MINRES Residual Norms of Diagonally Translated Linear Systems

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1. Motivation

- Solution of large sparse symmetric indefinite systems remains a challenging task.
- Solution of large sparse symmetric positive definite systems can be done efficiently with the CG method.

Rhetorical question: Can we transform solution of an indefinite system in solution of positive definite systems?

Example: Diagonal translation. We consider a linear system

\[ \mathbf{Ax} = \mathbf{b} \]
• $A$ is nonsingular, symmetric and indefinite

• $\lambda_1 < 0$ is the smallest eigenvalue of $A$

• Consider the positive definite system $(A - \lambda I)z = b$, where $I$ is the identity matrix and $\lambda < \lambda_1$

• Problem: If we have found the solution $z$ of the translated system, the solution of the original system is $x = \left( I + \lambda (A - \lambda I)^{-1} \right)^{-1} z$

Computation of iterates from iterates of a translated system is not feasible. But we can formulate a concise relationship between the residuals.
2. An equality for MINRES residual vectors

The MINRES method [Paige, Saunders - 1975]: Starting with an initial guess $x_0$, iterates $x_k$ minimize the residual norm $\|r_k\| = \|b - Ax_k\|$ according to

$$\|r_k\| = \min_{s \in AK_k(A,r_0)} \|r_0 - s\|,$$

where $r_0 = b - Ax_0$ and

$$K_k(A,r_0) \equiv \text{span}\{r_0, Ar_0, \ldots, A^{k-1}r_0\}.$$

Hence $r_0$ is projected onto $AK_k(A,r_0)$,

$$r_k \perp AK_k(A,r_0).$$
Theorem: Let \( [r_0, Ar_0, \ldots, A^k r_0] \) have full column rank. Then

\[ r_k^T = \|r_k\|^2 e_1^T [r_0, Ar_0, \ldots, A^k r_0]^+, \]  

(1)

where \([X]^+\) denotes the Moore-Penrose pseudoinverse of a matrix \(X\).

First proof of this equality by Stewart, later also by [Ipsen - 2000], [Zítko - 2000], [Liesen, Rozložník, Strakoš - 2002]. The elegant proof in the latter article exploits

\begin{itemize}
  \item \(X \cdot X^+ = (X \cdot X^+)^T\)
  \item \(X\) has full column rank \(\Rightarrow X^+ \cdot X = I\)
\end{itemize}
Proof: \[ r_k = r_0 - [A r_0, \ldots, A^k r_0] y_k, \] for some \( y_k \in \mathbb{R}^k \). Hence

\[
r_k = [r_0, \ldots, A^k r_0] \begin{pmatrix} 1 \\ -y_k \end{pmatrix} = [r_0, \ldots, A^k r_0] [r_0, \ldots, A^k r_0] + [r_0, \ldots, A^k r_0] \begin{pmatrix} 1 \\ -y_k \end{pmatrix} \\
= ([r_0, \ldots, A^k r_0] [r_0, \ldots, A^k r_0]^+)^T r_k = ([r_0, \ldots, A^k r_0]^+)^T [r_0, \ldots, A^k r_0]^T r_k.
\]

- \( r_k \perp [A r_0, \ldots, A^k r_0] \)
- \( r_0^T r_k = (r_k + [A r_0, \ldots, A^k r_0] y_k)^T r_k \)
- \( [r_0, \ldots, A^k r_0]^T r_k = \|r_k\|^2 e_1 \)

\[
\Rightarrow \quad r_k = ([r_0, \ldots, A^k r_0]^+)^T \|r_k\|^2 e_1. \quad \square
\]
3. An equality for MINRES residual vectors for diagonally translated systems

An equality for the special case of splitting of tridiagonal Toeplitz matrices is given in [Liesen, Strakoš - 2004]:

\[ T = \begin{pmatrix}
\lambda & \gamma & & & \\
\gamma & \lambda & \gamma & & \\
& \ddots & \ddots & \ddots & \\
& & \gamma & \lambda & \gamma \\
& & & \gamma & \lambda
\end{pmatrix} = \gamma S + \gamma S^T + \lambda I, \]

where \( S \) is the downshift matrix \( S = (e_2, \ldots, e_n, 0) \).
**Theorem:** Residual vectors generated by the MINRES method applied to a system $T x = b$ with a given initial residual $r_0 = b - Ax_0$ such that $[r_0, Tr_0, \ldots, T^k r_0]$ has full column rank, satisfy

$$r_k^T = \|r_k\|^2 [1, -\lambda, \ldots, (-\lambda)^k] \cdot [r_0, (\gamma S + \gamma S^T)r_0, \ldots, (\gamma S + \gamma S^T)^k r_0]^+.$$ 

Generalization for arbitrary diagonally translated systems:
**Theorem:** Let $\lambda \in \mathbb{R}$ and let $B = A - \lambda I$. Then the residual vectors generated by MINRES applied to $Ax = b$ with initial residual $r_0$ such that $[r_0, Ar_0, \ldots, A^kr_0]$ has full column rank, satisfy

$$r_k^T = \|r_k\|^2 [1, -\lambda, \ldots, (-\lambda)^k] \cdot [r_0, Br_0, \ldots, B^kr_0]^+,$$

and

$$\|r_k\| = \frac{1}{\| [1, -\lambda, \ldots, (-\lambda)^k] [r_0, Br_0, \ldots, B^kr_0]^+ \|}.$$
Proof:

\[ r_k^T = \|r_k\|^2 e_1^T [r_0, Ar_0, \ldots, A^k r_0]^+ = \|r_k\|^2 g_k^T. \]

\[ \Rightarrow g_k^T [r_0, Ar_0, \ldots, A^k r_0] = e_1^T \quad (2) \]

We can prove

\[ g_k^T [r_0, Br_0, \ldots, B^k r_0] = [1, -\lambda, \ldots, (-\lambda)^k] : \quad (3) \]

- Second entry: \( 0 = g_k^T Ar_0 = g_k^T (B + \lambda I) r_0 = g_k^T Br_0 + \lambda \Rightarrow g_k^T Br_0 = -\lambda \)

- Next entries: \( 0 = g_k^T A^j r_0 = g_k^T (B + \lambda I)^j r_0 = g_k^T \left( \sum_{i=0}^{j} \binom{j}{i} \lambda^i B^{j-i} \right) r_0 \ldots \Rightarrow g_k^T B^j r_0 = (-\lambda)^j \)

Multiply (3) from the right with \([r_0, Br_0, \ldots, B^k r_0]^+:\)

\[ g_k^T = [1, -\lambda, \ldots, (-\lambda)^k][r_0, Br_0, \ldots, B^k r_0]^+. \quad \square \]
**Corollary:** Let \( \mathbf{B} = \mathbf{A} - \lambda \mathbf{I} \) and, in addition to the assumptions of the preceding theorem, \( \mathbf{B} \) be nonsingular. Let \( r^A_k \) denote the MINRES residuals for \( \mathbf{A} \mathbf{x} = \mathbf{b} \) and the initial residual \( r_0 \) and let \( r^B_k \) denote the MINRES residuals for \( \mathbf{B} \mathbf{y} = \mathbf{c} \), with the same initial residual \( r_0 \). Then

\[
\frac{(r^A_k)^T}{\|r^A_k\|^2} = \frac{(r^B_k)^T}{\|r^B_k\|^2} + [0, -\lambda, \ldots, (-\lambda)^k] \cdot [r_0, \mathbf{B}r_0, \ldots, \mathbf{B}^k r_0]^+.
\]

**Proof:** Subtract

\[
\frac{(r^A_k)^T}{\|r^A_k\|^2} = [1, -\lambda, \ldots, (-\lambda)^k] \cdot [r_0, \mathbf{B}r_0, \ldots, \mathbf{B}^k r_0]^+
\]

and

\[
\frac{(r^B_k)^T}{\|r^B_k\|^2} = [1, 0, \ldots, 0] \cdot [r_0, \mathbf{B}r_0, \ldots, \mathbf{B}^k r_0]^+. \quad \square
\]
4. The equality in practice

1. The relation

\[
\frac{(r_k^A)^T}{\|r_k^A\|^2} = \frac{(r_k^B)^T}{\|r_k^B\|^2} + [0, -\lambda, \ldots, (-\lambda)^k] \cdot [r_0, Br_0, \ldots, B^k r_0]^+
\]

shows that the residuals are connected in a rather complicated way, in spite of equality of the Krylov subspaces

\[
\mathcal{K}_k(A, r_0) = \text{span}\{r_0, Ar_0, \ldots, A^{k-1} r_0\}
\]

\[
= \text{span}\{r_0, (A - \lambda I)r_0, \ldots, (A - \lambda I)^{k-1} r_0\} = \mathcal{K}_k(B, r_0).
\]

But

\[
A \mathcal{K}_k(A, r_0) \neq (A - \lambda I) \mathcal{K}_k(A, r_0) = B \mathcal{K}_k(B, r_0),
\]
and the distance of $r_0$ to these spaces determines convergence speed.

Concerning norms we have

$$
\|r^A_k\| = \frac{\|r^B_k\|^2}{\|r^B_k + [0, -\lambda, \ldots, (-\lambda)^k] \cdot \begin{bmatrix} r_0, B r_0, \ldots, B^k r_0 \end{bmatrix}^+ \|}. 
$$

Example: Shifted 2D Laplacian.
We choose $B \equiv L_{60}$, the 2D Laplacian of dimension 3600 from a $60 \times 60$ grid, and $A \equiv L_{60} - \frac{1}{10} I$. Then $\lambda = -0.1$ and $[0, -\lambda, \ldots, (-\lambda)^k] \approx [0, 0.1, 0, \ldots, 0]$ but still the difference in convergence behavior is remarkable.
Laplacian and Shifted Laplacian (3600 × 3600)

Dashed line: $\frac{\|r_k^{L60}\|}{\|r_0\|}$ - Solid line: $\frac{\|r_k^A\|}{\|r_0\|}$. 
2. Derivation of residual bounds? We have

$$\frac{\|r_k\|}{\|r_0\|} \leq \min_{p \in \pi_k} \max_{\lambda_i \in \sigma(A)} |p(\lambda_i)|,$$

where $\pi_k$ denotes the polynomials of maximal degree $k$ with the value 1 at the origin. In the positive definite case this gives the well-known bound

$$\frac{\|r_k\|}{\|r_0\|} \leq \min_{p \in \pi_k} \max_{\lambda \in [\lambda_{\min}, \lambda_{\max}]} |p(\lambda)| \leq 2 \left( \frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right)^k, \quad \kappa = \frac{\lambda_{\max}}{\lambda_{\min}}.$$

In the indefinite case the interval $[\lambda_{\min}, \lambda_{\max}]$ contains zero and the bound becomes useless. Hence one has to divide the interval into

$$[\lambda_{\min}, \lambda_s] \cup [\lambda_{s+1}, \lambda_{\max}], \quad \lambda_{\min} \leq \lambda_s < 0 < \lambda_{s+1} \leq \lambda_{\max}.$$

This makes it very difficult to handle the bound.
If we can choose $\mathbf{B} = \mathbf{A} - \lambda \mathbf{I}$ such that $\mathbf{B}$ is positive definite and $\|r_k^\mathbf{B} + [0, -\lambda, \ldots, (-\lambda)^k] \cdot [r_0, \mathbf{B}r_0, \ldots, \mathbf{B}^kr_0]^+\| \geq \|r_k^\mathbf{B}\|$, then

$$\|r_k^\mathbf{A}\| = \frac{\|r_k^\mathbf{B}\|^2}{\|r_k^\mathbf{B} + [0, -\lambda, \ldots, (-\lambda)^k] \cdot [r_0, \mathbf{B}r_0, \ldots, \mathbf{B}^kr_0]^+\|} \leq \|r_k^\mathbf{B}\|.$$

This should be worked out more in detail.

3. Our equality holds for any residual minimizing method. Originally: developed for the GMRES method to explain the following convergence behavior (solid line) for a convection diffusion model problem (see e.g. [Liesen, Strakoš - 2004]):
Discretized convection diffusion model problem

Solid line: GMRES residual norm reduction.
The system matrix $A$ of dimension $15^2 \times 15^2$ is block tridiagonal with blocks of dimension $15 \times 15$:

$$A = \begin{pmatrix}
\lambda_1 I & \mu_1 I \\
\gamma_1 I & \lambda_2 I & \mu_2 I \\
& \ddots & \ddots & \ddots \\
& & \gamma_{14} I & \lambda_{14} I & \mu_{14} I \\
& & & \gamma_{15} I & \lambda_{15} I
\end{pmatrix},$$

where all $|\mu_i| << 1$ and $\lambda_i$ are close.

We apply our theorem with $B = A - \lambda I$ for a $\lambda$ close to all $\lambda_i$. Then $B$ is close to the matrix with only the blocks $\gamma_i I$. Hence $B^{15} r_0 \approx 0$ for any $r_0$. Now our equality

$$||r_k|| = \frac{1}{||[1,-\lambda,\ldots,(-\lambda)^k][r_0,Br_0,\ldots,B^k r_0]^+||}$$
yields the bounds

\[
\frac{\sigma_{\text{min}}([r_0, B r_0, \ldots, B^k r_0])}{\sqrt{\sum_{j=0}^{k} |\lambda|^{2j}} \leq \|r_k\| \leq \frac{\|B^k r_0\|}{|\lambda|^k}}
\]

displayed above. For details we refer to a future article [DT, Greenbaum, Strakoš - 2005 ?].

4. From the proof it is clear that we can generalize as follows: **Theorem:** Let us consider the residual vectors generated by MINRES applied to \(Ax = b\) with an initial residual \(r_0\) such that \([r_0, A r_0, \ldots, A^k r_0]\) has full column rank. If \(A = B + U\) with \(UB = BU\) and \(Ur_0 = \lambda r_0\), then

\[
r_k^T = \|r_k\|^2 [1, -\lambda, \ldots, (-\lambda)^k] \cdot [r_0, B r_0, \ldots, B^k r_0]^+.
\]
Thank you for your attention.

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