Towards Practical Estimation of the A-norm of the error in CG

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joint work with
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The conjugate gradient method

$\mathbf{A}x = b$, $\mathbf{A}$ is real, symmetric, positive definite, $x_0 = 0$.

input $\mathbf{A}$, b
$r_0 = b$, $p_0 = r_0$
for $k = 1, 2, \ldots$ **do**

$$\gamma_{k-1} = \frac{r_{k-1}^T r_{k-1}}{p_{k-1}^T \mathbf{A}\, p_{k-1}}$$

$$x_k = x_{k-1} + \gamma_{k-1} p_{k-1}$$

$$r_k = r_{k-1} - \gamma_{k-1} \mathbf{A}\, p_{k-1}$$

$$\delta_k = \frac{r_k^T r_k}{r_{k-1}^T r_{k-1}}$$

$$p_k = r_k + \delta_k p_{k-1}$$

end for

exact arithmetic

↓

orthogonality

$r_i \perp r_j \qquad p_i \perp_{\mathbf{A}} p_j$

optimality of x_k

$$\min_{y \in \mathcal{K}_k} \|x - y\|_{\mathbf{A}} \,.$$

Estimating the $\mathbf{A}$-norm of the error

A brief history

- $\|x - x_k\|^2_{\mathbf{A}}$ can be used as a **measure of the "goodness"** of x_k as an estimate of x. [Hestenes, Stiefel 1952]

- G. Golub & collaborators: [Dahlquist, Golub, Nash 1978], **GQL** [Golub, Meurant 1994] error bounds and **Gauss quadrature**.

- Estimating errors in CG [Golub, Strakoš 1994], **CGQL** [Golub, Meurant, 1997] $\rightarrow$ **CGQ** [Meurant, T. 2013].

- Behavior in **finite precision arithmetic** [Golub, Strakoš 1994], Why it works [Strakoš, T. 2002].

- [Meurant, Strakoš 2006], [Golub, Meurant 2010], [Liesen, Strakoš 2013].

Quadrature bounds

Gauss and Gauss-Radau quadrature bounds

- Given $\mu \leq \lambda_{\min}$, it holds that

$$\gamma_k \|r_k\|^2 < \|x - x_k\|_A^2 < \gamma_k^{(\mu)} \|r_k\|^2$$

where $\gamma_k^{(\mu)}$ is easily computable.

- For some $d > 0$, we can improve the bound using

$$\|x - x_k\|_{\mathbf{A}}^2 = \sum_{j=k}^{k+d-1} \gamma_j \|r_j\|^2 + \|x - x_{k+d}\|_{\mathbf{A}}^2 .$$

[Golub, Strakoš 1994], [Strakoš, T. 2002], [Meurant, T. 2013]

Gauss-Radau upper bound

Given $\mu \le \lambda_{\min}$, it holds that [Meurant, T. 2013]

$$\|x - x_k\|_A^2 \ < \ \gamma_k^{(\mu)} \|r_k\|^2$$

where

$$\gamma_{k+1}^{(\mu)} \ = \ \frac{\left(\gamma_k^{(\mu)} - \gamma_k\right)}{\mu \left(\gamma_k^{(\mu)} - \gamma_k\right) \ + \ \delta_{k+1}}\,, \qquad \gamma_0^{(\mu)} = \frac{1}{\mu}\,.$$

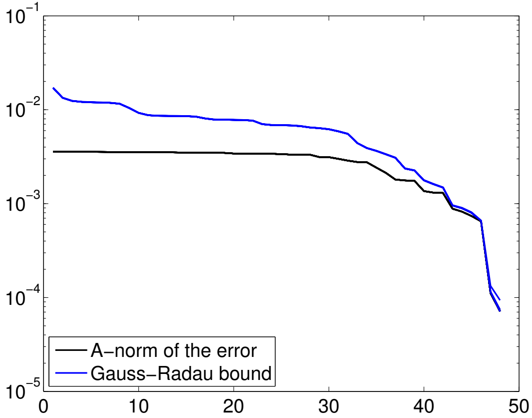
Practically relevant questions:

- Having μ, we can compute it almost **for free**.
- How to get μ?
- **Sensitivity** of the bound on μ?
- **Quality** of the bound?
- Numerical **behavior**?

Sensitivity in exact arithmetic

Gauss-Radau bound, bcsstk01 matrix, $n = 48$

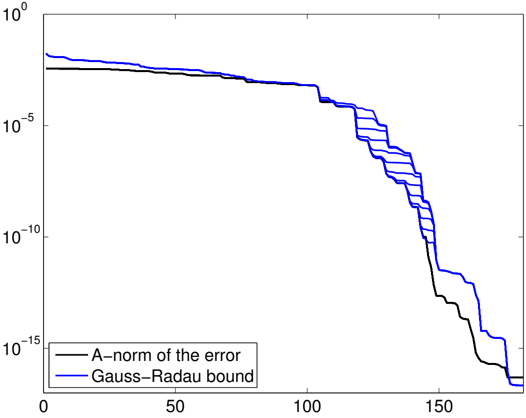
$$\mu = \frac{\lambda_{\min}}{1 + 10^{-m}}, \quad m = 2, \ldots, 14$$



Sensitivity in finite precision arithmetic

Gauss-Radau bound, bcsstk01 matrix, $n = 48$

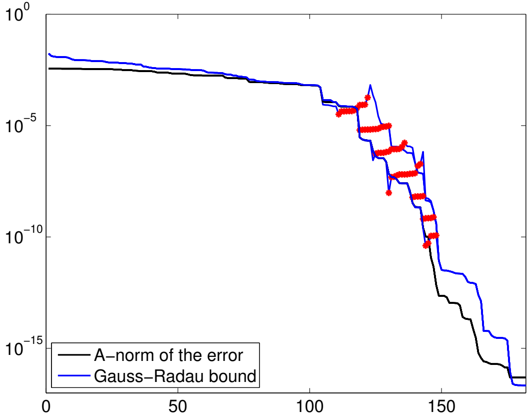
$$\mu = \frac{\lambda_{\min}}{1 + 10^{-m}}, \quad m = 2, \ldots, 14$$



Sensitivity in finite precision arithmetic

$\mu > \lambda_{\min}$, bcsstk01 matrix, $n = 48$

$$\mu = \frac{\lambda_{\min}}{1 - 10^{-m}}, \quad m = 2:2:14, \quad \gamma_k^{(\mu)} < 0$$



An upper bound on the Gauss-Radau bound

An upper bound on the Gauss-Radau bound

It holds that $\gamma_k < \gamma_k^{(\mu)}$ and

$$\mu \gamma_{k+1}^{(\mu)} = \frac{\mu \left(\gamma_k^{(\mu)} - \gamma_k \right)}{\mu \left(\gamma_k^{(\mu)} - \gamma_k \right) + \delta_{k+1}} < \frac{\mu \gamma_k^{(\mu)}}{\mu \gamma_k^{(\mu)} + \delta_{k+1}} .$$

From the induction hypothesis

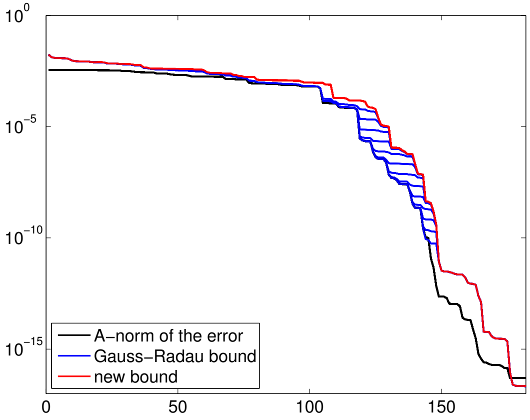
$$\mu \gamma_k^{(\mu)} \ \leq \ \frac{\|r_k\|^2}{\|p_k\|^2}$$

we obtain

$$\mu \gamma_{k+1}^{(\mu)} < \frac{\frac{\|r_k\|^2}{\|p_k\|^2}}{\frac{\|r_k\|^2}{\|p_k\|^2} + \delta_{k+1}} = \frac{\|r_{k+1}\|^2}{\|p_{k+1}\|^2} .$$

An upper bound on the Gauss-Radau bound, $\mu \leq \lambda_{\min}$

$$\|x - x_k\|_{\mathbf{A}}^2 \; < \; \gamma_k^{(\mu)} \|r_k\|^2 \; < \; \frac{\|r_k\|^2}{\mu} \frac{\|r_k\|^2}{\|p_k\|^2}$$



The new bound

$$\|x - x_k\|_{\mathbf{A}}^2 \; < \; \gamma_k^{(\mu)} \|r_k\|^2 \; < \; \frac{\|r_k\|^2}{\mu} \frac{\|r_k\|^2}{\|p_k\|^2}$$

- Having μ, we can compute it almost **for free**.
- Monotonically decreasing.
- **Not sensitive** to the choice of μ.
- As good as Gauss-Radau in many cases.
- It can be used even if $\mu > \lambda_{\min}$ (heuristics).

The new bound and connections, $\mu \leq \lambda_{\min}$

Using local orthogonality,

$$\|x - x_k\|_{\mathbf{A}}^2 < \frac{\|r_k\|^2}{\mu} \frac{\|r_k\|^2}{\|p_k\|^2} = \frac{1}{\mu} \left(\sum_{j=0}^{k} \|r_j\|^{-2} \right)^{-1}.$$

Connection between **orthogonal residual** and **minimal residual** methods in **exact arithmetic** (using global orthogonality)

$$\underbrace{\min_{y \in \mathcal{K}_k} \|b - \mathbf{A}y\|_{\mathbf{A}^{-1}}^2}_{\|x - x_k^{OR}\|_{\mathbf{A}}^2} \leq \frac{1}{\mu} \underbrace{\min_{y \in \mathcal{K}_k} \|b - \mathbf{A}y\|^2}_{\|r_k^{MR}\|^2}$$

The **red term** is used in **residual smoothing techniques**.

[Gutknecht, Rozložník 2001]

Approximating the extreme Ritz values in CG

Why? $\rightarrow$ $\lambda_{\min}$, $\|\mathbf{A}\|$, $\kappa(\mathbf{A})$

The conjugate gradient method

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input $\mathbf{A}$, b
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for $k = 1, 2, \ldots$ **do**

$$
\begin{aligned}
\gamma_{k-1} &= \frac{r_{k-1}^T r_{k-1}}{p_{k-1}^T \mathbf{A}\, p_{k-1}} \\
x_k &= x_{k-1} + \gamma_{k-1} p_{k-1} \\
r_k &= r_{k-1} - \gamma_{k-1} \mathbf{A}\, p_{k-1} \\
\delta_k &= \frac{r_k^T r_k}{r_{k-1}^T r_{k-1}} \\
p_k &= r_k + \delta_k p_{k-1}
\end{aligned}
$$

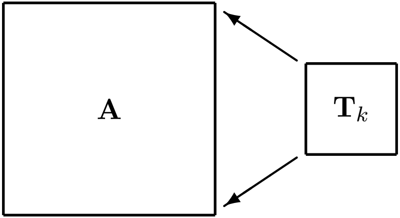
end for

$\mathbf{U}_k$

$$
\begin{bmatrix}
\frac{1}{\sqrt{\gamma_0}} & \sqrt{\frac{\delta_1}{\gamma_0}} & & \\
& \ddots & \ddots & \\
& & \ddots & \sqrt{\frac{\delta_{k-1}}{\gamma_{k-2}}} \\
& & & \frac{1}{\sqrt{\gamma_{k-1}}}
\end{bmatrix}
$$

$$\mathbf{T}_k = \mathbf{U}_k^T \mathbf{U}_k$$

Approximation of $\lambda_{\min}$ and $\lambda_{\max}$ in CG



$$\mathbf{T}_k = \mathbf{U}_k^T \mathbf{U}_k \quad \rightarrow \quad \begin{aligned} \lambda_{\max}(\mathbf{T}_k) &= \|\mathbf{U}_k\|^2 \\ \lambda_{\min}(\mathbf{T}_k) &= 1/\|\mathbf{U}_k^{-1}\|^2 \end{aligned}$$

How to approximate $\|\mathbf{U}_k\|^2$ and $\|\mathbf{U}_k^{-1}\|^2$?

Incremental estimation

of the largest and the smallest Ritz value in CG

- **Structure**: $\mathbf{U}_k$ and $\mathbf{U}_k^{-1}$ are **upper triangular**.

- $\mathbf{U}_k$ is bidiagonal,

$$\mathbf{U}_k \quad \rightarrow \quad \mathbf{U}_{k+1}, \qquad \mathbf{U}_k^{-1} \quad \rightarrow \quad \mathbf{U}_{k+1}^{-1}$$

  by **adding one column and one row**.

- **Incremental norm estimation**: incrementally improve an approximation of the maximum right singular vector. [Bischof 1990], [Duff, Vömmel 2002], [Duintjer Tebbens, Tůma 2014].

The idea of incremental norm estimation

$\mathbf{U}$ is general, upper triangular

Given $\mathbf{U} \in \mathbb{R}^{k \times k}$ upper triangular and a unit norm z. Form

$$\hat{\mathbf{U}} = \begin{bmatrix} \mathbf{U} & v \\ & q \end{bmatrix}, \qquad \hat{z} = \begin{bmatrix} sz \\ c \end{bmatrix},$$

where $s^2 + c^2 = 1$ are chosen such that

$$\| \hat{\mathbf{U}} \hat{z} \|^2 = \begin{bmatrix} s \\ c \end{bmatrix}^T \begin{bmatrix} \rho & \sigma \\ \sigma & \tau \end{bmatrix} \begin{bmatrix} s \\ c \end{bmatrix}$$

is maximal. Here

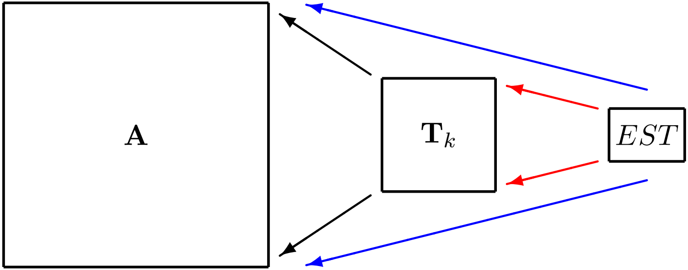
$$\rho = \|\mathbf{U}z\|^2, \qquad \sigma = v^T \mathbf{U} z, \qquad \tau = v^T v + q^2.$$

Specialization to bidiagonal matrices and their inverses

- Very cheap, no need to store vectors or coefficients.

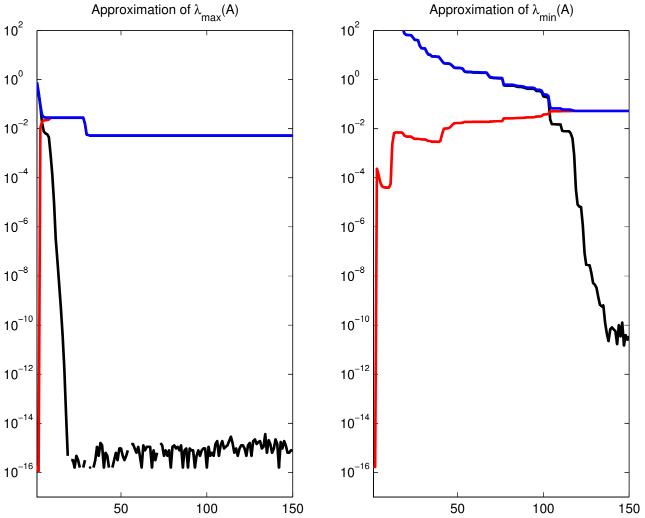
Estimation of $\|\mathbf{U}_k^{-1}\|^2$ in CG: Having γ_k and δ_k, update

$$
\begin{aligned}
\sigma_k &= -\sqrt{\frac{\gamma_k \delta_k}{\gamma_{k-1}}}\,(s_{k-1}\sigma_{k-1} + c_{k-1}\tau_{k-1}) \\
\tau_k &= \gamma_k \left(b_k^2 \tau_{k-1} + 1\right) \\
\omega_k^2 &= (\rho_k - \tau_k)^2 + 4\sigma_k^2 \\
c_k^2 &= \frac{1}{2}\left(1 - \frac{\rho_k - \tau_k}{\omega_k}\right) \\
\rho_{k+1} &= \rho_k + \omega_k c_k^2 \\
s_k &= \sqrt{1 - c_k^2}, \\
c_k &= |c_k| \operatorname{sign}(\sigma_k)
\end{aligned}
$$



Numerical experiments

bcsstk01, $n = 48$, relative accuracy of the approximations



How to improve the accuracy?

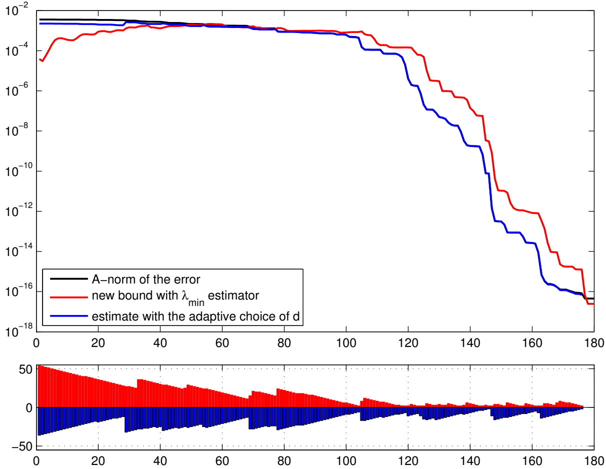
Store $\mathbf{U}_k$, z_k, one shifted inverse iteration applied to $\mathbf{T}_{k+1} - \theta I$.

Adaptive choice of d

$$\|x - x_k\|_{\mathbf{A}}^2 = \underbrace{\sum_{j=k}^{k+d-1} \gamma_j \|r_j\|^2}_{\nu_{j,d}} + \|x - x_{k+d}\|_{\mathbf{A}}^2$$

Experiment: Adaptive choice of d

$$\left(\nu_{j,d} \ > \ 2\,\|x - x_{k+d}\|^2_{\mathbf{A}}\right) \quad \approx \quad \left(\nu_{j,d} \ > \ 2\,\frac{\|r_{k+d}\|^2}{\mu_{k+d}}\,\frac{\|r_{k+d}\|^2}{\|p_{k+d}\|^2}\right)$$



Conclusions

- A **new bound** for the $\mathbf{A}$-norm of the error:
  - not sensitive to the choice of μ,
  - in many cases as good as Gauss-Radau bound,
  - it can be used even for $\mu > \lambda_{\min}$ (heuristics).
- Approximating the **extreme Ritz values** in CG $\approx$
  - the $\mathbf{A}$-norm of the error,
  - the level of maximal attainable accuracy,
  - the normwise backward error, $\kappa(\mathbf{A})$, etc.
- **Adaptive choice** of d?

Related papers

- G. H. Golub and G. Meurant, [Matrices, moments and quadrature. II. BIT, 37 (1997), pp. 687–705.]
- G. H. Golub and Z. Strakoš, [Estimates in quadratic formulas, Numer. Algorithms, 8 (1994), pp. 241–268.]
- G. Meurant and P. Tichý, [Practical estimation of the A-norm of the error in CG, in preparation, 2017]
- G. Meurant and P. Tichý, [On computing quadrature-based bounds for the $\mathbf{A}$-norm of the error in CG, Numer. Algorithms, 62 (2013), pp. 163-191]
- Z. Strakoš and P. Tichý, [On error estimation in CG and why it works in FP computations, Electron. Trans. Numer. Anal., 13 (2002), pp. 56–80.]

Thank you for your attention!