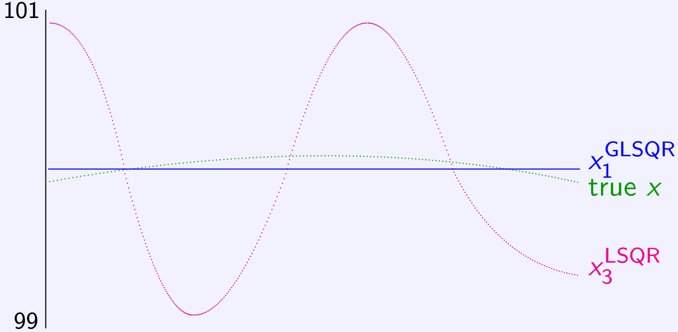
- GLSQR: choose $c = \begin{pmatrix}1 & 1 & \dots & 1\end{pmatrix}^T$ because true $x \approx 100c$



Numerical results (Reichel and Ye 2008)

Example 2 (Star cluster)

- 470 stars, $\hat{x} = 256 \times 256$ pixels, $\hat{b} = A\hat{x}$, $n = 65536$
- Solve $Ax = b$, $\|b - \hat{b}\| = 10^{-2} \|\hat{b}\|$

Numerical results (Reichel and Ye 2008)

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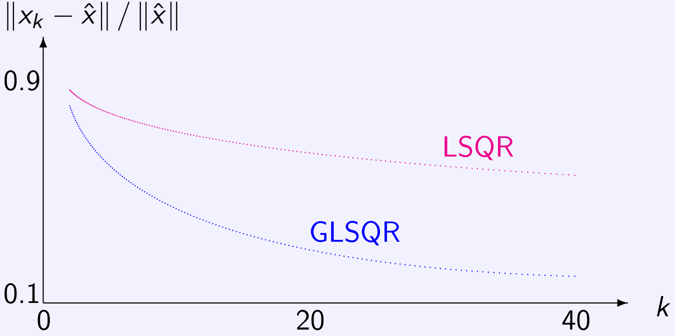
- Solve $Ax = b$, $\|b - \hat{b}\| = 10^{-2}\,\|\hat{b}\|$
- Choose $c = b$ (because $b \approx x$)
- Compare error in x_k^{LSQR} and x_k^{GLSQR} for 40 iterations



Numerical results (Reichel and Ye 2008)

Example 3 (Fredholm equation)

$$\int_0^1 k(s,t)x(t)dt = \exp(s) + (1-e)s - 1, \qquad 0 \leq s \leq 1$$

$$k(s,t) = \begin{cases} s(t-1), & s < t \\ t(s-1), & s \geq t \end{cases}$$

- Discretize to get $A\hat{x} = \hat{b}$, $n = 1024$
- Solve $Ax = b$, $\|b - \hat{b}\| = 10^{-3}\|\hat{b}\|$
- x_{22}^{LSQR} has smallest error, but oscillates around $\hat{x}$

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- x_{22}^{LSQR} has smallest error, but oscillates around $\hat{x}$
- Discretize coarsely to get $A_c x_c = b_c$, $n = 4$
- Prolongate x_c to get $x_{\text{prl}} \in \mathbb{R}^{1024}$ and starting vector $c = x_{\text{prl}}$
- x_4^{GLSQR} is very close to $\hat{x}$

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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- Orthogonal tridiagonalization generates

$$U_{2k} \in \operatorname{span}\{b \;\; AA^T b \quad \dots \quad (AA^T)^{k-1} b \;\; Ac \quad (AA^T)Ac \quad \dots\}$$
$$V_{2k} \in \operatorname{span}\{c \;\; A^T A c \quad \dots \quad (A^T A)^{k-1} c \;\; A^T b \;\; (A^T A) A^T b \quad \dots\}$$

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- Reichel and Ye 2008:
  Richer subspace for ill-posed $Ax \approx b$ (can choose $c \approx x$)
  A can be rectangular
  Check for early termination of $\{u_k\}$ or $\{v_k\}$ sequence

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 $c^T x = b^T y$ 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 1998
    Nine ways to compute the scattering amplitude (1): Estimating $c^T x$ iteratively

Block Lanczos

Orthogonal tridiagonalization is equivalent to

- block Lanczos on A^TA with starting block $(c \;\; A^Tb)$
  Parlett 1987

Block Lanczos

Orthogonal tridiagonalization is equivalent to

- block Lanczos on A^TA with starting block $\begin{pmatrix} c & A^Tb \end{pmatrix}$
  Parlett 1987
- block Lanczos on $\begin{pmatrix} & A \\ A^T & \end{pmatrix}$ with starting block $\begin{pmatrix} b & \\ & c \end{pmatrix}$
  Golub, Stoll, and Wathen 2008

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There are two ways of spreading light.
To be the candle
or the mirror that reflects it.

– Edith Wharton

References

- M. A. Saunders, H. D. Simon, and E. L. Yip (1988).
  Two conjugate-gradient-type methods for unsymmetric linear equations,
  SIAM J. Numer. Anal. 25:4, 927–940.
- L. Reichel and Q. Ye (2008).
  A generalized LSQR algorithm,
  Numer. Linear Algebra Appl. 15, 643–660.
- G. H. Golub, M. Stoll, and A. Wathen (2008).
  Approximation of the scattering amplitude and linear systems,
  ETNA 31, 178–203.

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  Two conjugate-gradient-type methods for unsymmetric linear equations,
  SIAM J. Numer. Anal. 25:4, 927–940.
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  Two conjugate-gradient-type methods for unsymmetric linear equations,
  SIAM J. Numer. Anal. 25:4, 927–940.
- L. Reichel and Q. Ye (2008).
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- G. H. Golub, M. Stoll, and A. Wathen (2008).
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Happy birthday Lothar!

Thanks for noticing A can be rectangular!

Gene is with us every day