On improving accuracy of the error estimates in the conjugate gradient method

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based on joint work with
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The conjugate gradient method

A is symmetric and positive definite, $Ax = b$

input A, b, x_0

$p_0 = r_0 = b - Ax_0$

for $k = 1, 2, \ldots$ **do**

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

end for

exact arithmetic

$\downarrow$

orthogonality

$r_i \perp r_j \qquad p_i \perp_A p_j$

optimality of x_k

$$\min_{y \in \mathcal{K}_k} \|x - y\|_A \,.$$

Estimating the A-norm of the error

A brief history

- $\|x - x_k\|_A^2$ ... **measure** of the “goodness” of x_k

  [Hestenes, Stiefel 1952]

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- Gauss **quadrature** error bounds (Lanczos) $\rightarrow$ **GQL**

  [Dahlquist, Golub, Nash 1978], [Golub, Meurant 1994]

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- Estimating errors in CG $\rightarrow$ **CGQL** $\rightarrow$ **CGQ**

  [Golub, Strakoš 1994], [Golub, Meurant, 1997], [Meurant, T. 2013]

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- Why it works in **finite precision** arithmetic

  [Golub, Strakoš 1994], [Strakoš, T. 2002, 2005].

Quadrature bounds

Gauss and Gauss-Radau quadrature bounds

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

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

where

$$\alpha_{k+1}^{(\mu)} = \frac{\left(\alpha_k^{(\mu)} - \alpha_k\right)}{\mu \left(\alpha_k^{(\mu)} - \alpha_k\right) + \beta_{k+1}}, \qquad \alpha_0^{(\mu)} = \frac{1}{\mu}.$$

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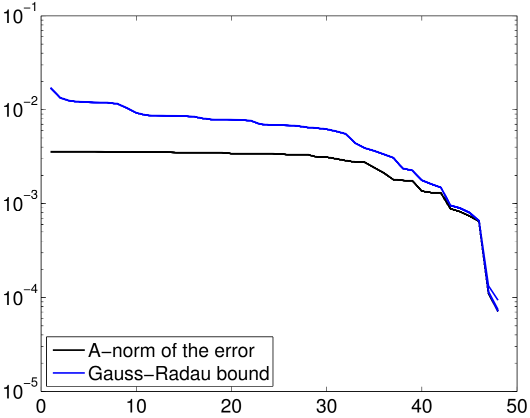
Practically relevant questions:

- How to get μ?
- **Quality** of the bound?
- Numerical **behavior**?

Upper bound in exact arithmetic

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

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



Upper bound in finite precision arithmetic

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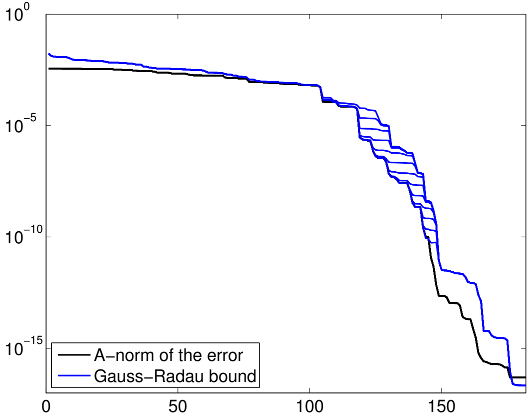
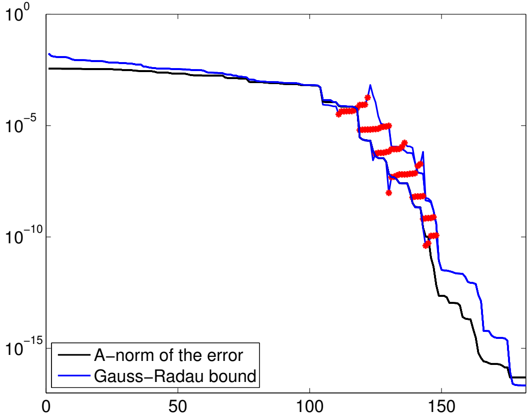


Upper bound in finite precision arithmetic

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

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

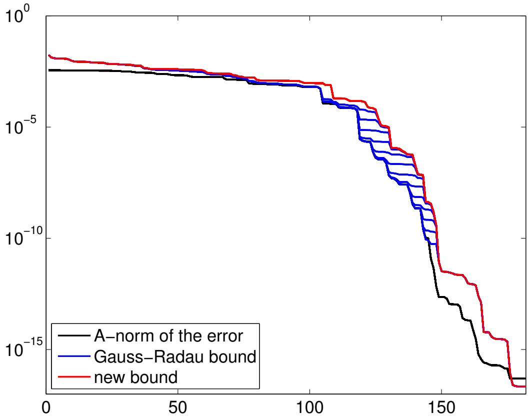


An upper bound on the upper bound

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

[Meurant, T. 2018?]

$$\|x - x_k\|_A^2 \; < \; \alpha_k^{(\mu)} \|r_k\|^2 \; < \; \frac{\|r_k\|^2}{\mu} \frac{\|r_k\|^2}{\|p_k\|^2}$$



The new bound

[Meurant, T. 2018?]

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

- 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).

How to approximate μ?

The conjugate gradient method

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p_k &= r_k + \beta_k p_{k-1}
\end{aligned}$$

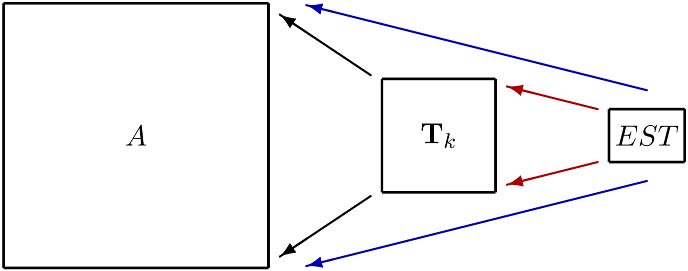
end for

$$\mathbf{U}_k$$

$$\begin{bmatrix} \frac{1}{\sqrt{\alpha_0}} & \sqrt{\frac{\beta_1}{\alpha_0}} & & \\ & \ddots & \ddots & \\ & & \ddots & \sqrt{\frac{\beta_{k-1}}{\alpha_{k-2}}} \\ & & & \frac{1}{\sqrt{\alpha_{k-1}}} \end{bmatrix}$$

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

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



$$\mathbf{T}_k = \mathbf{U}_k^T \mathbf{U}_k \quad \to \quad \lambda_{\min}(\mathbf{T}_k) \quad = \quad 1/\|\mathbf{U}_k^{-1}\|^2$$

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

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

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

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

Incremental estimation

of the smallest Ritz value in CG

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

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  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].

Approximation of the smallest Ritz value in CG

Having α_k and β_k, update

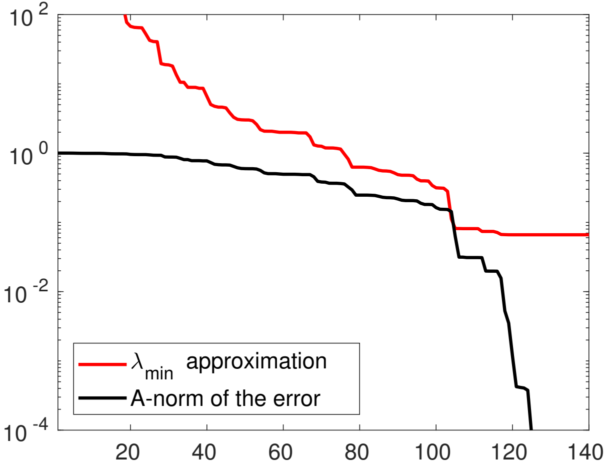
$$
\begin{aligned}
\sigma_k &= -\sqrt{\frac{\alpha_k \beta_k}{\alpha_{k-1}}}\,(s_{k-1}\sigma_{k-1} + c_{k-1}\tau_{k-1}) \\
\tau_k &= \alpha_k \left(b_k^2 \tau_{k-1} + 1\right) \\
\omega_k^2 &= (\rho_k - \tau_k)^2 + 4\sigma_k^2 \\
c_k^2 &= \frac{1}{2}\left(1 - \frac{\rho_k - \tau_k}{\omega_k}\right) \\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

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

[Meurant, T. 2018?]

Approximation of $\lambda_{\min}$

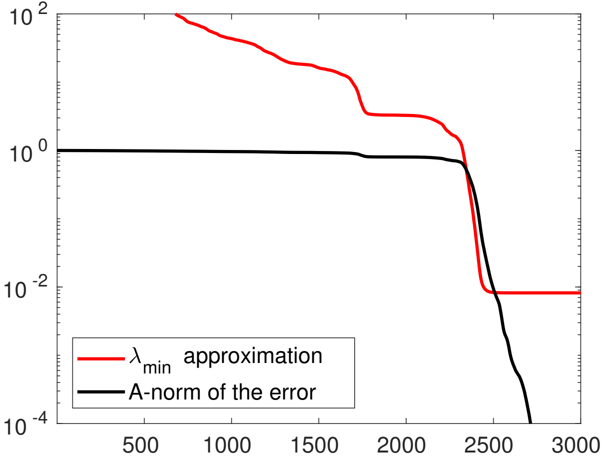
bcsstk01, $n = 48$



$$\frac{\lambda_{\min} - \mu_k}{\lambda_{\min}}$$

Approximation of $\lambda_{\min}$

s3dkt3m2, $n = 90449$, ichol

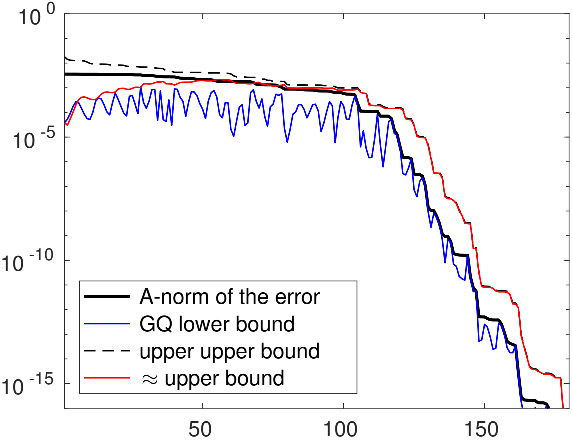


$$\frac{\lambda_{\min} - \mu_k}{\lambda_{\min}}$$

Bounds summary

bcsstk01, $n = 48$

$$\alpha_k \|r_k\|^2 < \|x - x_k\|_A^2 \lesssim \frac{\|r_k\|^2}{\mu_k} \frac{\|r_k\|^2}{\|p_k\|^2}$$



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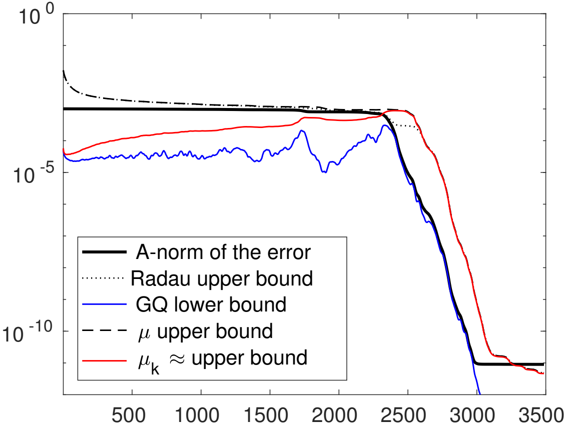


Improving accuracy of the estimates

$$\|x - x_k\|_A^2 \;=\; \alpha_k \|r_k\|^2 \;+\; \|x - x_{k+1}\|_A^2$$

[Golub, Strakoš 1994, Golub, Meurant 1997, Strakoš, T. 2002]

Use a delay and bound $(k+d)$th error

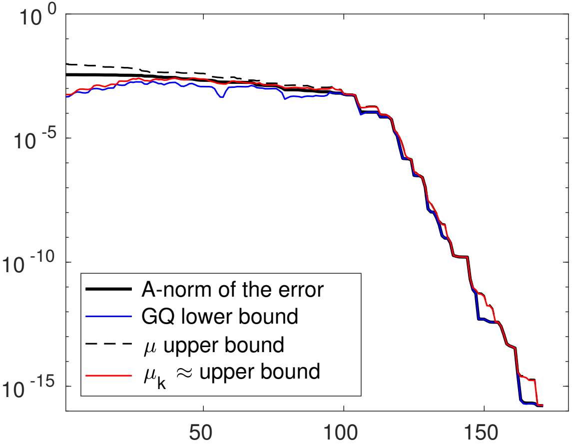
bcsstk01, $n = 48$, $d = 10$

$$\|x - x_k\|_A^2 \;=\; \sum_{j=k}^{k+d-1} \alpha_j \|r_j\|^2 \;+\; \|x - x_{k+d}\|_A^2$$

Use a delay and bound $(k+d)$th error

bcsstk01, $n = 48$, $d = 10$

$$\|x - x_k\|_A^2 = \sum_{j=k}^{k+d-1} \alpha_j \|r_j\|^2 + \|x - x_{k+d}\|_A^2$$



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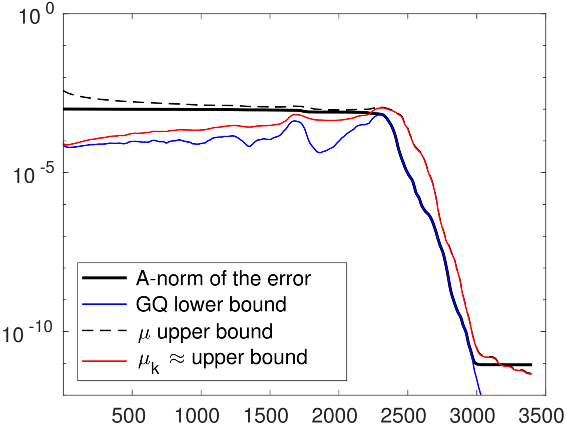

How to choose d adaptively?

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

$$= \nu_{k,d} + \frac{\|x - x_{k+d}\|_A^2}{\|x - x_k\|_A^2} \|x - x_k\|_A^2,$$

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If

$$\frac{\|x - x_{k+d}\|_A}{\|x - x_k\|_A} < \varepsilon,$$

then

$$\nu_{k,d}^{1/2} < \|x - x_k\|_A < \frac{\nu_{k,d}^{1/2}}{\sqrt{1-\varepsilon^2}}, \quad \text{e.g.,} \quad \varepsilon = 0.8.$$

Pseudo algorithm - adaptive choice of d

$go = 1$
$d = d + 1$
while $((d \geq 1)$ and $(go))$ **do**
    compute $\nu_{k-d+1,d}$
    if $\left(\frac{\|x-x_k\|_A}{\|x-x_{k-d}\|_A} < \varepsilon\right)$ **then**
        compute lower or upper bounds at iteration $k-d$
        $d = d - 1$
    else
        $go = 0$
    end if
end while

Adaptive choice of d

μ_k upper bound approach, bcsstk01

$$\frac{\|x - x_{k+d}\|_A}{\|x - x_k\|_A} \lesssim \frac{\frac{\|r_{k+d}\|}{\sqrt{\mu_{k+d}}} \frac{\|r_{k+d}\|}{\|p_{k+d}\|}}{\sqrt{\nu_{k,d}}} < \varepsilon = 0.5,$$

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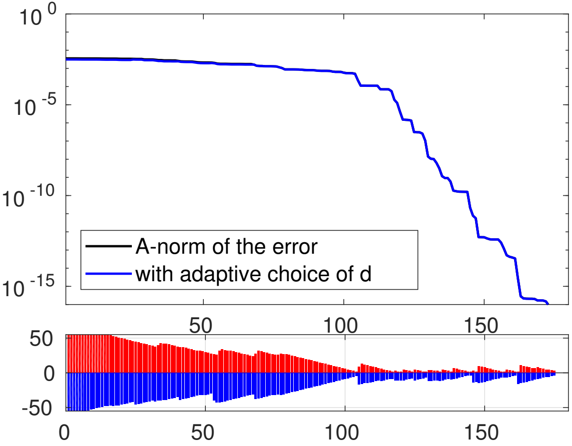

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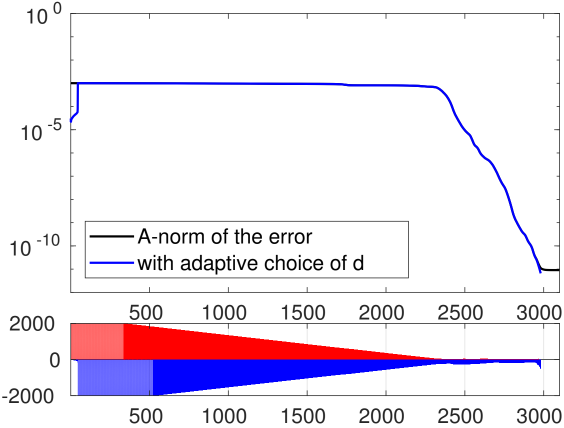

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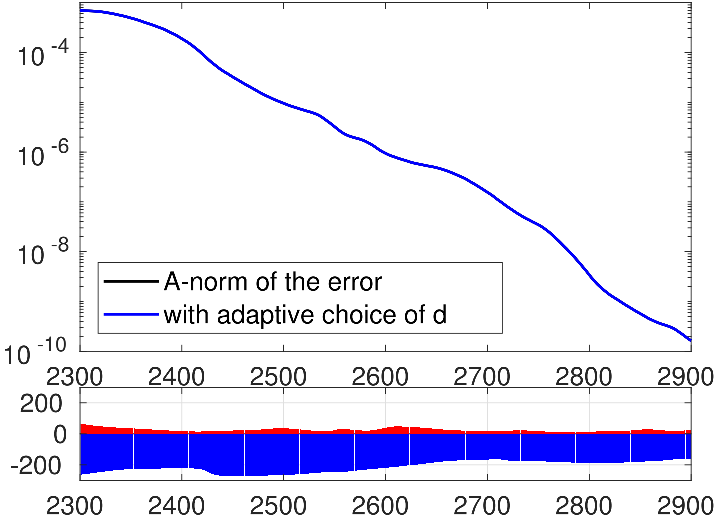

Another approach

superliner, linear, sublinear CG convergence

Let $\alpha > \beta > \gamma > 0$. Then

$$\frac{\beta - \gamma}{\alpha - \beta} > \frac{\beta}{\alpha} \quad \Leftrightarrow \quad \frac{\beta}{\alpha} > \frac{\gamma}{\beta}.$$

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Apply to $\|x - x_{k-d}\|_A^2 > \|x - x_k\|_A^2 > \|x - x_{k+d}\|_A^2$. Then

$$\frac{\nu_{k,d}}{\nu_{k-d,d}} > \frac{\|x - x_k\|_A^2}{\|x - x_{k-d}\|_A^2} \quad \Leftrightarrow \quad \frac{\|x - x_k\|_A}{\|x - x_{k-d}\|_A} > \frac{\|x - x_{k+d}\|_A}{\|x - x_k\|_A}.$$

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CG convergence:

- **linear** $\rightarrow$ **good** approximation
- **superliner** $\rightarrow$ **upper** bound
- **sublinear** $\rightarrow$ **lower** bound

Yet another approach

decrease formula

For $\ell + e < k$ and $d > 0$, one can relate

$$\frac{\|x - x_{k+d}\|_A^2}{\|x - x_k\|_A^2} \quad \text{and} \quad \frac{\|x - x_{\ell+e}\|_A^2}{\|x - x_\ell\|_A^2} \; .$$

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It holds that

$$\frac{\|x - x_{k+d}\|_A^2}{\|x - x_k\|_A^2} = \left(1 - \frac{1}{\left(1 - \frac{1}{\frac{\|x - x_{\ell+e}\|_A^2}{\|x - x_\ell\|_A^2}}\right) \frac{\sum_{j=\ell+e}^{k-1} g_j}{\sum_{j=\ell}^{\ell+e-1} g_j} + 1} \right) \frac{\sum_{j=k}^{k+d-1} g_j}{\sum_{j=\ell+e}^{k-1} g_j} + 1$$

where

$$g_j = \alpha_j \|r_j\|^2 \,.$$

Conclusions

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Future work $\rightarrow$ **combine** approaches, numerical experiments

Related papers

- 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, to be submitted soon, 2018]
- G. Meurant and P. Tichý, [On computing quadrature-based bounds for the 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!