On computing quadrature-based bounds for the $\mathbf{A}$-norm of the error in conjugate gradients

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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**.

Without loss of generality, $\|b\| = 1$, $x_0 = 0$.

The conjugate gradient method

input $\mathbf{A}$, b

$r_0 = b$, $p_0 = r_0$

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

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

test quality of x_k

end for

Mathematical properties of CG

optimality property

CG $\rightarrow x_k,\ r_k,\ p_k$

The kth Krylov subspace,

$$\mathcal{K}_k(\mathbf{A}, b) \equiv \operatorname{span}\{b, \mathbf{A}b, \ldots, \mathbf{A}^{k-1}b\}\,.$$

- Residuals $r_0, \ldots, r_{k-1}$ form an orthogonal basis of $\mathcal{K}_k(\mathbf{A}, b)$.
- The CG approximation x_k is optimal

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

A practically relevant question

How to measure quality of an approximation?

- **using residual information,**
  - normwise backward error,
  - relative residual norm.

  "Using of the residual vector r_k as a measure of the "goodness" of the estimate x_k is not reliable" [Hestenes & Stiefel 1952]

- **using error estimates,**
  - estimate of the $\mathbf{A}$-norm of the error,
  - estimate of the Euclidean norm of the error.

  "The function $(x - x_k, \mathbf{A}(x - x_k))$ can be used as a measure of the "goodness" of x_k as an estimate of x." [Hestenes & Stiefel 1952]

The (relative) $\mathbf{A}$-norm of the error plays an important role in stopping criteria in many problems [Deuflhard 1994], [Arioli 2004], [Jiránek, Strakoš, Vohralík 2006]

The Lanczos algorithm

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

input $\mathbf{A}$, b
$v_1 = b/\|b\|$, $\delta_1 = 0$
$\beta_0 = 0$, $v_0 = 0$
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

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

The Lanczos algorithm can be represented by

$$\mathbf{A}\mathbf{V}_k = \mathbf{V}_k \mathbf{T}_k + \beta_k v_{k+1} e_k^T, \qquad \mathbf{V}_k^* \mathbf{V}_k = \mathbf{I}.$$

CG versus Lanczos

Let $\mathbf{A}$ be symmetric, positive definite

The CG approximation is the given by

$$x_k = \mathbf{V}_k\, y_k \quad \text{where} \quad \mathbf{T}_k\, y_k = \|b\| e_1\,.$$

It holds that

$$v_{k+1} = (-1)^k \frac{r_k}{\|r_k\|}\,, \qquad \mathbf{T}_k = \mathbf{L}_k \mathbf{D}_k \mathbf{L}_k^T\,,$$

where

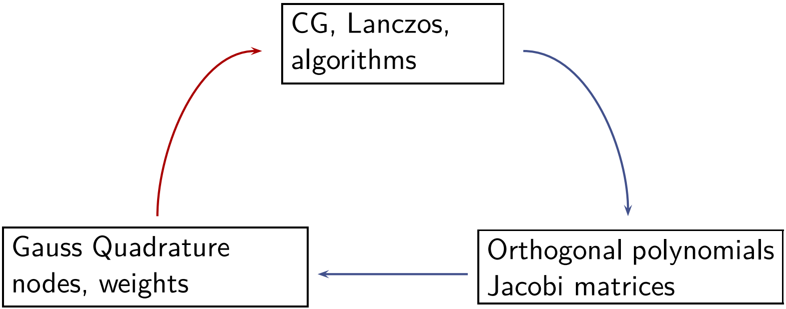
$$\mathbf{L}_k \equiv \begin{bmatrix} 1 & & & \\ \sqrt{\delta_1} & \ddots & & \\ & \ddots & \ddots & \\ & & \sqrt{\delta_{k-1}} & 1 \end{bmatrix}, \quad \mathbf{D}_k \equiv \begin{bmatrix} \gamma_0^{-1} & & & \\ & \ddots & & \\ & & \ddots & \\ & & & \gamma_{k-1}^{-1} \end{bmatrix}.$$

- Both algorithms generate an orthogonal basis of the Krylov subspace $\mathcal{K}_k(\mathbf{A}, b)$.
- Lanczos generates an orthonormal basis $v_1, \ldots, v_k$ using a three-term recurrence $\rightarrow \mathbf{T}_k$.
- CG generates an orthogonal basis $r_0, \ldots, r_{k-1}$ using a coupled two-term recurrence $\rightarrow \mathbf{T}_k = \mathbf{L}_k \mathbf{D}_k \mathbf{L}_k^T$.
- It holds that

$$v_{k+1} = (-1)^k \frac{r_k}{\|r_k\|} .$$

CG, Lanczos and Gauss quadrature

Overview



CG, Lanczos and Gauss quadrature

Corresponding formulas

At any iteration step k, CG (implicitly) determines weights and nodes of the k-point Gauss quadrature

$$\int_{\zeta}^{\xi} f(\lambda)\, d\omega(\lambda) \;=\; \sum_{i=1}^{k} \omega_i^{(k)} f(\theta_i^{(k)}) \;+\; \mathcal{R}_k[f]\,.$$

$\mathbf{T}_k$ ... Jacobi matrix, $\theta_i^{(k)}$ ... eigenvalues of $\mathbf{T}_k$, $\omega_i^{(k)}$ ... scaled and squared first components of the normalized eigenvectors of $\mathbf{T}_k$.

$f(\lambda) \equiv \lambda^{-1}$. **Lanczos-related** quantities:

$$\left(\mathbf{T}_n^{-1}\right)_{1,1} \;=\; \left(\mathbf{T}_k^{-1}\right)_{1,1} + \mathcal{R}_k[\lambda^{-1}].$$

CG-related quantities

$$\|x\|_{\mathbf{A}}^2 \;=\; \sum_{j=0}^{k-1} \gamma_j \|r_j\|^2 + \|x - x_k\|_{\mathbf{A}}^2\,.$$

Gauss-Radau quadrature

$$\int_{\zeta}^{\xi} f \, d\omega(\lambda) = \sum_{i=1}^{k} w_i f(\nu_i) + \sum_{j=1}^{m} \widetilde{w}_j f(\widetilde{\nu}_j) + \mathcal{R}_k[f],$$

the weights $[w_i]_{i=1}^k$, $[\widetilde{w}_j]_{j=1}^m$ and the nodes $[\nu_i]_{i=1}^k$ are unknowns, $[\widetilde{\nu}_j]_{j=1}^m$ are prescribed outside the open integration interval.

$m = 1$: **Gauss-Radau** quadrature. Algebraically: Given $\mu \equiv \widetilde{\nu}_1$, find $\widetilde{\alpha}_{k+1}$ so that μ is an eigenvalue of the extended matrix

$$\widetilde{\mathbf{T}}_{k+1} = \begin{bmatrix} \alpha_1 & \beta_1 & & & \\ \beta_1 & \ddots & \ddots & & \\ & \ddots & \ddots & \beta_{k-1} & \\ & & \beta_{k-1} & \alpha_k & \beta_k \\ & & & \beta_k & \widetilde{\alpha}_{k+1} \end{bmatrix}.$$

Quadrature for $f(\lambda) = \lambda^{-1}$ is given by $\left(\widetilde{\mathbf{T}}_{k+1}^{-1}\right)_{1,1}$.

Quadrature formulas
Golub - Meurant - Strakoš approach

Quadrature formulas for $f(\lambda) = \lambda^{-1}$ take the form

$$\begin{aligned} \left(\mathbf{T}_n^{-1}\right)_{1,1} &= \left(\mathbf{T}_k^{-1}\right)_{1,1} + \mathcal{R}_k^{(G)}, \\ \left(\mathbf{T}_n^{-1}\right)_{1,1} &= \left(\widetilde{\mathbf{T}}_k^{-1}\right)_{1,1} + \mathcal{R}_k^{(R)}, \end{aligned}$$

and $\mathcal{R}_k^{(G)} > 0$ while $\mathcal{R}_k^{(R)} < 0$ if $\mu \leq \lambda_{\min}$. Equivalently

$$\begin{aligned} \|x\|_{\mathbf{A}}^2 &= \tau_k + \|x - x_k\|_{\mathbf{A}}^2, \\ \|x\|_{\mathbf{A}}^2 &= \widetilde{\tau}_k + \mathcal{R}_k^{(R)}. \end{aligned}$$

where $\tau_k \equiv \left(\mathbf{T}_k^{-1}\right)_{1,1}$, $\widetilde{\tau}_k \equiv \left(\widetilde{\mathbf{T}}_k^{-1}\right)_{1,1}$.

[Golub & Meurant 1994, 1997, 2010, Golub & Strakoš 1994]

Idea of estimating the $\mathbf{A}$-norm of the error

Consider two quadrature rules at steps k and $k+d$, $d>0$,

$$\begin{aligned} \|x\|_{\mathbf{A}}^2 &= \tau_k + \|x-x_k\|_A^2\,, \\ \|x\|_{\mathbf{A}}^2 &= \widehat{\tau}_{k+d} + \widehat{\mathcal{R}}_{k+d}\,. \end{aligned} \tag{1}$$

Then

$$\|x-x_k\|_{\mathbf{A}}^2 = \widehat{\tau}_{k+d} - \tau_k + \hat{\mathcal{R}}_{k+d}\,.$$

Gauss quadrature: $\hat{\mathcal{R}}_{k+d} = \mathcal{R}_{k+d}^{(G)} > 0 \rightarrow$ lower bound,

Radau quadrature: $\hat{\mathcal{R}}_{k+d} = \mathcal{R}_{k+d}^{(R)} < 0 \rightarrow$ upper bound.

How to compute efficiently

$$\widehat{\tau}_{k+d} - \tau_k\,?$$

How to compute $\widehat{\tau}_{k+d} - \tau_k$?

For numerical reasons, it is not good to compute explicitly τ_k, $\widehat{\tau}_{k+d}$, and subtract .

Instead, we use the formula,

$$
\begin{aligned}
\widehat{\tau}_{k+d} - \tau_k &= \sum_{j=k}^{k+d-2} \left(\tau_{j+1} - \tau_j\right) + \left(\widehat{\tau}_{j+d} - \tau_{j+d-1}\right) \\
&\equiv \sum_{j=k}^{k+d-2} \Delta_j + \widehat{\Delta}_{k+d-1}\,,
\end{aligned}
$$

and update the Δ's without subtraction. Recall that

$$
\begin{aligned}
\Delta_j &= \left(\mathbf{T}_{j+1}^{-1}\right)_{1,1} - \left(\mathbf{T}_j^{-1}\right)_{1,1}\,, \\
\widehat{\Delta}_{k+d-1} &= \left(\widehat{\mathbf{T}}_{k+d}^{-1}\right)_{1,1} - \left(\mathbf{T}_{k+d-1}^{-1}\right)_{1,1}\,.
\end{aligned}
$$

Golub and Meurant approach

[Golub & Meurant 1994, 1997]: Use tridiagonal matrices,

$$\boxed{\text{CG}} \rightarrow \boxed{\mathbf{T}_k} \rightarrow \boxed{\mathbf{T}_k - \mu \mathbf{I}} \rightarrow \boxed{\widetilde{\mathbf{T}}_k}$$

Compute the Δ's,

$$\Delta_{k-1} \equiv \left(\mathbf{T}_k^{-1}\right)_{1,1} - \left(\mathbf{T}_{k-1}^{-1}\right)_{1,1},$$

$$\Delta_k^{(\mu)} \equiv \left(\widetilde{\mathbf{T}}_{k+1}^{-1}\right)_{1,1} - \left(\mathbf{T}_k^{-1}\right)_{1,1}.$$

Use the formulas

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

$$\|x - x_k\|_{\mathbf{A}}^2 = \sum_{j=k}^{k+d-2} \Delta_j + \Delta_{k+d-1}^{(\mu)} + \mathcal{R}_{k+d}^{(R)}.$$

CGQL (Conjugate Gradients and Quadrature via Lanczos)

input $\mathbf{A}$, b, x_0, μ
$r_0 = b - \mathbf{A}x_0$, $p_0 = r_0$
$\delta_0 = 0$, $\gamma_{-1} = 1$, $c_1 = 1$, $\beta_0 = 0$, $d_0 = 1$, $\tilde{\alpha}_1^{(\mu)} = \mu$,
for $k = 1, \ldots,$ until convergence **do**
CG-iteration (k)

$$\begin{aligned}
\alpha_k &= \frac{1}{\gamma_{k-1}} + \frac{\delta_{k-1}}{\gamma_{k-2}}, \; \beta_k^2 = \frac{\delta_k}{\gamma_{k-1}^2} \\
d_k &= \alpha_k - \frac{\beta_{k-1}^2}{d_{k-1}}, \; \Delta_{k-1} = \|r_0\|^2 \frac{c_k^2}{d_k}, \\
\tilde{\alpha}_{k+1}^{(\mu)} &= \mu + \frac{\beta_k^2}{\alpha_k - \tilde{\alpha}_k^{(\mu)}}, \\
\Delta_k^{(\mu)} &= \|r_0\|^2 \frac{\beta_k^2 c_k^2}{d_k\left(\tilde{\alpha}_{k+1}^{(\mu)} d_k - \beta_k^2\right)}, \quad c_{k+1}^2 = \frac{\beta_k^2 c_k^2}{d_k^2}
\end{aligned}$$

Estimates(k,d)
end for

Our approach

[Meurant & T. 2012]

- We use tridiagonal matrices only implicitly.
- CG generates LDL^T factorization of $\mathbf{T}_k$.
- Update LDL^T factorizations of the tridiagonal matrices

$$\boxed{\widetilde{\mathbf{T}}_k}$$

- Quite complicated algebraic manipulations, but, in the end,
- we get **very simple formulas** for updating Δ_{k-1} and $\Delta_k^{(\mu)}$.
- This idea can be used also for other types of quadratures (Gauss-Lobatto, Anti-Gauss).

CGQ (Conjugate Gradients and Quadrature)

[Meurant & T. 2012]

input $\mathbf{A}$, b, x_0, μ,
$r_0 = b - \mathbf{A}x_0$, $p_0 = r_0$
$\Delta_0^{(\mu)} = \frac{\|r_0\|^2}{\mu}$,
for $k = 1, \ldots,$ until convergence **do**
CG-iteration(k)

$$\begin{aligned} \Delta_{k-1} &= \gamma_{k-1}\|r_{k-1}\|^2, \\ \Delta_k^{(\mu)} &= \frac{\|r_k\|^2 \left(\Delta_{k-1}^{(\mu)} - \Delta_{k-1}\right)}{\mu\left(\Delta_{k-1}^{(\mu)} - \Delta_{k-1}\right) + \|r_k\|^2} \end{aligned}$$

Estimates(k,d)
end for

Practically relevant questions

The estimation is based on formulas

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

$$\|x - x_k\|_{\mathbf{A}}^2 = \sum_{j=k}^{k+d-2} \Delta_j + \Delta_{k+d-1}^{(\mu)} + \mathcal{R}_{k+d}^{(R)}$$

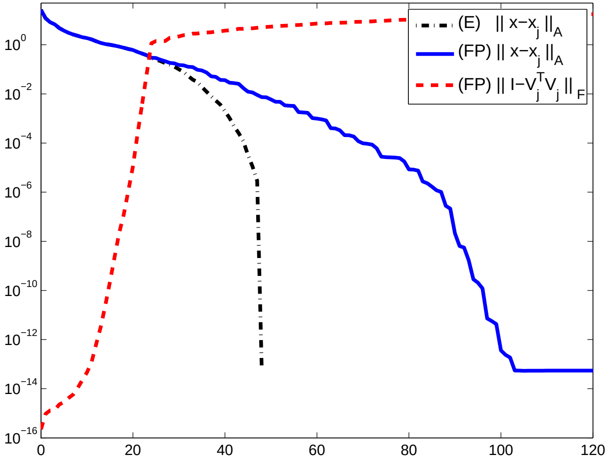
We are able to compute Δ_j and $\Delta_j^{(\mu)}$ almost for free.

Practically relevant questions:

- What happens in finite precision arithmetic ?
- How to choose d ?
- How to choose μ ?

Finite precision arithmetic
CG behavior

Orthogonality is lost, convergence is delayed!



Identities need not hold in finite precision arithmetic!

Rounding error analysis

- Lower bound [Strakoš & T. 2002, 2005]: The equality

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

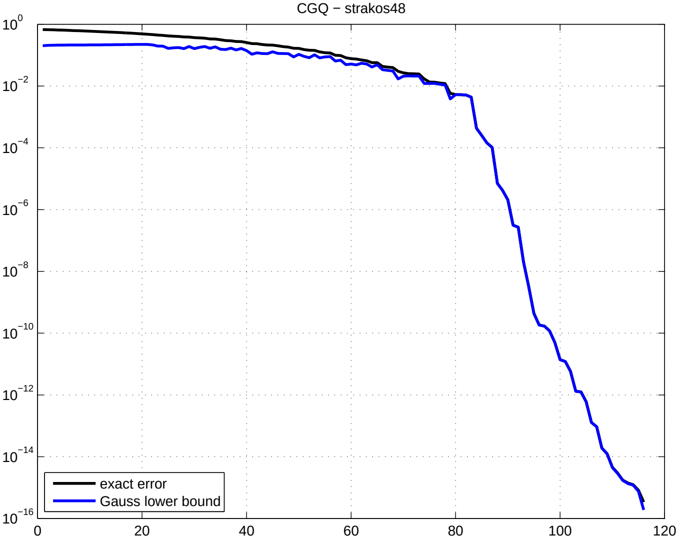
  holds (up to a small inaccuracy) also in finite precision arithmetic for computed vectors and coefficients.

- Upper bound: There is no rounding error analysis of

$$\|x - x_k\|_{\mathbf{A}}^2 = \sum_{j=k}^{k+d-2} \Delta_j + \Delta_{k+d-1}^{(\mu)} \;+\; \mathcal{R}_{k+d}^{(R)}\,.$$

The choice of d - Experiment 1

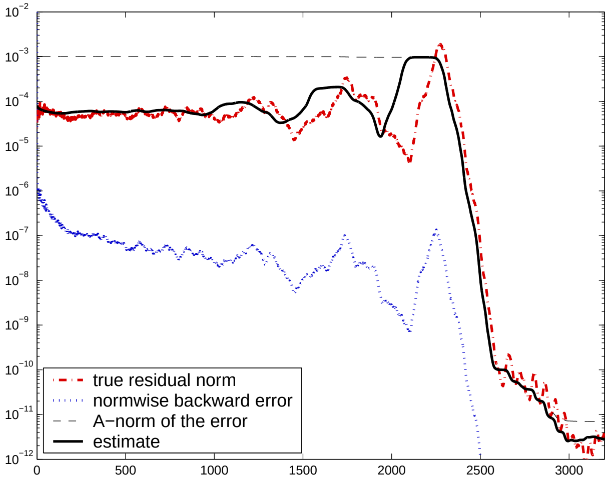
Strakos matrix, $n = 48$, $\lambda_1 = 0.1$, $\lambda_n = 1000$, $\rho = 0.9$, $d = 4$



The choice of d - Experiment 2

R. Kouhia: Cylindrical shell (Matrix Market), matrix s3dkt3m2

PCG, $\kappa(\mathbf{A}) = 3.62e+11\,,\;\; n = 90499\,,\;\; d = 200\,,$ cholinc$(\mathbf{A}, 0)\,.$



The choice of d

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

We get a tight lower bound if

$$\|x - x_k\|_{\mathbf{A}}^2 \;\gg\; \|x - x_{k+d}\|_{\mathbf{A}}^2 \,.$$

How to detect a reasonable decrease of the $\mathbf{A}$-norm od the error?

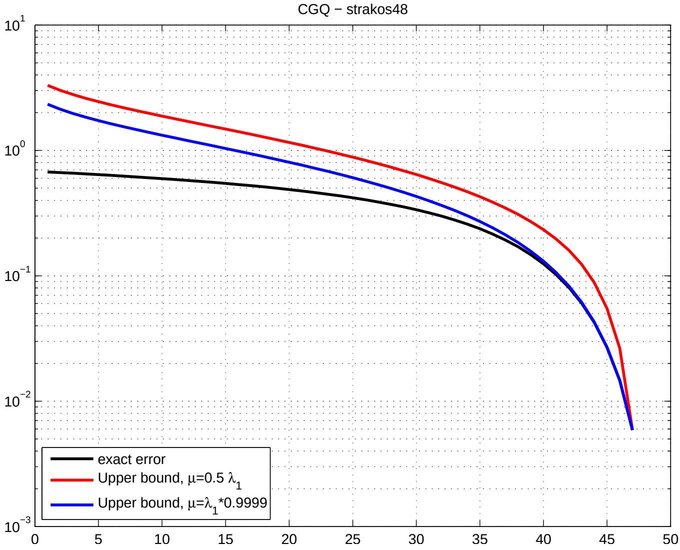
Theoretically, one could use the upper bound,

$$\frac{\|x - x_{k+d}\|_{\mathbf{A}}^2}{\|x - x_k\|_{\mathbf{A}}^2} \;\leq\; \frac{\Delta_{k+d}^{(\mu)}}{\sum_{j=k}^{k+d-1} \Delta_j} \;<\; \mathrm{tol}\,.$$

But, **can we trust the upper bound**?

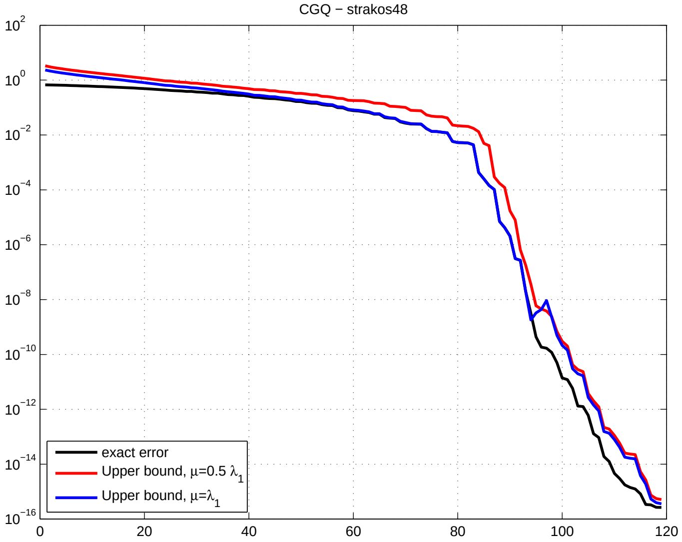
The choice of μ, upper bound, exact arithmetic

Strakos matrix, $n = 48$, $\lambda_1 = 0.1$, $\lambda_n = 1000$, $\rho = 0.9$, $d = 1$



The choice of μ, upper bound, finite precision arithmetic

Strakos matrix, $n = 48$, $\lambda_1 = 0.1$, $\lambda_n = 1000$, $\rho = 0.9$, $d = 1$



Numerical troubles with the upper bound

Given μ, we look for $\widetilde{\alpha}_{k+1}$ (explicitly or implicitly) so that μ is an eigenvalue of the extended matrix

$$\widetilde{\mathbf{T}}_{k+1} = \begin{bmatrix} \alpha_1 & \beta_1 & & & \\ \beta_1 & \ddots & \ddots & & \\ & \ddots & \ddots & \beta_{k-1} & \\ & & \beta_{k-1} & \alpha_k & \beta_k \\ & & & \beta_k & \widetilde{\alpha}_{k+1} \end{bmatrix}.$$

To find such a $\widetilde{\alpha}_{k+1}$, we need to solve the system

$$(\mathbf{T}_k - \mu\mathbf{I})y = e_k\,.$$

If μ is close to the smallest eigenvalue of $\mathbf{T}_k$, we can get into numerical troubles!

Conclusions and questions

- The upper bound as well as the lower bound on the $\mathbf{A}$-norm of the error can be **computed in a simple way**.
- Unfortunately, the computation of the upper bound is **not always numerically stable**.
  - μ is far from $\lambda_1 \rightarrow$ overestimation,
  - μ is close to $\lambda_1 \rightarrow$ numerical troubles.
- The estimation of the $\mathbf{A}$-norm of the error **should be based** on the numerical stable **lower bound**.
- **How to detect** a reasonable decrease of the $\mathbf{A}$-norm of the error? (How to choose d adaptively?).
- Is there any way how to **involve** the upper bound? Understanding of numerical behaviour of the upper bound?

Related papers

- G. Meurant and P. Tichý, [On computing quadrature-based bounds for the $\mathbf{A}$-norm of the error in conjugate gradients, Numer. Algorithms, (2012)]
- G. H. Golub and G. Meurant, [Matrices, moments and quadrature with applications, Princeton University Press, USA, 2010.]
- Z. Strakoš and P. Tichý, [On error estimation in the conjugate gradient method and why it works in finite precision computations, Electron. Trans. Numer. Anal., 13 (2002), pp. 56–80.]
- 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.]

Thank you for your attention!