Approximating the extremal Ritz values in CG

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joint work with
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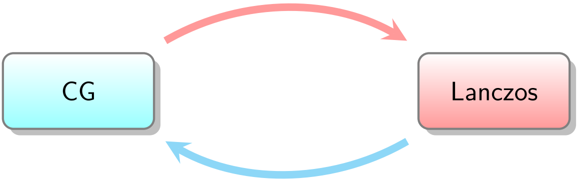
Problem formulation

Consider a system

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

where $\mathbf{A} \in \mathbb{R}^{n \times n}$ is **symmetric, positive definite**.



Approximations to $\lambda_{\min}$ **and** $\lambda_{\max}$ during CG computations?

(for free, as a by-product, without storing coefficients)

Motivation

- Error bounds

$$\frac{\|x - x_k\|_{\mathbf{A}}}{\|x - x_0\|_{\mathbf{A}}} \le 2\left(\frac{\sqrt{\kappa(\mathbf{A})} - 1}{\sqrt{\kappa(\mathbf{A})} + 1}\right)^k .$$

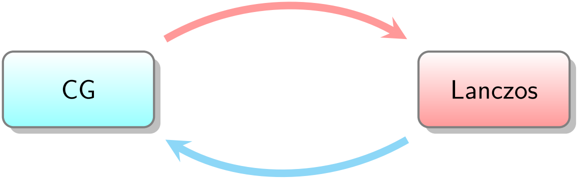
- Gauss-Radau quadrature-based bounds, $\mu \le \lambda_{\min}$,

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

- Normwise backward error

$$\frac{\|r_k\|}{\|\mathbf{A}\|\|x_k\| + \|b\|} .$$

- $\|\mathbf{A}\| \to$ maximum attainable accuracy.
- Sequences of linear systems $\to \kappa(\mathbf{A}_k)$.


CG
Lanczos

The conjugate gradient method (CG)

input $\mathbf{A}$, b, x_0
$r_0 = b - Ax_0$, $p_0 = r_0$
for $k = 1, 2, \ldots$ **do**

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

test quality of x_k

end for

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

Orthogonality

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

Coefficients $\to \mathbf{R}_k$

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

The Lanczos algorithm

Let $\mathbf{A}$ be symmetric, compute orthonormal basis of $\mathcal{K}_k(\mathbf{A}, r_0)$

input $\mathbf{A}$, r_0
$v_1 = r_0/\|r_0\|$
$\beta_0 = 0,\ v_0 = 0$
for $k = 1, 2, \ldots$ **do**
  $\alpha_k = v_k^T \mathbf{A} v_k$
  $w = \mathbf{A} v_k - \alpha_k v_k - \beta_{k-1} v_{k-1}$
  $\beta_k = \|w\|$
  $v_{k+1} = w/\beta_k$
end for

$$\mathbf{T}_k = \begin{bmatrix} \alpha_1 & \beta_1 & & \\ \beta_1 & \ddots & & \\ & & \ddots & \beta_{k-1} \\ & & \beta_{k-1} & \alpha_k \end{bmatrix}$$

$$\mathbf{V}_k^* \mathbf{V}_k = \mathbf{I}$$

$$\mathbf{A}\mathbf{V}_k = \mathbf{V}_k \mathbf{T}_k + \beta_k v_{k+1} e_k^T$$

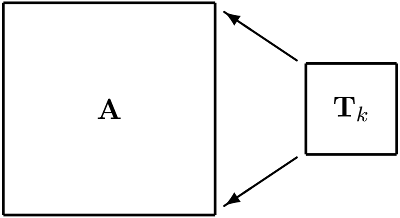
The Lanczos method

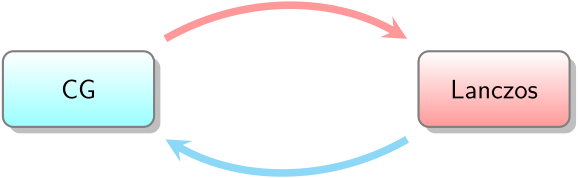
and the eigenvalue approximations

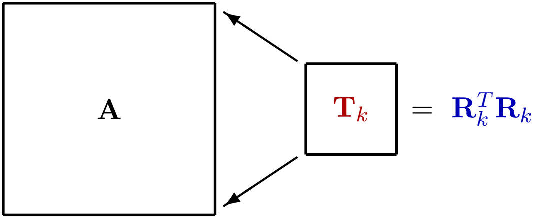
$$\mathbf{A}\mathbf{V}_k = \mathbf{V}_k \underbrace{\mathbf{T}_k}_{\mathbf{T}_k\, y = \mu\, y} + \beta_k v_{k+1} e_k^T$$

and

$$\mathbf{A} \overbrace{\mathbf{V}_k y}^{z} = \mu \overbrace{\mathbf{V}_k y}^{z} + \beta_k\, v_{k+1} e_k^T\, y$$







$$\lambda_{\max}(\mathbf{T}_k) = \|\mathbf{R}_k\|^2$$
$$\lambda_{\min}(\mathbf{T}_k) = 1/\|\mathbf{R}_k^{-1}\|^2$$

Approximating extremal Ritz values in CG

Incremental estimation

of the largest and the smallest Ritz value in CG

- Want to estimate $\|\mathbf{R}_k\|$ and $\|\mathbf{R}_k^{-1}\|$.

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

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

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

  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

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

Specialization to upper bidiagonal matrices

and their inverses

$$\mathbf{R}_{k+1} = \left[\begin{array}{cccc|c} a_1 & b_1 & & & 0 \\ & \ddots & \ddots & & \vdots \\ & & \ddots & b_{k-1} & 0 \\ & & & a_k & b_k \\ \hline & & & & a_{k+1} \end{array}\right]$$

$$\mathbf{R}_{k+1}^{-1} = \begin{bmatrix} \mathbf{R}_k^{-1} & -w_k \frac{b_k}{a_{k+1}} \\ & \frac{1}{a_{k+1}} \end{bmatrix}$$

where w_k is the last column of $\mathbf{R}_k^{-1}$.

Find **updating formulas** for the entries of the 2×2 matrices.

Incremental estimation of $\|\mathbf{R}_k\|^2$ in CG

Approximation ρ_{k+1} to the largest Ritz value

input $\mathbf{A}$, b

$r_0 = b$, $p_0 = r_0$

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

CG iteration(k) $\rightarrow \gamma_{k-1}$, x_k, r_k, δ_k, p_k

$c_0^2 = 1$, $\rho_1 = {\gamma_0}^{-1}$ for $k = 1$

$\sigma_k = \frac{\sqrt{\delta_k}}{\gamma_{k-1}}\, c_{k-1}$,

$\tau_k = \frac{\delta_k}{\gamma_{k-1}} + \frac{1}{\gamma_k}$

$\Delta_k = (\rho_k - \tau_k)^2 + 4\sigma_k^2$

$c_k^2 = \frac{1}{2}\left(1 - \frac{\rho_k - \tau_k}{\sqrt{\Delta_k}}\right)$

$\rho_{k+1} = \rho_k + \sqrt{\Delta_k}\, c_k^2$

end for

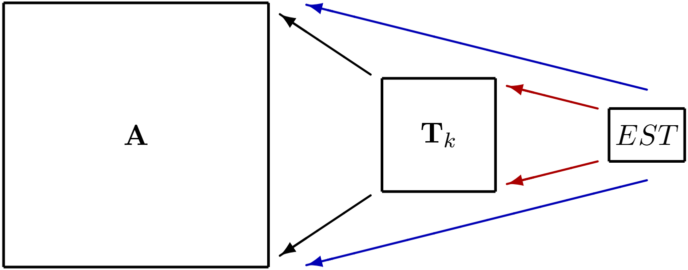
Incremental estimation of $\|\mathbf{R}_k^{-1}\|^2$ in CG

Approximation $\rho_{k+1}^{\min}$ to the smallest Ritz value

Having γ_{k-1}, γ_k and δ_k, update

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

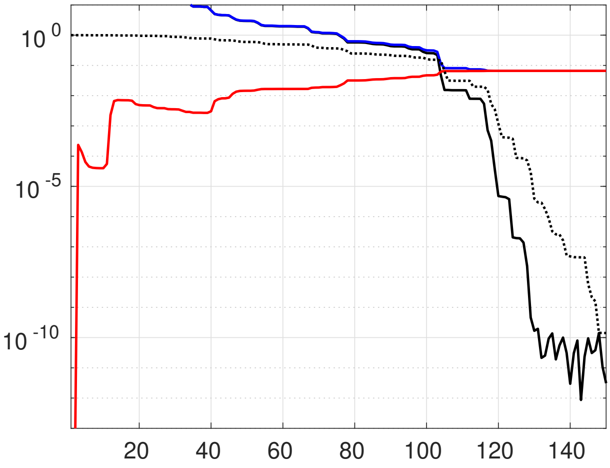
Very cheap, no need to store vectors or coefficients [Meurant, T. 2018]



Numerical experiments

Approximation of $\lambda_{\min}$

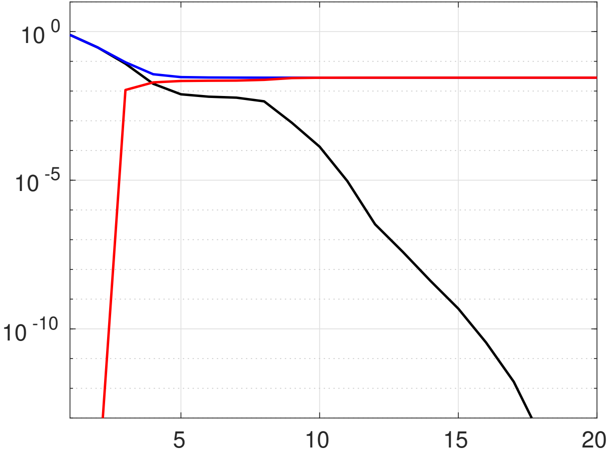
bcsstk01, $n = 48$



$$\frac{\theta_k^{\min} - \rho_k^{\min}}{\theta_k^{\min}}, \quad \frac{\lambda_{\min} - \theta_k^{\min}}{\lambda_{\min}}, \quad \frac{\lambda_{\min} - \rho_k^{\min}}{\lambda_{\min}}$$

Approximation of $\lambda_{\max}$

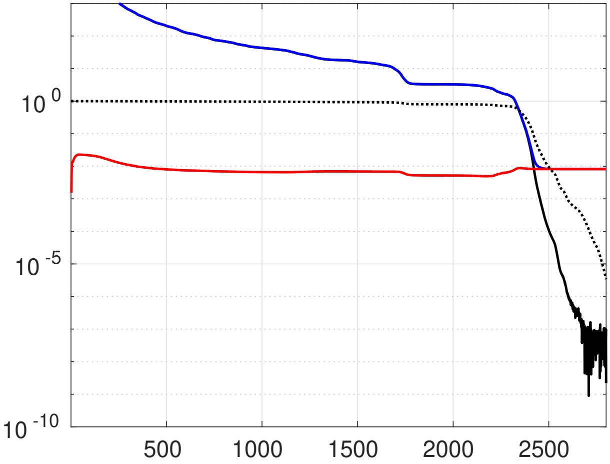
bcsstk01, $n = 48$



$$\frac{\theta_k^{\max} - \rho_k^{\max}}{\theta_k^{\min}}, \quad \frac{\lambda_{\max} - \theta_k^{\max}}{\lambda_{\min}}, \quad \frac{\lambda_{\max} - \rho_k^{\max}}{\lambda_{\max}}$$

Approximation of $\hat{\lambda}_{\min}$

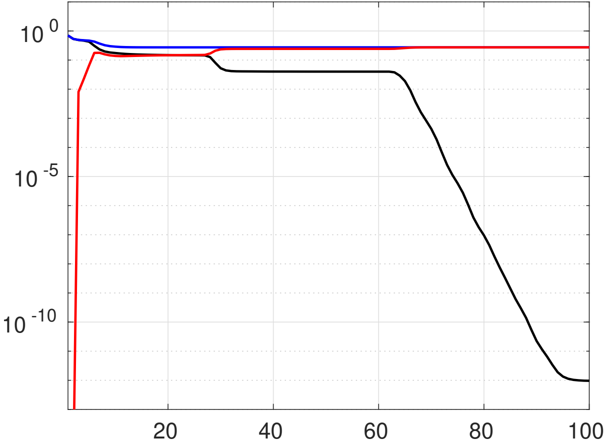
s3dkt3m2, $n = 90449$, preconditioned using `ichol`



$$\frac{\theta_k^{\min} - \rho_k^{\min}}{\theta_k^{\min}}, \quad \frac{\lambda_{\min} - \theta_k^{\min}}{\lambda_{\min}}, \quad \frac{\lambda_{\min} - \rho_k^{\min}}{\lambda_{\min}}$$

Approximation of $\hat{\lambda}_{\max}$

s3dkt3m2, $n = 90449$, preconditioned using `ichol`



$$\frac{\theta_k^{\max} - \rho_k^{\max}}{\theta_k^{\min}}, \quad \frac{\lambda_{\max} - \theta_k^{\max}}{\lambda_{\min}}, \quad \frac{\lambda_{\max} - \rho_k^{\max}}{\lambda_{\max}}$$

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

Cheap bounds on the $\mathbf{A}$-norm of the error

Let $0 < \mu \leq \lambda_{\min}$. Then

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

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

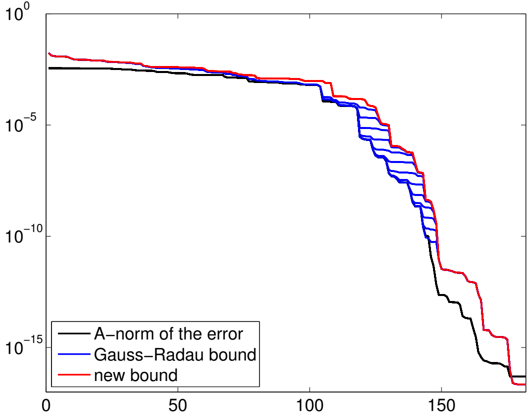
$$\gamma_{k+1}^{(\mu)} \; = \; \frac{\left(\gamma_k^{(\mu)} - \gamma_k\right)}{\mu \left(\gamma_k^{(\mu)} - \gamma_k\right) \; + \; \delta_{k+1}} \, , \qquad \gamma_0^{(\mu)} = \frac{1}{\mu} \, .$$

[Golub, Meurant 1997], [Meurant, T. 2013, 2018]

Bounds for $\mu < \lambda_{\min}$

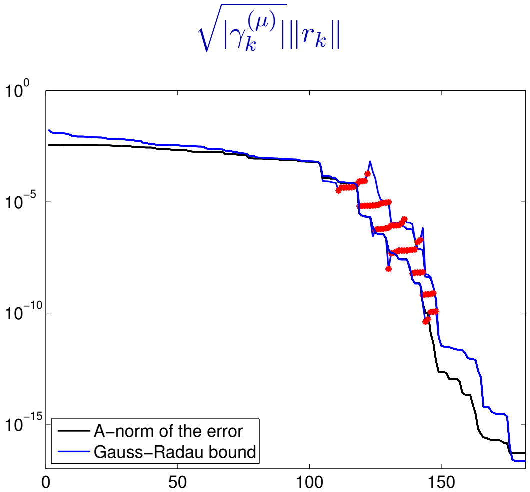
`bcsstk01`, $n = 48$, $\mu = \frac{\lambda_{\min}}{1+10^{-m}}$, $m = 2, 4, \ldots, 14$

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



Gauss-Radau bound for $\mu > \lambda_{\min}$

bcsstk01, $n = 48$, $\mu = \frac{\lambda_{\min}}{1-10^{-m}}$, $m = 2, 4, \ldots, 14$



Bounds on the $\mathbf{A}$-norm of the error

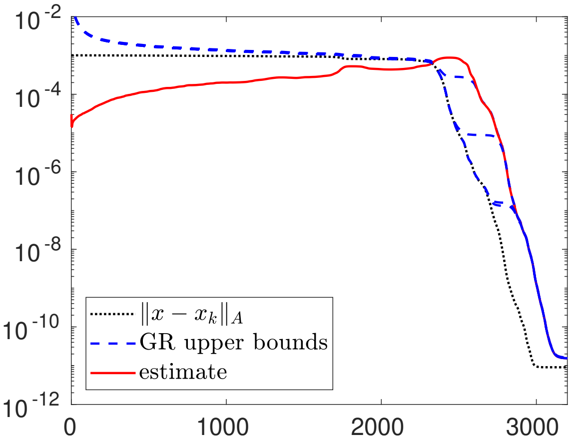
Let $0 < \mu \leq \lambda_{\min}$. Then

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

- **First bound** can be used only for $\mu \leq \lambda_{\min}$, sensitive!
- **Second bound**
  - monotonically decreasing
  - not sensitive to the choice of μ
  - as good as Gauss-Radau in many cases
  - can be used even if $\mu > \lambda_{\min}$ (heuristics
  - μ can be changed at every iteration

Approximating $\|x - x_k\|_{\mathbf{A}}$ using $\mu = \rho_k^{\min}$

s3dkt3m2, $n = 90449$, ichol, $\mu = \frac{\lambda_{\min}(\widehat{A})}{(1+10^{-m})}$, $m = 1, 4, 8, 12$



$$\|x - x_k\|_{\mathbf{A}} < \sqrt{\gamma_k^{(\mu)}}\|r_k\| \lesssim \frac{\|r_k\|}{\sqrt{\rho_k^{\min}}} \frac{\|r_k\|}{\|p_k\|}$$

Summary

- $\mathbf{R}_k \rightarrow$ an important **source of information**.
- We developed **cheap estimators** of $\lambda_{\min}(\mathbf{A})$ and $\lambda_{\max}(\mathbf{A})$.
- The reached relative **accuracy** $\approx$ usually 10^{-1} or 10^{-2}.
- The accuracy **can be improved** when storing $\mathbf{R}_k$.
- These estimates can be used, e.g., to approximate
  - the normwise backward error,
  - condition number of $\mathbf{A}$,
  - attainable level of accuracy,
  - **the $\mathbf{A}$-norm of the error**. [Meurant, T. 2018]

Related papers

- C. H. Bischof, [Incremental condition estimation, SIAM J. Matrix Anal. Appl., 35 (1990), pp. 312-322.]
- I. S. Duff and C. Vömel, [Incremental norm estimation for dense and sparse matrices, BIT 42 (2002), pp. 300-322.]
- J. Duintjer Tebbens and M. Tůma, [On incremental condition estimators in the 2-norm. SIAM J. Matrix Anal. Appl. 35 (2014), pp. 174-197.]
- 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]
- G. Meurant and P. Tichý, [Approximating the extreme Ritz values and upper bounds for the A-norm of the error in CG, Numer. Algor. (2018).]