MINRES-QLP: a Krylov subspace method for indefinite or singular symmetric systems

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Abstract

CG, SYMMLQ, and MINRES are Krylov subspace methods for solving symmetric systems of linear equations. When these methods are applied to an incompatible system (that is, a singular symmetric least-squares problem), CG could break down and SYMMLQ’s solution could explode, while MINRES would give a least-squares solution but not necessarily the minimum-length (pseudoinverse) solution. This understanding motivates us to design a MINRES-like algorithm to compute minimum-length solutions to singular symmetric systems.

MINRES uses QR factors of the tridiagonal matrix from the Lanczos process (where $R$ is upper-tridiagonal). MINRES-QLP uses a QLP decomposition (where rotations on the right reduce $R$ to lower-tridiagonal form). On ill-conditioned systems (singular or not), MINRES-QLP can give more accurate solutions than MINRES. We derive preconditioned MINRES-QLP, new stopping rules, and better estimates of the solution and residual norms, the matrix norm, and the condition number.
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Outline

- Symmetric Lanczos
- CG, SYMMLQ, MINRES
- Theorem
- Joke
- MINRES-QLP
- Numerical example
Tridiagonalization of symmetric $A$

Direct (product of Householder transformations):

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

Direct (product of Householder transformations):

\[
\begin{pmatrix}
1 \\ V^T
\end{pmatrix}
\begin{pmatrix}
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\begin{pmatrix}
1 \\ V
\end{pmatrix}
= \begin{pmatrix}
0 & x & x & x \\
 x & x & x & x \\
 x & x & x & x
\end{pmatrix}
\]

Iterative (symmetric Lanczos process):

\[
( b \\ AV_k ) = V_{k+1} \begin{pmatrix}
\beta e_1 \\ T_k
\end{pmatrix}
\]

\[
V_k = \begin{pmatrix}
v_1 & \ldots & v_k
\end{pmatrix} \quad T_k = \begin{pmatrix}
T_k \\ 0 \ldots 0 \beta_{k+1}
\end{pmatrix}
\]
Lanczos for solving $Ax = b$

$\beta v_1 = b$

$V_k = (v_1 \ldots v_k) \quad n \times k$

$x_k = V_k y_k \quad \text{for some } y_k$
Lanczos for solving $Ax = b$

\[
\beta v_1 = b
\]

\[
V_k = \begin{pmatrix} v_1 & \ldots & v_k \end{pmatrix} \quad n \times k
\]

\[
x_k = V_k y_k \quad \text{for some } y_k
\]

\[
\begin{pmatrix} b & AV_k \end{pmatrix} = V_{k+1} \begin{pmatrix} \beta e_1 & T_k \end{pmatrix}
\]

\[
b - AV_k y_k = V_{k+1} \begin{pmatrix} \beta e_1 - T_k y_k \end{pmatrix}
\]

\[
\|b - Ax_k\| \leq \|V_{k+1}\| \left\| \beta e_1 - T_k y_k \right\| \quad \text{make small}
\]
Lanczos properties

For most iterations, \( AV_k = V_{k+1} T_k \)

**Theorem**

\( T_k \) has full column rank for all \( k < \ell \) (so the MINRES subproblem \( \min ||\beta e_1 - T_k y_k|| \) is well defined)
Lanczos properties

For most iterations, \( AV_k = V_{k+1} T_k \)

**Theorem**

\( T_k \) has full column rank for all \( k < \ell \)
(so the MINRES subproblem \( \min \| \beta e_1 - T_k y_k \| \) is well defined)

At the last iteration, \( AV_\ell = V_\ell T_\ell \)

**Theorem**

\( T_\ell \) is nonsingular iff \( b \in \text{range}(A) \), and rank \( T_\ell = \ell \) or \( \ell - 1 \)
(so MINRES is ok only if \( Ax = b \))
Four ways to make $T_k y_k \approx \beta e_1$

\[
\begin{pmatrix}
\alpha_1 & \beta_2 \\
\beta_2 & \alpha_2 & \beta_3 \\
\vdots & \ddots & \ddots \\
\beta_{k-1} & \alpha_{k-1} & \beta_k
\end{pmatrix}
\begin{pmatrix}
\beta \\
0 \\
\vdots \\
0
\end{pmatrix}
= \begin{pmatrix} y_k \end{pmatrix}
\]

\[y_k =
\begin{pmatrix}
\beta \\
0 \\
\vdots \\
0
\end{pmatrix}
\]

SYMMLQ \hspace{1cm} \min \| y_k \| \hspace{1cm} \text{st} \hspace{1cm} T_{k-1}^T y_k = \beta e_1
Four ways to make $T_k y_k \approx \beta e_1$

$$\begin{pmatrix}
\alpha_1 & \beta_2 \\
\beta_2 & \alpha_2 & \beta_3 \\
& \ddots & \ddots & \ddots \\
& & \ddots & \ddots & \ddots \\
& & & \beta_{k-1} & \alpha_{k-1} & \beta_k \\
& & & \beta_k & \alpha_k & \\
\end{pmatrix}
\begin{pmatrix}
y_k \\
\beta \\
0 \\
\vdots \\
\vdots \\
0 \\
0 \\
\end{pmatrix}
= T_k y_k = \beta e_1$$
Four ways to make $T_k y_k \approx \beta e_1$

$$
\begin{pmatrix}
\alpha_1 & \beta_2 \\
\beta_2 & \alpha_2 & \beta_3 \\
\vdots & \ddots & \ddots & \ddots \\
\vdots & \ddots & \ddots & \ddots \\
\beta_{k-1} & \alpha_{k-1} & \beta_k \\
\beta_k & \alpha_k \\
\beta_{k+1}
\end{pmatrix}
\begin{pmatrix}
y_k \approx \\
\beta \\
0 \\
\vdots \\
0 \\
0 \\
0 
\end{pmatrix}
$$

MINRES

$$
\min_{y_k} \| T_k y_k - \beta e_1 \|
$$
Four ways to make \( T_k y_k \approx \beta e_1 \)

\[
\begin{pmatrix}
\alpha_1 & \beta_2 \\
\beta_2 & \alpha_2 & \beta_3 \\
\vdots & \ddots & \ddots & \ddots \\
\beta_{k-1} & \alpha_{k-1} & \beta_k \\
\beta_k & \alpha_k \\
\beta_{k+1}
\end{pmatrix}
\begin{pmatrix}
\beta \\
0 \\
\vdots \\
0 \\
0
\end{pmatrix}
\approx
\begin{pmatrix}
y_k \\
\vdots \\
0
\end{pmatrix}
\]

MINRES \[ \min \| T_k y_k - \beta e_1 \| \]

MINRES-QLP \[ \min \| y_k \| \text{ s.t. } \min \| T_k y_k - \beta e_1 \| \]

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QLP decomposition of $T_k$:

$$Q_k T_k = \begin{pmatrix} R_k \\ 0 \end{pmatrix} , \quad R_k P_k = L_k \quad \Rightarrow \quad Q_k T_k P_k = \begin{pmatrix} L_k \\ 0 \end{pmatrix}$$

$$y = P_k u \quad \Rightarrow \quad Q_k (T_k y - \beta e_1) = \begin{pmatrix} L_k \\ 0 \end{pmatrix} u - \begin{pmatrix} t_k \\ \phi_k \end{pmatrix}$$
QLP decomposition of $T_k$:

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$k < \ell$:

$$L_k u_k = t_k, \quad x_k = V_k P_k u_k$$

orthogonal steps like SYMMLQ
QLP decomposition of $T_k$:

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$k < \ell$:

$$L_k u_k = t_k, \quad x_k = V_k P_k u_k \quad \text{orthogonal steps like SYMMLQ}$$

$k = \ell$:

$$L_\ell u_\ell = t_\ell \quad \text{or} \quad \min \| u_\ell \| \quad \text{st} \quad \min \| L_\ell u_\ell - t_\ell \|$$
Theorem

In MINRES-QLP, \( x_\ell = V_\ell P_\ell u_\ell \) is the min-length solution of \( Ax \approx b \)
Theorem

In MINRES-QLP, $x_\ell = V_\ell P_\ell u_\ell$ is the min-length solution of $Ax \approx b$

Additional features:

- Two-sided spd preconditioner (reduce number of iterations)
- Transfer from MINRES to MINRES-QLP when $T_k$ is moderately ill-conditioned
Theorem

In MINRES-QLP, \( x_\ell = V_\ell P_\ell u_\ell \) is the min-length solution of \( Ax \approx b \)

Additional features:

- Two-sided spd preconditioner (reduce number of iterations)
- Transfer from MINRES to MINRES-QLP when \( T_k \) is moderately ill-conditioned

Per iteration costs:

- Storage: \( 7n - 8n \) vectors
- Matrix-vector multiply: 1
- Work: \( 9n - 14n \) flops
- (Solve a system with preconditioner)
Numerical example

\[ A = \text{tridiag} \left( T \ T \ T \right) \in \mathbb{R}^{400 \times 400}, \quad T = \text{tridiag} \left( 1 \ 1 \ 1 \right) \in \mathbb{R}^{20 \times 20} \]

\[ |\lambda_1|, |\lambda_2| = O(\varepsilon), \quad |\lambda_3|, \ldots, |\lambda_{400}| \in [0.2, 4.3], \quad b_i \sim \text{i.i.d. } U(0, 10) \]
S.-C. T. Choi, C. C. Paige and M. A. Saunders,
“MINRES-QLP: A Krylov subspace method for indefinite or

S.-C. T. Choi, C. C. Paige and M. A. Saunders,
“ALGORITHM: MINRES-QLP for singular symmetric and
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S.-C. T. Choi, “CS-MINRES: a Krylov subspace method for
Complex Symmetric Linear Equations and Least-Squares
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We dedicate MINRES-QLP
to the memory of Gene Golub

Gene’s 75th + Stanford CS 50th
March 30, 2007