On the next-to-last CG and MR iteration step

(with application to symmetric tridiagonal Toeplitz matrices)

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joint work with

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A system of linear algebraic equations

Consider a system of linear algebraic equations

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

$\mathbf{A} \in \mathbb{R}^{n \times n}$ is nonsingular and normal, $b \in \mathbb{R}^n$.

- How to construct an approximation to the solution?

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Krylov subspace methods $\mapsto$ Given $x_0 \in \mathbb{R}^n$, $r_0 = b - \mathbf{A}x_0$. Find x_i,

$$x_i \in x_0 + \mathcal{K}_i(\mathbf{A}, r_0) \qquad \texttt{such that} \qquad r_i \perp \mathcal{C}_i,$$

where $r_i = b - \mathbf{A}x_i$, $\mathcal{K}_i(\mathbf{A}, r_0) \equiv \mathrm{span}\,\{r_0, \cdots, \mathbf{A}^{i-1}r_0\}$.

OR and MR Krylov subspace methods

Let $x_0 = 0$, i.e. $r_0 = b - \mathbf{A}x_0 = b$ (for simplicity).

Orthogonal Residual (OR) and Minimal Residual (MR) approach

(OR) `Find` $x_i \in \mathcal{K}_i(\mathbf{A}, b)$ `such that` $r_i \perp \mathcal{K}_i(\mathbf{A}, b)$.

(MR) `Find` $x_i \in \mathcal{K}_i(\mathbf{A}, b)$ `such that` $r_i \perp \mathbf{A}\mathcal{K}_i(\mathbf{A}, b)$.

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Optimality properties

(OR) $$\|e_i\|_{\mathbf{A}} = \min_{p \in \pi_i} \|p(\mathbf{A})x\|_{\mathbf{A}}$$ `(if A is SPD)`,

(MR) $$\|r_i\| = \min_{p \in \pi_i} \|p(\mathbf{A})b\|,$$

where $e_i \equiv x - x_i$, $\pi_i \equiv \{\, p$ is a polynomial; $\deg(p) \leq i;\ p(0) = 1 \}$.

The problem of convergence

MR constructs approximations $x_i \in \mathcal{K}_i(\mathbf{A}, b)$ to the solution x of the system $\mathbf{A}x = b$ such that

$$\|r_i\| = \min_{p \in \pi_i} \|p(\mathbf{A})\, b\| \,.$$

- **Our aim:**

  Description and understanding of this minimization process.

- **Considered classes of matrices in this talk:**

  Normal matrices, symmetric and positive definite matrices, symmetric positive definite tridiagonal Toeplitz matrices.

- We denote the OR method for SPD matrices as the CG method (Conjugate Gradient).

Outline

1. Introduction
2. Convergence bounds
3. Formulas for the next-to-last CG and MR iteration step
4. Application to symmetric tridiagonal Toeplitz matrices
5. Model problem: 1D Poisson equation
6. Conclusions

Convergence of the MR method

Let $\mathbf{A}$ be normal, $L \equiv \{\lambda_1, \ldots, \lambda_n\}$, $\|b\| = 1$. Then

$$\|r_i\| \quad = \quad \min_{p \in \pi_i} \|p(\mathbf{A})b\|$$

Convergence of the MR method

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$$\begin{aligned} \|r_i\| &= \min_{p \in \pi_i} \|p(\mathbf{A})b\| \\ &\leq \max_{\|b\|=1} \min_{p \in \pi_i} \|p(\mathbf{A})b\| \qquad \text{(worst-case)} \\ &= \min_{p \in \pi_i} \|p(\mathbf{A})\| \\ &= \min_{p \in \pi_i} \max_{\lambda_j \in L} |p(\lambda_j)| \end{aligned}$$

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- In this sense we understand the MR-CG worst-case behaviour.
- How to describe $\|r_i\|$ or the worst-case bound in terms of input data?

General formula for the MR residual

Krylov matrix

$$\mathbf{K}_{i+1} \equiv [b, \mathbf{A}b, \ldots, \mathbf{A}^i b] \, .$$

Residual r_i can be written as (Assumption: $\mathbf{K}_{i+1}$ has full column rank)

$$r_i = \|r_i\|^2 \, (\mathbf{K}_{i+1}^{+})^H \, e_1 \quad \Rightarrow \quad \|r_i\| = \frac{1}{\|(\mathbf{K}_{i+1}^{+})^H \, e_1\|} \, .$$

[Ipsen ’00, Liesen & Rozložník & Strakoš ’02]

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We consider $\mathbf{A}$ and b in the form

$$\mathbf{A} \;=\; \mathbf{Q}\boldsymbol{\Lambda}\mathbf{Q}^H, \qquad b \;=\; \mathbf{Q}\,[\varrho_1, \ldots, \varrho_n]^T\,.$$

We will assume that all eigenvalues of $\mathbf{A}$ are **distinct**.

The next-to-last MR iteration step

Let $\varrho_j \neq 0$ for all j. Then

$$\|r_{n-1}\| = \left(\sum_{j=1}^{n} \left| \frac{l_j}{\varrho_j} \right|^2 \right)^{-1/2}, \qquad l_j \equiv \prod_{\substack{k=1 \\ k \neq j}}^{n} \frac{\lambda_k}{\lambda_k - \lambda_j}.$$

[Liesen & T. '04, Ipsen '00]

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[Liesen & T. ’04, Ipsen ’00]

Using Cauchy’s inequality,

$$\frac{\|r_{n-1}^w\|}{\|b_{MR}^w\|} = \left(\sum_{j=1}^{n} |l_j| \right)^{-1},$$

where

$$b_{MR}^w = \mathbf{Q} \, [\varrho_1^w, \ldots, \varrho_n^w]^T, \qquad |\varrho_k^w|^2 = \gamma \, |l_k|, \quad k = 1, \ldots, n \, ,$$

$\gamma > 0$ is any scaling factor. [Liesen & T. ’04]

The next-to-last CG iteration step

CG can be seen as MR for a special right hand side $\tilde{b}$,

$$\min_{p\in\pi_i} \|p(\mathbf{A})x\|_{\mathbf{A}} = \min_{p\in\pi_i} \|p(\mathbf{A})\mathbf{A}^{1/2}x\| = \min_{p\in\pi_i} \|p(\mathbf{A})\tilde{b}\| \,.$$

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Then

$$\|e_{n-1}\|_{\mathbf{A}} \;=\; \left(\sum_{j=1}^{n} \left| \frac{\lambda_j^{1/2}\, l_j}{\varrho_j} \right|^2 \right)^{-1/2}, \qquad \frac{\|e_{n-1}^w\|_{\mathbf{A}}}{\|x_{CG}^w\|_{\mathbf{A}}} \;=\; \left(\sum_{j=1}^{n} |l_j| \right)^{-1},$$

$$b_{CG}^w \;=\; \mathbf{Q}\,[\varrho_1^w, \ldots, \varrho_n^w]^T, \qquad |\varrho_k^w|^2 = \gamma\, |\lambda_k\, l_k|, \quad k = 1, \ldots, n\,,$$

$\gamma > 0$ is any scaling factor.

[Liesen & T. '05]

Summary (the next-to-last iteration step)

The next-to-last step of CG and MR is completely understood!

We know

- the convergence quantities,
- the worst-case convergence quantities and corresponding b^w.

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How to use this information?

- We can study the influence of the right hand side,
- we can compare the worst-case bound with classical bounds,
- we can determine right hand sides leading to the slowest convergence and identify the worst input data of our original problem.

Symmetric tridiagonal Toeplitz matrices

Consider linear algebraic systems $\mathbf{A}x = b$, where

$$\mathbf{A} = \begin{bmatrix} \alpha & \beta & & \\ \beta & \ddots & \ddots & \\ & \ddots & \ddots & \beta \\ & & \beta & \alpha \end{bmatrix} \in \mathbb{R}^{n \times n}.$$

Let α and β be such that $\mathbf{A}$ is **symmetric and positive definite** matrix.

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Let α and β be such that $\mathbf{A}$ is **symmetric and positive definite** matrix.

Eigenvalues and eigenvectors of $\mathbf{A}$ are known

$$\begin{aligned} \lambda_k &= \alpha + 2\,\beta\,\cos(k\pi h)\,, \\ q_k &= (2h)^{1/2}\ \left[\sin\left(k\pi h\right), \sin\left(2k\pi h\right), \ldots, \sin\left(nk\pi h\right)\right]^T, \end{aligned}$$

where $h \equiv (n+1)^{-1}$.

Worst-case bound versus classical κ-bound

Now we are able to determine l_j and the worst-case bound

$$\frac{\|e_{n-1}^w\|_A}{\|e_0^w\|_A} = \left(\sum_{j=1}^{n} |l_j| \right)^{-1} \approx \frac{2\,\nu^{n-1}}{1+\nu^2+\cdots+\nu^{2(n-1)}+\nu^{2n}},$$

where

$$\nu \equiv \frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}, \quad \kappa = \frac{\lambda_{max}}{\lambda_{min}}.$$

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where

$$\nu \;\equiv\; \frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}, \quad \kappa = \frac{\lambda_{max}}{\lambda_{min}}.$$

The classical κ-bound is given by

$$\frac{\|e_{n-1}^w\|_A}{\|e_0^w\|_A} \;\leq\; \frac{2\nu^{n-1}}{1+\nu^{2(n-1)}} \;\leq\; 2\nu^{n-1}.$$

Model problem: Poisson equation

$$-u''(z) \;=\; f(z), \qquad z \in (0,1)\,, \qquad u(0) = u_0, \;\; u(1) = u_1\,.$$

The central finite difference approximation on the uniform grid kh, $k = 1, \ldots, n$, $h = 1/(n+1)$, leads to a system $\mathbf{A}x = b$

$$\overbrace{\begin{bmatrix} 2 & -1 & & \\ -1 & \ddots & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & 2 \end{bmatrix}}^{\mathbf{A}} x \;=\; \overbrace{h^2 \begin{bmatrix} f(h) \\ \vdots \\ \vdots \\ f(nh) \end{bmatrix} + \begin{bmatrix} u_0 \\ \\ \\ u_1 \end{bmatrix}}^{b}.$$

The eigenvalues λ_k and the eigenvectors q_k of $\mathbf{A}$ are known,

$$\lambda_k = 4\sin^2\left(\frac{k\pi h}{2}\right) \quad \Rightarrow \quad l_j = 2\cos^2\left(\frac{j\pi h}{2}\right).$$

[Liesen & T. '05]

Various right hand sides

Formulas for the next-to-last step

$$\|r_{n-1}\| = \left(\sum_{j=1}^{n} \left| \frac{l_j}{\varrho_j} \right|^2 \right)^{-1/2}, \qquad \|e_{n-1}\|_{\mathbf{A}} = \left(\sum_{j=1}^{n} \left| \frac{\lambda_j^{1/2}\, l_j}{\varrho_j} \right|^2 \right)^{-1/2}.$$

We consider two types of right hand sides:

- worst-case b's: right hand sides leading to maximal relative convergence quantities in the next-to-last step $\rightarrow b^w_{MR}$, b^w_{CG}.
- unbiased $b \rightarrow b^u$, all ϱ_j are of equal size.

Some results for MR

Let $\|b^w_{MR}\| = \|b^u\| = 1.$ [Liesen & T. '05]

Worst-case $\times$ unbiased case (MR)

$$\|r^w_{n-1}\| \;=\; \frac{1}{n}\,, \qquad \|r^u_{n-1}\| \;>\; \sqrt{\frac{2}{3}}\,\frac{1}{n}\,.$$

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Worst data for MR

$$u(0) = 0,\ u(1) = 0,\ f(z) \approx \cot\left(\frac{\pi z}{2}\right)$$

yield a worst right-hand side for MR.

Worst data for CG

We are able to determine worst-case ϱ_{CG}^{w},

$$\varrho_{CG}^{w} \qquad b_{CG}^{w} = \mathbf{Q}\varrho_{CG}^{w} \qquad \text{diff. eq.}$$

$$\begin{bmatrix} \sin(\pi h) \\ \vdots \\ \sin(n\pi h) \end{bmatrix} \quad \leftrightarrow \quad \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \quad \leftrightarrow \quad \begin{aligned} f(z) &= 0\,, \\ u(0) &= 1\,, \\ u(1) &= 0\,. \end{aligned}$$

CG started with $x_0 = 0$ and b_{CG}^{w} attains the worst-case relative A-norm of the error in the $(n-1)$st iteration step.

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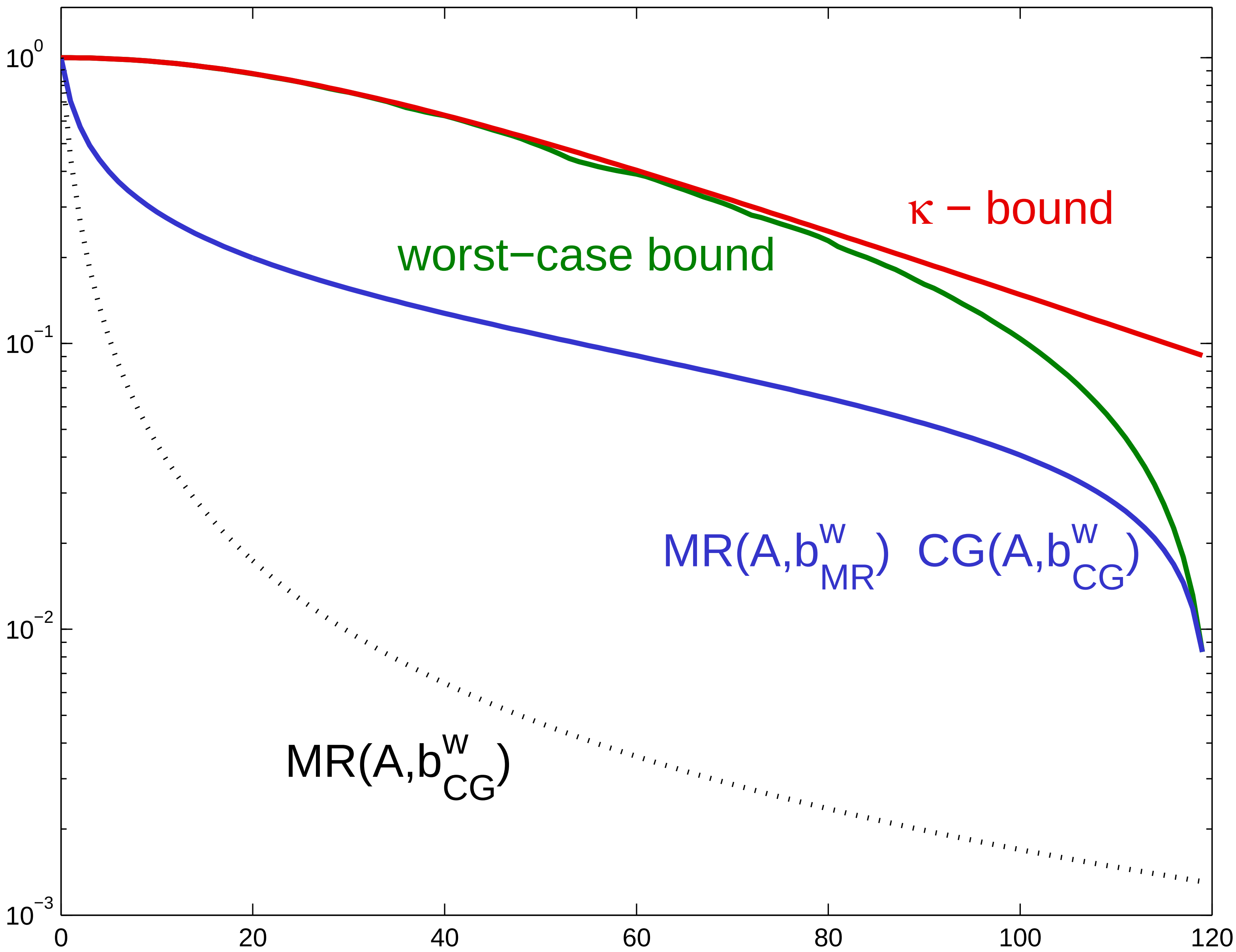
Another example: Let n be even.

$$u''(z) = 0\,,\ u(0) = 1\,,\ u(1) = 1 \quad \Longrightarrow \quad b = [1, 0, \ldots, 0, 1]^T.$$

Then $\|x - x_{n/2}\|_A / \|x\|_A$ is the worst possible one and CG finds the solution in the following step. [Liesen & T. '05]

Numerical experiment



Conclusions

[Liesen & T. '05]

For MR ($\mathbf{A}$ is normal) and for CG ($\mathbf{A}$ is SPD):

- **The next-to-last iteration step is completely understood!**
- Our results allow to study **model problems with known eigenvalues** .
- For **1-D Poison equation** we obtained interesting results:

  $\longrightarrow$ particular worst-case quantities in the next-to-last step,

  $\longrightarrow$ implications for the connection between the differential equation and the linear solver for the discretized problem.

Thank you for your attention!

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More details can be found in

Liesen, J. and Tichý, P., **The worst-case GMRES for normal matrices**, BIT Numerical Mathematics, Volume 44, pp. 79-98, 2004.

Liesen, J. and Tichý, P., **On the next-to-last CG and MR iteration step**, submitted to ETNA, January 2005.

See also `http://www.math.tu-berlin.de/~tichy`