UNIVERSITÀ
DEGLI STUDI DI TRIESTE

Iterative Methods for Sparse Linear Systems

Solution of symmetric indefinite Linear Systems

The Minimal Residual (MINRES) method

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The MINRES method

MINRES, introduced by Paige and Saunders in:

C. C. Paige and M. A. Saunders
Solution of sparse indefinite systems of linear equations
SIAM J. Numerical Analysis 12, 617-629, 1975

is an efficient variant of the GMRES method for solving symmetric (not SPD) linear systems.

If A is symmetric from the Arnoldi relation

$$V_m^T A V_m = H_m$$

it follows that H_m must be also symmetric and therefore **tridiagonal**.

We will denote $T_m \equiv H_m$ and $T_{m+1,m} \equiv H_{m+1,m}$ the $m+1 \times m$ matrix of the Arnoldi process.

The tridiagonal matrix $T_{m+1,m}$ takes the form

$$T_{m+1,m} = \begin{bmatrix} \alpha_1 & \beta_2 & & & \\ \beta_2 & \alpha_2 & \beta_3 & & \\ & \beta_3 & \alpha_3 & \ldots & \\ & & \ldots & \ldots & \beta_m \\ & & & \beta_m & \alpha_m \\ & & & & \beta_{m+1} \end{bmatrix}.$$

Arnoldi for symmetric matrices: Lanczos

The Arnoldi relation simplifies for symmetric matrices as

$$AV_m = V_{m+1} T_{m+1,m}$$

or

$$A \begin{bmatrix} \boldsymbol{v}_1 & \dots & \boldsymbol{v}_m \end{bmatrix} = \begin{bmatrix} \boldsymbol{v}_1 & \dots & \boldsymbol{v}_{m+1} \end{bmatrix} \begin{bmatrix} \alpha_1 & \beta_2 & & & \\ \beta_2 & \alpha_2 & \beta_3 & & \\ & \beta_3 & \alpha_3 & \dots & \\ & & \dots & \dots & \beta_m \\ & & & \beta_m & \alpha_m \\ & & & & \beta_{m+1} \end{bmatrix}.$$

Equating e.g. column k of the previous relation we obtain

$$A\boldsymbol{v}_k = \beta_k \boldsymbol{v}_{k-1} + \alpha_k \boldsymbol{v}_k + \beta_{k+1} \boldsymbol{v}_{k+1}$$

and thus

$$\beta_{k+1} \boldsymbol{v}_{k+1} = A\boldsymbol{v}_k - \alpha_k \boldsymbol{v}_k - \beta_k \boldsymbol{v}_{k-1}$$

so that any Krylov basis vector $\boldsymbol{v}_{k+1}$ can be obtained using a 3-term recurrence.

Derivation of the MINRES method: the Lanczos algorithm

When A is symmetric the Arnoldi algorithm can be simplified to a 3-term recurrence known as **Lanczos** algorithm:

1: $\boldsymbol{v}_0 = 0, \boldsymbol{w}_1 = \boldsymbol{r}_0, \beta_1 = \|\boldsymbol{w}_1\|_2$
2: **for** $k = 1 : m$ **do**
3: $\quad \boldsymbol{v}_k = \boldsymbol{w}_k / \beta_k$
4: $\quad \boldsymbol{w}_{k+1} = A\boldsymbol{v}_k - \beta_k \boldsymbol{v}_{k-1}$
5: $\quad \alpha_k = \boldsymbol{w}_{k+1}^T \boldsymbol{v}_k$
6: $\quad \boldsymbol{w}_{k+1} = \boldsymbol{w}_{k+1} - \alpha_k \boldsymbol{v}_k$
7: $\quad \beta_{k+1} = \|\boldsymbol{w}_{k+1}\|_2$
8: **end for**

Note that β_k (norm of $\boldsymbol{w}_k$) is used instead of $\boldsymbol{v}_{k-1}^T A \boldsymbol{v}_k$ at step 4.

We will prove in the next slides that these two quantities are the same and that the outcome of this algorithm is an orthonormal basis of $\mathcal{K}_m(A, \boldsymbol{r}_0)$.

The Lanczos method generates an orthonormal krylov basis

Theorem

The Lanczos algorithm constructs an orthonormal basis $\{\boldsymbol{v}_1, \dots, \boldsymbol{v}_m\}$ *of* $\mathcal{K}_m(A, \boldsymbol{r}_0)$.

Sketch of the proof.

The vectors $\{\boldsymbol{v}_1, \dots, \boldsymbol{v}_m\}$ all clearly belong to the Krylov subspace generated by $\boldsymbol{r}_0$ and they have unit norm by construction.

We have to prove that for each $k \geq 1$, $\boldsymbol{v}_j^T \boldsymbol{v}_{k+1} = 0, \ \forall j \leq k$, through the following steps:

(a) $\boldsymbol{v}_k^T \boldsymbol{v}_{k+1} = 0$. This property comes directly from the choice of α_k.

Then we need to prove by induction that $\boldsymbol{v}_j^T \boldsymbol{v}_{k+1} = 0, \ \forall j \leq k-1$:

(b) $\boldsymbol{v}_{k-1}^T \boldsymbol{v}_{k+1} = 0$,

(c) $\boldsymbol{v}_j^T \boldsymbol{v}_{k+1} = 0, \ \forall j < k-1$.

□

Proof.

Proof (continued) By induction. For $k = 1$ the statement is obviously true since $\boldsymbol{v}_0 = 0 \Longrightarrow \boldsymbol{v}_0^T \boldsymbol{v}_2 = 0$.

Assume $\boldsymbol{v}_j^T \boldsymbol{v}_k = 0, \ j \leq k - 2$.

Proof of (b). Premultiplying by $\boldsymbol{v}_{k-1}^T$ the relation

$$\beta_{k+1} \boldsymbol{v}_{k+1} = A\boldsymbol{v}_k - \alpha_k \boldsymbol{v}_k - \beta_k \boldsymbol{v}_{k-1} \tag{1}$$

yields

$$\begin{aligned}
\beta_{k+1} \boldsymbol{v}_{k-1}^T \boldsymbol{v}_{k+1} &= \boldsymbol{v}_{k-1}^T A\boldsymbol{v}_k - \alpha_k \boldsymbol{v}_{k-1}^T \boldsymbol{v}_k - \beta_k \boldsymbol{v}_{k-1}^T \boldsymbol{v}_{k-1} = \\
&= \boldsymbol{v}_k^T A\boldsymbol{v}_{k-1} - \beta_k = \\
&= \boldsymbol{v}_k^T \left(\beta_k \boldsymbol{v}_k + \alpha_{k-1} \boldsymbol{v}_{k-1} + \beta_{k-1} \boldsymbol{v}_{k-2}\right) - \beta_k \\
&= \beta_k - \beta_k = 0.
\end{aligned}$$

Proof of (c). Premultiplying (1) by $\boldsymbol{v}_j^T$, with $j < k - 1$, yields

$$\begin{aligned}
\beta_{k+1} \boldsymbol{v}_j^T \boldsymbol{v}_{k+1} &= \boldsymbol{v}_j^T A\boldsymbol{v}_k - \alpha_k \boldsymbol{v}_j^T \boldsymbol{v}_k - \beta_k \boldsymbol{v}_j^T \boldsymbol{v}_{k-1} = \\
&= \boldsymbol{v}_k^T A\boldsymbol{v}_j = \\
&= \boldsymbol{v}_k^T \left(\beta_{j+1} \boldsymbol{v}_{j+1} + \alpha_j \boldsymbol{v}_j + \beta_j \boldsymbol{v}_{j-1}\right) = 0.
\end{aligned}$$

$\square$

Derivation of MINRES: Residual Minimization

As in the case of GMRES, the MINRES method minimizes the 2-norm of the residual $\boldsymbol{r}_k$

$$\begin{aligned}
\min \|\boldsymbol{r}_k\|_2 &= \min_{\boldsymbol{y}} \|\boldsymbol{r}_0 - AV_k\boldsymbol{y}\|_2 = \\
&= \min_{\boldsymbol{y}} \|\beta_1 \boldsymbol{v}_1 - V_{k+1} T_{k+1,k}\boldsymbol{y}\|_2 = \\
&= \min_{\boldsymbol{y}} \| V_{k+1} \left(\beta_1 \boldsymbol{e}_1 - T_{k+1,k}\boldsymbol{y}\right) \|_2 \\
&= \min_{\boldsymbol{y}} \|\beta_1 \boldsymbol{e}_1 - T_{k+1,k}\boldsymbol{y}\|_2
\end{aligned}$$

Differently from the GMRES method, for MINRES **there is no need to save the Krylov basis** generated by the Lanczos algorithm.

The current iterate $\boldsymbol{x}_k$ can be directly recovered from $\boldsymbol{x}_{k-1}$ as: $\boldsymbol{x}_k = \boldsymbol{x}_{k-1} + a_{k-1}\boldsymbol{p}_{k-1}$

- Let $T_{k+1,k} = Q_{k+1}R_{k+1,k}$ be the QR factorization of the tridiagonal matrix at iteration k and $\tilde{R}$ the square $k \times k$ submatrix of $R_{k+1,k}$ obtained eliminating the last row.
- Define $P_k = \begin{bmatrix} \boldsymbol{p}_0 & \dots & \boldsymbol{p}_{k-1} \end{bmatrix} = V_k\tilde{R}^{-1} \implies P_k\tilde{R} = V_k$.
- Since $\tilde{R}$ has only three nonzero diagonals, we have

$$\boldsymbol{p}_{k-1} = \frac{\boldsymbol{v}_k - r_{k-1,k}\boldsymbol{p}_{k-2} - r_{k-2,k}\boldsymbol{p}_{k-3}}{r_{kk}}$$

Derivation of MINRES

The previous relation comes from equating the last column of the following equation:

$$\begin{pmatrix} \boldsymbol{v}_1 & \boldsymbol{v}_2 & \dots & \boldsymbol{v}_k \end{pmatrix} = \begin{pmatrix} \boldsymbol{p}_0 & \dots & \boldsymbol{p}_{k-3} & \boldsymbol{p}_{k-2} & \boldsymbol{p}_{k-1} \end{pmatrix} \begin{pmatrix} r_{11} & r_{12} & r_{13} & 0 & \dots & 0 \\ 0 & r_{22} & r_{23} & r_{24} & \dots & 0 \\ \dots & 0 & r_{33} & r_{34} & \dots & 0 \\ \dots & \dots & 0 & r_{44} & \dots & r_{k-2,k} \\ \dots & \dots & \dots & 0 & \dots & r_{k-1,k} \\ 0 & 0 & 0 & 0 & 0 & r_{k,k} \end{pmatrix}$$

Now, recalling that the solution of the least squares problem using the QR factorization of $T_{k+1,k}$ is the vector $y = \tilde{R}^{-1}\beta_1\tilde{Q}^T\boldsymbol{e}_1$, where $\tilde{Q} = Q_{k+1,k}(1:k, 1:k)$, we have that:

$$\begin{aligned} \boldsymbol{x}_k &= \boldsymbol{x}_0 + V_k\tilde{R}^{-1}\beta_1\tilde{Q}^T\boldsymbol{e}_1 = \\ &= \boldsymbol{x}_0 + P_k\beta_1 \begin{bmatrix} q_{11} \\ \dots \\ q_{1,k-1} \\ q_{1k} \end{bmatrix} = \\ &= \boldsymbol{x}_0 + \beta_1 P_{k-1} \begin{bmatrix} q_{11} \\ \dots \\ q_{1,k-1} \end{bmatrix} + \beta_1\boldsymbol{p}_{k-1}q_{1k} = \\ &= \boldsymbol{x}_{k-1} + a_{k-1}\boldsymbol{p}_{k-1}. \end{aligned}$$

MINRES convergence

The optimality property of MINRES can be stated as

$$\frac{\|\boldsymbol{r}_k\|_2}{\|\boldsymbol{r}_0\|_2} \le \min_{\substack{P_k \in \Pi_k \\ P_k(0)=1}} \max_{\lambda_i \in \sigma(A)} |P_k(\lambda_i)|$$

Being A symmetric but indefinite zero belongs to the spectral interval $[\lambda_{\min}, \lambda_{\max}]$.

Worst-case MINRES convergence behavior: replace the discrete set of the eigenvalues by the union of two intervals containing all of them and excluding the origin, say

$$I_- \bigcup I_+ \equiv [\lambda_{\min}, \lambda_s] \bigcup [\lambda_{s+1}, \lambda_{\max}]$$

with $\lambda_{\min} \le \lambda_s < 0 < \lambda_{s+1} \le \lambda_{\max}$.

When both intervals are of the same length, i.e., $\lambda_{\max} - \lambda_{s+1} = \lambda_s - \lambda_{\min}$, the following bound for the min-max value holds

$$\frac{\|\boldsymbol{r}_k\|_2}{\|\boldsymbol{r}_0\|_2} \le \min_{\substack{P_k \in \Pi_k \\ P_k(0)=1}} \max_{x \in I_- \bigcup I_+} |P_k(x)| \le 2 \left(\frac{\sqrt{|\lambda_{\min}\lambda_{\max}|} - \sqrt{|\lambda_s \lambda_{s+1}|}}{\sqrt{|\lambda_{\min}\lambda_{\max}|} + \sqrt{|\lambda_s \lambda_{s+1}|}} \right)^{\lfloor k/2 \rfloor} \tag{2}$$

Illustration of the bound

Calling κ the product of the ratio between the endpoints of the intervals,

$$\kappa = \frac{|\lambda_{\max}\lambda_{\min}|}{|\lambda_s \lambda_{s+1}|}$$

("pseudo" condition number relative to I_- and I_+), the bound in (2) reduces to

$$\frac{\|\boldsymbol{r}_k\|_2}{\|\boldsymbol{r}_0\|_2} \leq 2\left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^{\lfloor k/2 \rfloor},$$

which corresponds to the value of the **CG bound** at step $\lfloor k/2 \rfloor$ for an SPD matrix having κ as the condition number.

In the general case when the two intervals are not of the same length, the explicit solution of the min-max approximation problem on $I_- \cup I_+$ becomes quite complicated,

and no simple and explicit bound on the MINRES convergence is known.

Convergence analysis of Krylov subspace methods
Jörg Liesen and Petr Tichy
GAMM, 2014

Preconditioning MINRES

- Even if A is symmetric and indefinite, any preconditioner for MINRES must be symmetric and positive definite. This is necessary since otherwise there is no equivalent symmetric system for the preconditioned matrix.

  Thus a nonsymmetric iterative method (e.g. GMRES) must be used when a **symmetric and indefinite** preconditioner is employed for a symmetric and indefinite matrix.

- A preconditioner for a symmetric indefinite matrix A for use with MINRES therefore can not be an approximation of the inverse of A, since this is also indefinite.

- With a symmetric and positive definite preconditioner, the preconditioned MINRES convergence bounds seen before become

$$\frac{\|\boldsymbol{r}_k\|_{M^{-1}}}{\|\boldsymbol{r}_0\|_{M^{-1}}} \leq \min_{\substack{P_k \in \Pi_k \\ P_k(0)=1}} \max_{\lambda_i \in \sigma(M^{-1}A)} |P_k(\lambda_i)| \leq \min_{\substack{P_k \in \Pi_k \\ P_k(0)=1}} \max_{x \in I_- \bigcup I_+} |P_k(x)|$$

  where the intervals I_- and I_+ now refer to the eigenvalue distribution of the preconditioned matrix.

In summary: a good preconditioner must yield two intervals $I_- = [-\beta, -\alpha]$, $I_+ = [a, b]$

$$\boxed{\text{for which the quantity } \frac{\beta \cdot b}{\alpha \cdot a} \text{ is as small as possible.}}$$

Block Diagonal preconditioner for indefinite linear systems

MINRES particularly suited for indefinite saddle point linear systems like $H\boldsymbol{x} = \boldsymbol{b}$ where

$$H = \begin{bmatrix} A & B^T \\ B & 0 \end{bmatrix}$$

with $A \in \mathbb{R}^{n\times n}$ SPD and $B \in \mathbb{R}^{m\times n}(m < n)$ rectangular with full row rank.

H is highly indefinite having exactly n positive and m negative eigenvalues.

Optimal preconditioner for MINRES:

$$M = \begin{bmatrix} A & 0 \\ 0 & S \end{bmatrix}$$

where $S = BA^{-1}B^T$ is the (SPD) Schur complement matrix.

Theorem

The preconditioned matrix $M^{-1}H$ has only three distinct eigenvalues, namely

$$\sigma(M^{-1}H) = \left\{1, \frac{1-\sqrt{5}}{2}, \frac{1+\sqrt{5}}{2}\right\}.$$

As a consequence MINRES converges in only three iterations!

Block Diagonal preconditioner for indefinite linear systems

Spectral distribution of $M^{-1}H$

Proof.

$\lambda \in \sigma(M^{-1}H)$ satisfies $H\boldsymbol{u} = \lambda M\boldsymbol{u}$, for some $\boldsymbol{u} \neq 0$:

$$\begin{bmatrix} A & B^T \\ B & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{u}_1 \\ \boldsymbol{u}_2 \end{bmatrix} = \lambda \begin{bmatrix} A & 0 \\ 0 & S \end{bmatrix} \begin{bmatrix} \boldsymbol{u}_1 \\ \boldsymbol{u}_2 \end{bmatrix}$$

Componentwise

$$\begin{cases} A\boldsymbol{u}_1 + B^T\boldsymbol{u}_2 & = & \lambda A\boldsymbol{u}_1 \\ B\boldsymbol{u}_1 & = & \lambda S\boldsymbol{u}_2 \end{cases}$$

If $\boldsymbol{u}_2 = 0$ then from the first equation we have $A\boldsymbol{u}_1 = \lambda A\boldsymbol{u}_1$ which implies $\lambda = 1$ (since $\boldsymbol{u}_1$ must be nonzero and A is nonsingular).

Assume now $\boldsymbol{u}_2 \neq 0$. Then multiplying the first equation by BA^{-1} on the left yields

$$B\boldsymbol{u}_1 + S\boldsymbol{u}_2 = \lambda B\boldsymbol{u}_1.$$

Now substituting $B\boldsymbol{u}_1$ with $\lambda S\boldsymbol{u}_2$ from the second equation we get

$$(\lambda^2 - \lambda - 1)S\boldsymbol{u}_2 = 0, \quad \text{which gives} \quad \lambda = \frac{1 \pm \sqrt{5}}{2},$$

since $\boldsymbol{u}_2 \neq 0$ by hypothesis and also $S\boldsymbol{u}_2 \neq 0$ being S SPD and therefore nonsingular. □

Block Diagonal preconditioner for indefinite linear systems

Practical implementations

Note. The previous block diagonal preconditioner is ideal since its applications requires two system solutions with A and S (also computing explicitly S is not convenient).

In practice $\tilde{A}$ and $\tilde{S}$ are computed as *cheap* approximations of A and S, respectively, and $\tilde{M}$ is defined as

$$\tilde{M} = \begin{bmatrix} \tilde{A} & 0 \\ 0 & \tilde{S} \end{bmatrix}$$

In constraint optimization problems A is replaced by its diagonal ($\tilde{A} = \mathrm{diag}(A)$) and $\tilde{S}$ is the corresponding Schur complement: $\tilde{S} = B\,\mathrm{diag}(A)^{-1}B^T$.

With the approximate block diagonal preconditioner the previous spectral results no longer holds.

It can be proved that the eigenvalues of $\tilde{M}^{-1}H$ are contained in two intervals

$$I_- = [\lambda_{\min}, \lambda_s] \bigcup I_+ = [\lambda_{s+1}, \lambda_{\max}]$$

whose lengths are small and λ_s, λ_{s+1} are bounded away from zero ($\Longrightarrow$ fast convergence) if $\tilde{A}$ and $\tilde{S}$ well approximate A and S, respectively.