Solving linear systems by orthogonal tridiagonalization (GMINRES and/or GLSQR)

Michael Saunders
Systems Optimization Laboratory (SOL)
Institute for Computational Mathematics and Engineering (ICME)
Stanford University

Workshop on Numerical Linear Algebra and Optimization
on the occasion of Michael Overton's 60th birthday

PIMS
University of British Columbia
Vancouver, BC

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

A general matrix A can be reduced to tridiagonal form by orthogonal transformations on the left and right: $U^T AV = T$. We can arrange that the first columns of U and V are proportional to given vectors b and c. An iterative form of this process was given by Saunders, Simon, and Yip (SINUM 1988) and used to solve square systems $Ax = b$ and $A^T y = c$ 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 $c^T x = b^T y$ without computing x or y. Golub, Stoll, and Wathen (ETNA 2008) revealed that the orthogonal tridiagonalization is equivalent to a certain block Lanczos process. This reminds us of Golub, Luk, and Overton (TOMS 1981): a block Lanczos approach to computing singular vectors.

Meeting for Michael (MXO)

First thought:

Block Lanczos process

(for eigenvectors)

Orthogonal matrix reductions

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

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

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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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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  Focus on $Ax = b$, $A^T y = c$ and estimation of $c^T x = b^T y$ without x, y

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  Focus on $Ax = b$, $A^T y = c$ and estimation of $c^T x = b^T y$ without x, y
- 2012 Patrick Küschner, Max Planck Institute, Magdeburg
  Eigenvalues
  Need to solve $Ax = b$ and $A^T y = c$

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- CG, SYMMLQ, MINRES work well for symmetric $Ax = b$
- 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 $\|r\| \leq 10^{-6}\|b\|$:

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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- Three numerical examples (all square!)
- 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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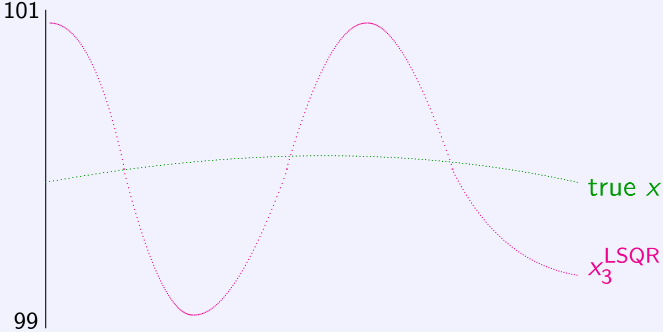
- Among $\{x_k^{\text{LSQR}}\}$, x_3^{LSQR} is closest to $\hat{x}$



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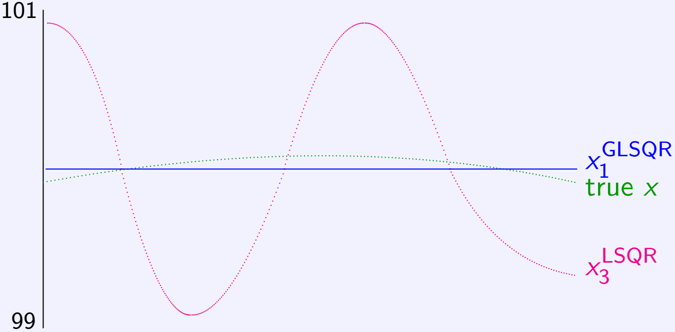
- Among $\{x_k^{\mathrm{LSQR}}\}$, x_3^{LSQR} is closest to $\hat{x}$
- GLSQR: choose $c = \begin{pmatrix}1 & 1 & \dots & 1\end{pmatrix}^T$ because true $x \approx 100c$



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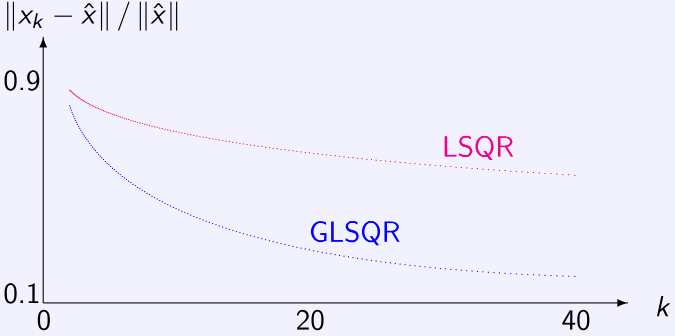
- Solve $Ax = b$, $\|b - \hat{b}\| = 10^{-2}\,\|\hat{b}\|$
- Choose $c = b$ (because $b \approx x$)
- Compare error in x_k^{LSQR} and x_k^{GLSQR} for 40 iterations



Numerical results (Reichel and Ye 2008)

Example 3 (Fredholm equation)

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

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

- 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^2 b \quad \dots \quad A^{k-1} b\} \\
V_k &\in \operatorname{span}\{c \quad A^T c \quad (A^T)^2 c \quad \dots \quad (A^T)^{k-1} c\}
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- Orthogonal tridiagonalization generates

$$U_{2k} \in \text{span}\{b \;\; AA^Tb \;\; \dots \;\; (AA^T)^{k-1}b \;\; Ac \;\; (AA^T)Ac \;\; \dots\}$$
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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

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

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  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

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Happy birthday Michael!

Gene is with us every day