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

$$\mathbf{A}x = b$$

- $\mathbf{A}$ is nonsingular, symmetric and indefinite
- $\lambda_1 < 0$ is the smallest eigenvalue of $\mathbf{A}$
- Consider the positive definite system $(\mathbf{A} - \lambda\mathbf{I})z = b$, where $\mathbf{I}$ 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 $x = \left(\mathbf{I} + \lambda(\mathbf{A} - \lambda\mathbf{I})^{-1}\right)^{-1} z$

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 $\|r_k\| = \|b - \mathbf{A}x_k\|$ according to

$$\|r_k\| = \min_{s \in \mathbf{A}\mathcal{K}_k(\mathbf{A}, r_0)} \|r_0 - s\|,$$

where $r_0 = b - \mathbf{A}x_0$ and

$$\mathcal{K}_k(\mathbf{A}, r_0) \equiv \mathrm{span}\{r_0, \mathbf{A}r_0, \ldots, \mathbf{A}^{k-1}r_0\}.$$

Hence r_0 is projected onto $\mathbf{A}\mathcal{K}_k(\mathbf{A}, r_0)$,

$$r_k \perp \mathbf{A}\mathcal{K}_k(\mathbf{A}, r_0).$$

Theorem: *Let* $[r_0, \mathbf{A}r_0, \ldots, \mathbf{A}^k r_0]$ *have full column rank. Then*

$$r_k^T = \|r_k\|^2 \, e_1^T [r_0, \mathbf{A}r_0, \ldots, \mathbf{A}^k r_0]^+, \tag{1}$$

where $[\mathbf{X}]^+$ *denotes the Moore-Penrose pseudoinverse of a matrix* $\mathbf{X}$.

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

- $\mathbf{X} \cdot \mathbf{X}^+ = (\mathbf{X} \cdot \mathbf{X}^+)^T$
- $\mathbf{X}$ has full column rank $\Rightarrow \mathbf{X}^+ \cdot \mathbf{X} = \mathbf{I}$

Proof: $r_k = r_0 - [\mathbf{A}r_0, \dots, \mathbf{A}^k r_0]\, y_k,$ for some $y_k \in \mathbb{R}^k$. Hence

$$r_k = [r_0, \dots, \mathbf{A}^k r_0] \begin{pmatrix} 1 \\ -y_k \end{pmatrix} = [r_0, \dots, \mathbf{A}^k r_0][r_0, \dots, \mathbf{A}^k r_0]^+ [r_0, \dots, \mathbf{A}^k r_0] \begin{pmatrix} 1 \\ -y_k \end{pmatrix}$$

$$= \left([r_0, \dots, \mathbf{A}^k r_0][r_0, \dots, \mathbf{A}^k r_0]^+\right)^T r_k = ([r_0, \dots, \mathbf{A}^k r_0]^+)^T [r_0, \dots, \mathbf{A}^k r_0]^T r_k.$$

- $r_k \perp [\mathbf{A}r_0, \dots, \mathbf{A}^k r_0]$
- $r_0^T r_k = (r_k + [\mathbf{A}r_0, \dots, \mathbf{A}^k r_0]\, y_k)^T r_k$
- $[r_0, \dots, \mathbf{A}^k r_0]^T r_k = \|r_k\|^2 e_1$

$$\Rightarrow \quad r_k = ([r_0, \dots, \mathbf{A}^k r_0]^+)^T \|r_k\|^2 e_1. \quad \square$$

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]:

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

where $\mathbf{S}$ is the downshift matrix $\mathbf{S} = (e_2, \ldots, e_n, 0)$.

Theorem: *Residual vectors generated by the MINRES method applied to a system* $\mathbf{T}x = b$ *with a given initial residual* $r_0 = b - \mathbf{A}x_0$ *such that* $[r_0, \mathbf{T}r_0, \ldots, \mathbf{T}^k r_0]$ *has full column rank, satisfy*

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

Generalization for arbitrary diagonally translated systems:

Theorem: *Let* $\lambda \in \mathbb{R}$ *and let* $\mathbf{B} = \mathbf{A} - \lambda \mathbf{I}$. *Then the residual vectors generated by MINRES applied to* $\mathbf{A}x = b$ *with initial residual* r_0 *such that* $[r_0, \mathbf{A}r_0, \ldots, \mathbf{A}^k r_0]$ *has full column rank, satisfy*

$$r_k^T = \|r_k\|^2 \, [1, -\lambda, \ldots, (-\lambda)^k] \cdot \left[r_0, \mathbf{B}r_0, \ldots, \mathbf{B}^k r_0 \right]^+,$$

and

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

Proof:

$$r_k^T = \|r_k\|^2 e_1^T [r_0, \mathbf{A} r_0, \ldots, \mathbf{A}^k r_0]^+ \equiv \|r_k\|^2 g_k^T.$$

$$\Rightarrow \quad g_k^T [r_0, \mathbf{A} r_0, \ldots, \mathbf{A}^k r_0] = e_1^T \qquad (2)$$

We can prove $g_k^T [r_0, \mathbf{B} r_0, \ldots, \mathbf{B}^k r_0] = [1, -\lambda, \ldots, (-\lambda)^k]$: (3)

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

Multiply (3) from the right with $[r_0, \mathbf{B} r_0, \ldots, \mathbf{B}^k r_0]^+$:

$$g_k^T = [1, -\lambda, \ldots, (-\lambda)^k][r_0, \mathbf{B} r_0, \ldots, \mathbf{B}^k r_0]^+. \quad \square$$

Corollary: *Let* $\mathbf{B} = \mathbf{A} - \lambda\mathbf{I}$ *and, in addition to the assumptions of the preceding theorem,* $\mathbf{B}$ *be nonsingular. Let* $r_k^{\mathbf{A}}$ *denote the MINRES residuals for* $\mathbf{A}x = b$ *and the initial residual* r_0 *and let* $r_k^{\mathbf{B}}$ *denote the MINRES residuals for* $\mathbf{B}y = c$*, with the same initial residual* r_0*. Then*

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

Proof: Subtract

$$\frac{(r_k^{\mathbf{A}})^T}{\|r_k^{\mathbf{A}}\|^2} = [1, -\lambda, \ldots, (-\lambda)^k] \cdot \left[r_0, \mathbf{B}r_0, \ldots, \mathbf{B}^k r_0\right]^+$$

and

$$\frac{(r_k^{\mathbf{B}})^T}{\|r_k^{\mathbf{B}}\|^2} = [1,\ 0\ ,\ \ldots\ ,\ 0\ ] \cdot \left[r_0, \mathbf{B}r_0, \ldots, \mathbf{B}^k r_0\right]^+. \quad \square$$

4. The equality in practice

1. The relation

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

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

$$\mathcal{K}_k(\mathbf{A}, r_0) = \text{span}\{r_0, \mathbf{A}r_0, \ldots, \mathbf{A}^{k-1}r_0\}$$

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

But

$$\mathbf{A}\mathcal{K}_k(\mathbf{A}, r_0) \neq (\mathbf{A} - \lambda\mathbf{I})\mathcal{K}_k(\mathbf{A}, r_0) = \mathbf{B}\,\mathcal{K}_k(\mathbf{B}, r_0),$$

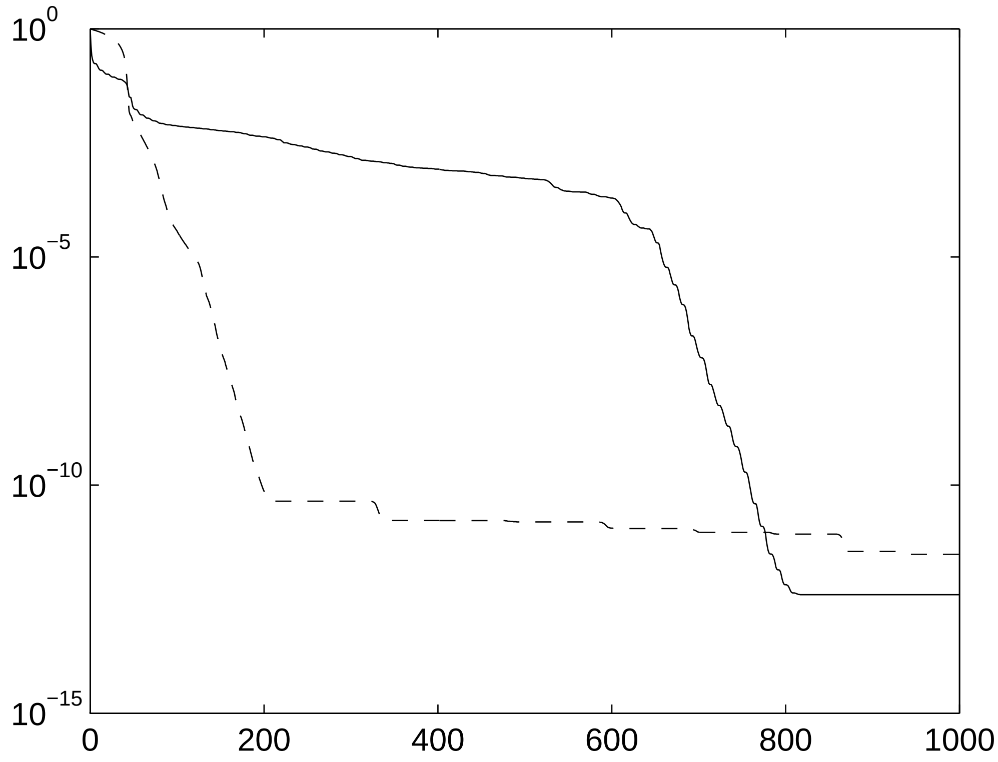
and the distance of r_0 to *these* spaces determines convergence speed.

Concerning norms we have

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

Example: Shifted 2D Laplacian.
We choose $\mathbf{B} \equiv \mathbf{L}_{60}$, the 2D Laplacian of dimension 3600 from a 60×60 grid, and $\mathbf{A} \equiv \mathbf{L}_{60} - \frac{1}{10}\mathbf{I}$. 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: $\frac{\|r_k^{\mathbf{L}_{60}}\|}{\|r_0\|}$ - Solid line: $\frac{\|r_k^{\mathbf{A}}\|}{\|r_0\|}$.

2. Derivation of residual bounds ? We have

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

where π_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

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

This makes it very difficult to handle the bound.

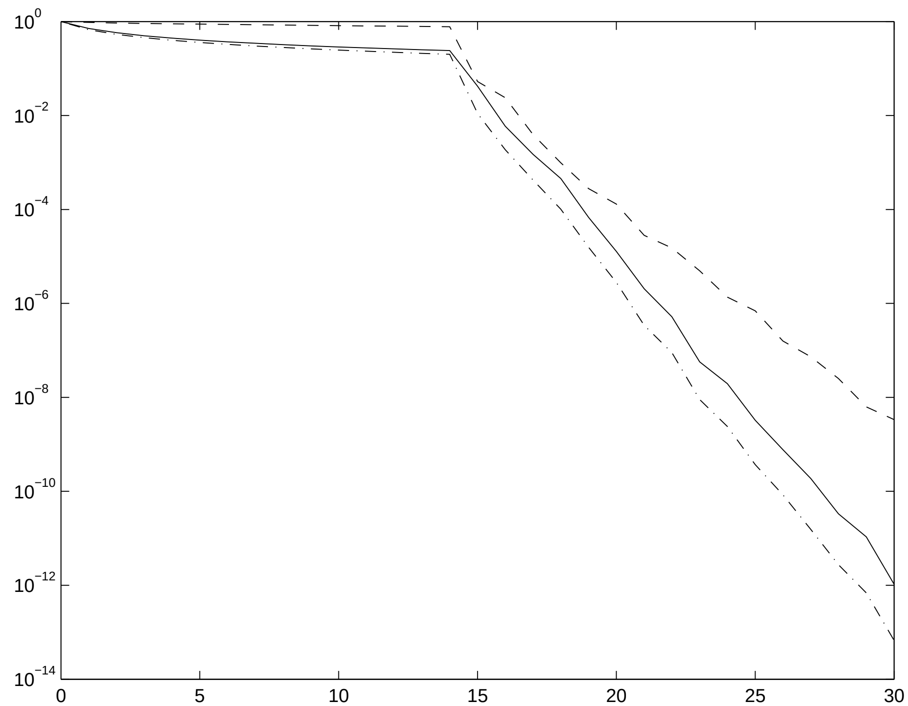
If we can choose $\mathbf{B} = \mathbf{A} - \lambda\mathbf{I}$ such that $\mathbf{B}$ is positive definite and $\|r_k^{\mathbf{B}} + [0, -\lambda, \ldots, (-\lambda)^k] \cdot \left[r_0, \mathbf{B}r_0, \ldots, \mathbf{B}^k r_0\right]^+\| \geq \|r_k^{\mathbf{B}}\|$, then

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

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 15×15:

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

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

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

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

yields the bounds

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

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* $\mathbf{A}x = b$ *with an initial residual* r_0 *such that* $[r_0, \mathbf{A}r_0, \ldots, \mathbf{A}^k r_0]$ *has full column rank. If* $\mathbf{A} = \mathbf{B} + \mathbf{U}$ *with* $\mathbf{UB} = \mathbf{BU}$ *and* $\mathbf{U}r_0 = \lambda r_0$*, then*

$$r_k^T = \|r_k\|^2 \, [1, -\lambda, \ldots, (-\lambda)^k] \cdot \left[r_0, \mathbf{B}r_0, \ldots, \mathbf{B}^k r_0\right]^+ .$$

Thank you for your attention.

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