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

Petr Tichý

joint work with

Gerard Meurant and Zdeněk Strakoš

Institute of Computer Science,
Academy of Sciences of the Czech Republic

September 13, 2012, Podbanské, Slovakia
ALGORITMY 2012

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]

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]

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]

Outline

1. CG and the Lanczos algorithm
2. CG, Lanczos and Quadrature
3. How to compute the estimates?
4. Experiments and questions

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 $k = 1, 2, \dots$ **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

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

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

```
input A, b
v_1 = b/||b||, δ_1 = 0
β_0 = 0, v_0 = 0
for k = 1, 2, ... do
    α_k = v_k^T A v_k
    w = A v_k − α_k v_k − β_{k−1} v_{k−1}
    β_k = ||w||
    v_{k+1} = w/β_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

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

CG versus Lanczos

Summary

- 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

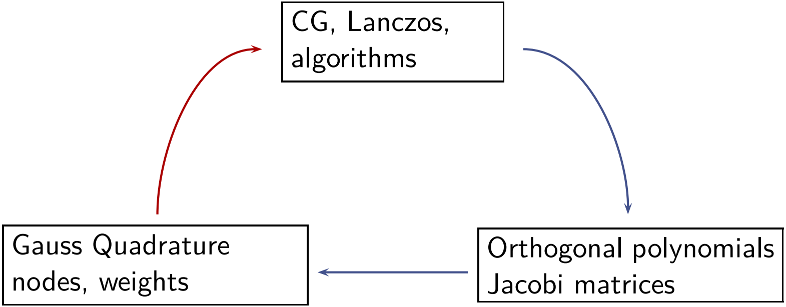
$$v_{k+1} = (-1)^k \frac{r_k}{\|r_k\|}\,.$$

Outline

1. CG and the Lanczos algorithm
2. CG, Lanczos and Quadrature
3. How to compute the estimates?
4. Experiments and questions

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 $\mathbf{T}_k$.

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 $\mathbf{T}_k$.

$f(\lambda) \equiv \lambda^{-1}$

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:

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

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

More general quadrature formulas

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

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.

Gauss-Radau quadrature

More general quadrature formulas

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

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.

Gauss-Radau quadrature

More general quadrature formulas

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

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 $\mu \leq \lambda_{\min}$.

Quadrature formulas

Golub - Meurant - Strakoš approach

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

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

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

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

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 $k+d$, $d > 0$,

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

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.

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

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

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

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

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

Outline

1. CG and the Lanczos algorithm
2. CG, Lanczos and Quadrature
3. How to compute the estimates?
4. Experiments and questions

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 .

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,

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

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,

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

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,

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

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,

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

Use the formulas

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

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 $\Delta_k^{(\mu)}$.

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)

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

  Estimates(k,d)
end for

Outline

1 CG and the Lanczos algorithm

2 CG, Lanczos and Quadrature

3 How to compute the estimates?

4 Experiments and questions

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

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.

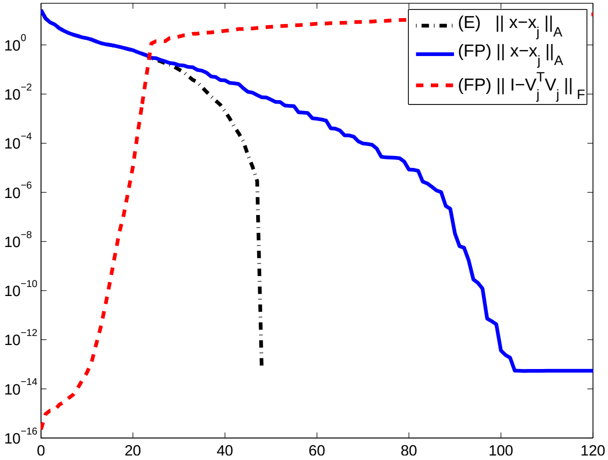
Practically relevant questions:

- 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.

Rounding error analysis

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

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

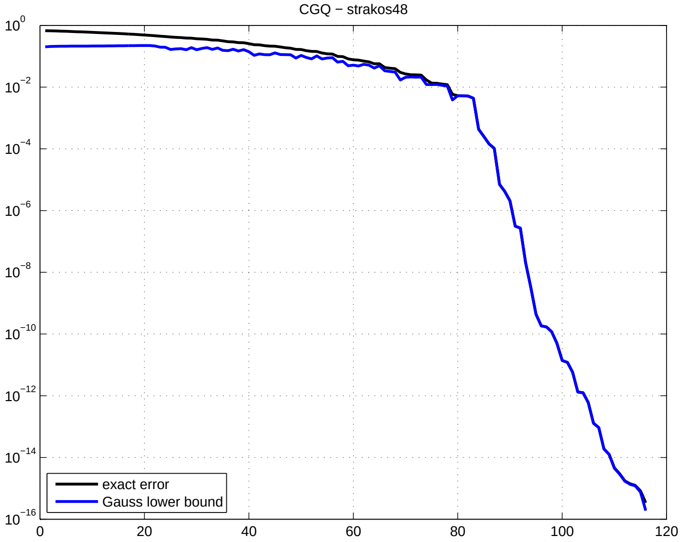
  holds (up to a small inaccuracy) also in finite precision arithmetic for computed vectors and coefficients.

- 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

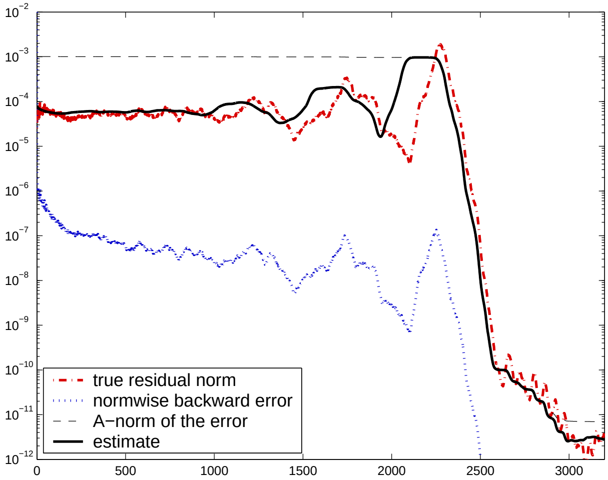
Strakos matrix, $n = 48$, $\lambda_1 = 0.1$, $\lambda_n = 1000$, $\rho = 0.9$, $d = 4$



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

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

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?

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,

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

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?

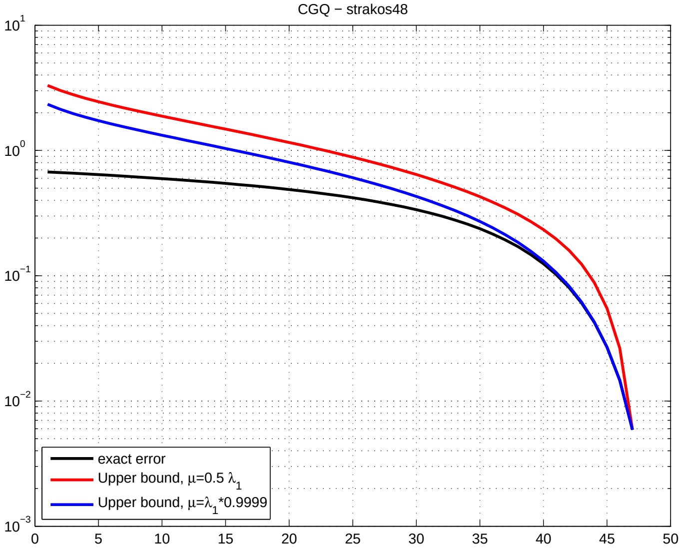
Theoretically, one could use the upper bound,

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

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

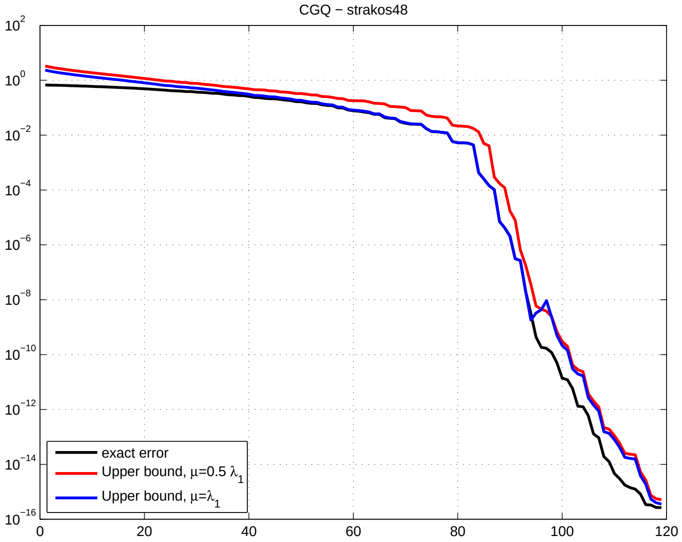
The choice of μ, upper bound, exact arithmetic

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

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

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**.

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 λ_1 $\rightarrow$ overestimation,
  - μ is close to λ_1 $\rightarrow$ 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 λ_1 $\rightarrow$ overestimation,
  - μ is close to λ_1 $\rightarrow$ numerical troubles.
- The estimation of the $\mathbf{A}$-norm of the error **should be based** on the numerical stable **lower bound**.

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?).

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 λ_1 $\rightarrow$ overestimation,
  - μ is close to λ_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!