Efficient Estimation of the $\mathbf{A}$-norm of the Error in the Preconditioned Conjugate Gradient Method

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A system of linear algebraic equations

Consider a system of linear algebraic equations

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

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

Discretization of elliptic self-adjoint partial differential equations:
Energy norm.

The conjugate gradient method minimizes at the jth step the energy norm of the error on the given j-dimensional Krylov subspace.

The conjugate gradient method (CG)

Given $x_0 \in \mathbb{R}^n$, $r_0 = b - \mathbf{A}x_0$.

CG computes a sequence of iterates x_j ,

$$x_j \in x_0 + \mathcal{K}_j(\mathbf{A}, r_0)$$

so that

$$\|x - x_j\|_{\mathbf{A}} = \min_{u \in x_0 + \mathcal{K}_j(\mathbf{A}, r_0)} \|x - u\|_{\mathbf{A}} \, ,$$

where

$$\begin{aligned} \mathcal{K}_j(\mathbf{A}, r_0) &\equiv \operatorname{span}\{r_0, \mathbf{A}r_0, \cdots, \mathbf{A}^{j-1}r_0\} \, , \\ \|x - x_j\|_{\mathbf{A}} &\equiv \big((x - x_j), \mathbf{A}(x - x_j)\big)^{\frac{1}{2}} . \end{aligned}$$

CG – Hestenes and Stiefel (1952)

given $x_0,\ r_0 = b - \mathbf{A}x_0,\ p_0 = r_0$,

for $j = 0, 1, 2, \ldots$

$$\gamma_j = \frac{(r_j, r_j)}{(p_j, \mathbf{A}p_j)}$$

$$\begin{aligned} x_{j+1} &= x_j + \gamma_j\, p_j \\ r_{j+1} &= r_j - \gamma_j\, \mathbf{A}p_j \end{aligned}$$

$$\delta_{j+1} = \frac{(r_{j+1}, r_{j+1})}{(r_j, r_j)}$$

$$p_{j+1} = r_{j+1} + \delta_{j+1}\, p_j$$

Preconditioned Conjugate Gradients (PCG)

The CG-iterates are thought of being applied to

$$\hat{\mathbf{A}}\hat{x} = \hat{b}\,.$$

We consider symmetric preconditioning

$$\hat{\mathbf{A}} = \mathbf{L}^{-1}\mathbf{A}\mathbf{L}^{-T}, \qquad \hat{b} = \mathbf{L}^{-1}b\,.$$

Change of variables

$$\mathbf{M} \equiv \mathbf{L}\mathbf{L}^T\,, \quad \gamma_j \equiv \hat{\gamma}_j\,, \quad \delta_j \equiv \hat{\delta}_j\,,$$

$$x_j \equiv \mathbf{L}^{-T}\hat{x}_j\,, \quad r_j \equiv \mathbf{L}\,\hat{r}_j\,, \quad s_j \equiv \mathbf{M}^{-1}r_j\,, \quad p_j \equiv \mathbf{L}^{-T}\hat{p}_j\,.$$

The preconditioner $\mathbf{M}$ is chosen so that a linear system with the matrix $\mathbf{M}$ is easy to solve while the matrix $\mathbf{L}^{-1}\mathbf{A}\mathbf{L}^{-T}$ should ensure fast convergence of CG.

Algorithm of PCG

given $x_0\,,\;\; r_0 = b - \mathbf{A}x_0\,,\;\; s_0 = \mathbf{M}^{-1}r_0\,,\;\; p_0 = s_0\,,$

for $j = 0, 1, 2, \ldots$

$$\gamma_j = \frac{(r_j\,, s_j)}{(p_j\,, \mathbf{A}p_j)}$$

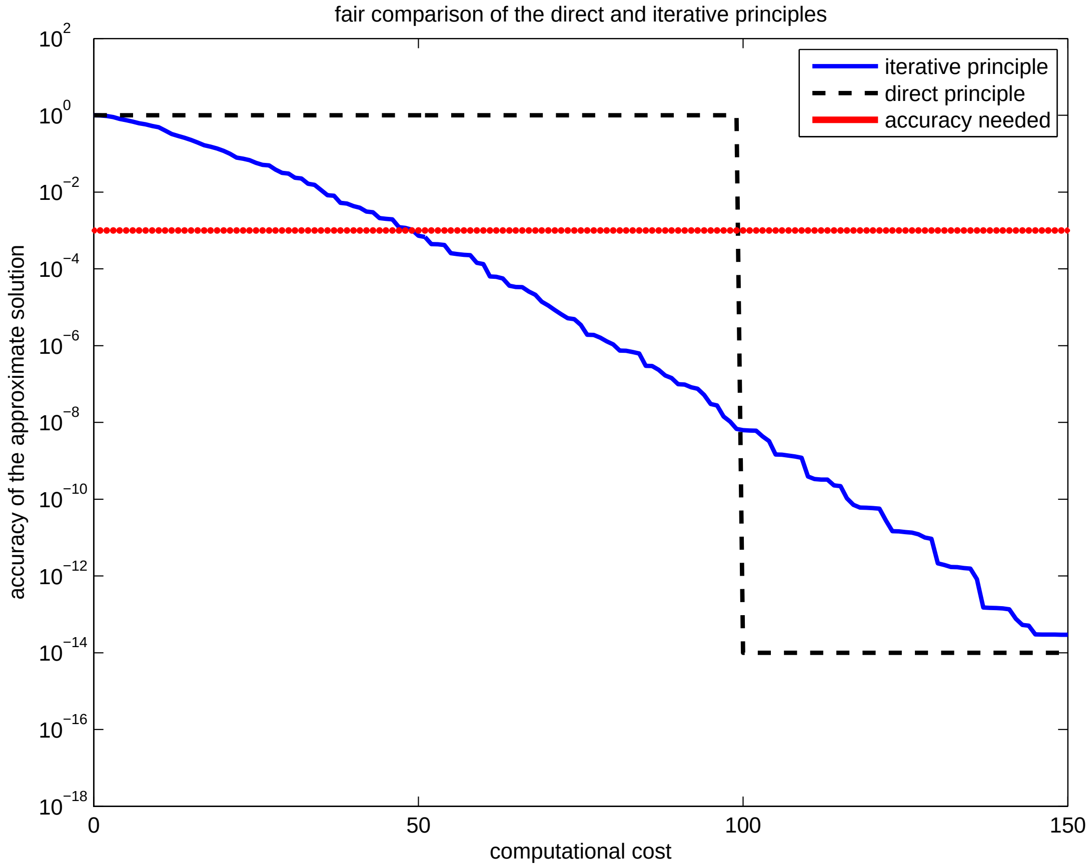
$$\begin{aligned} x_{j+1} &= x_j + \gamma_j\, p_j \\ r_{j+1} &= r_j - \gamma_j\, \mathbf{A}p_j \\ s_{j+1} &= \mathbf{M}^{-1}r_{j+1} \end{aligned}$$

$$\delta_{j+1} = \frac{(r_{j+1}\,, s_{j+1})}{(r_j\,, s_j)}$$

$$p_{j+1} = s_{j+1} + \delta_{j+1}\, p_j$$

When to stop?

When to stop? Should we bother?



How to measure a quality of approximation?

Measuring accuracy? . . . it depends on a problem.

- **using residual information,**
  - normwise backward error,
  - relative residual norm.
- **using error estimates,**
  - estimate of the $\mathbf{A}$-norm of the error,
  - estimate of the Euclidean norm of the error.

If the original system is well-conditioned - it does not matter.

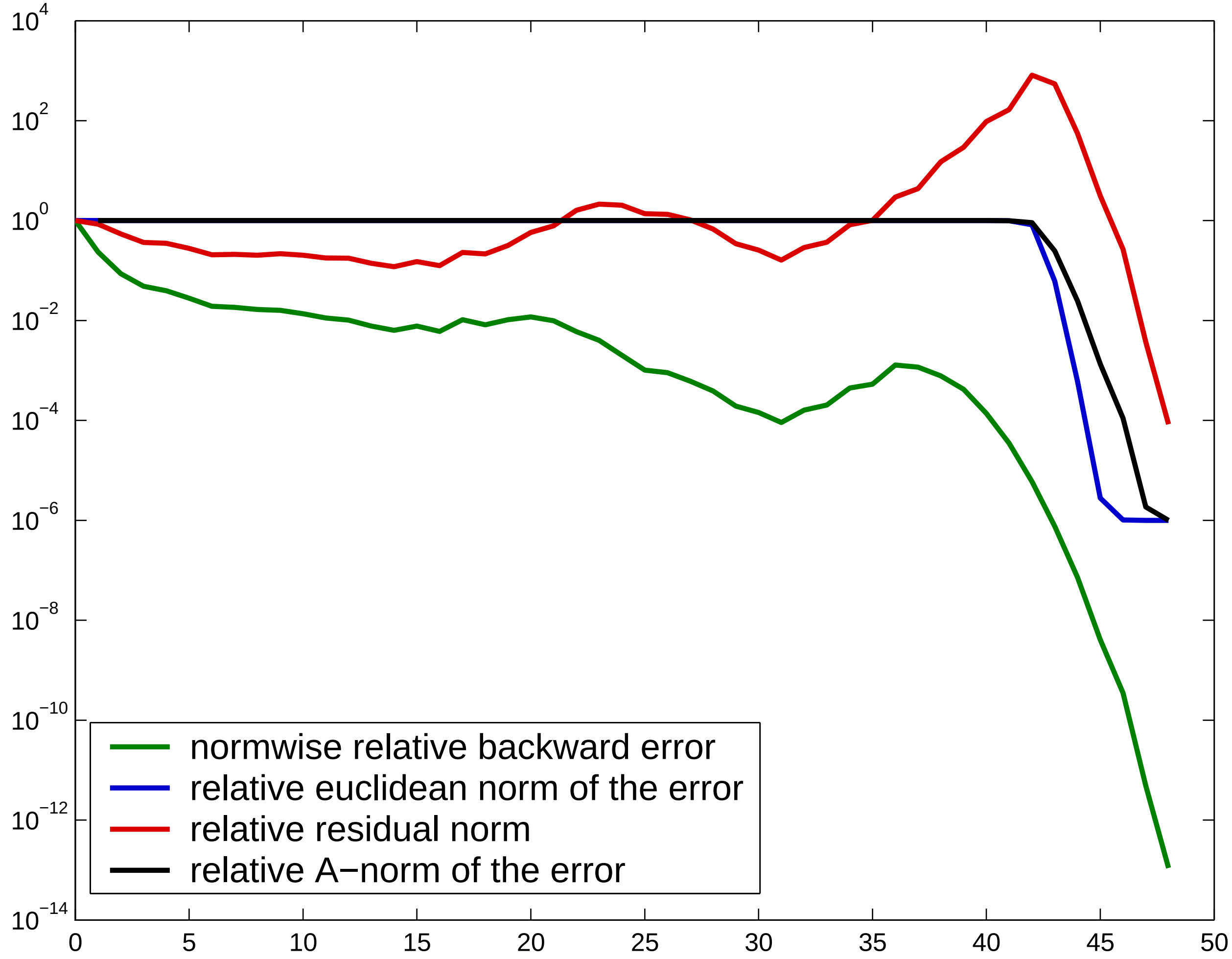
A message from history

- Using of the residual vector r_j as a measure of the "goodness" of the estimate x_j is not reliable [HeSt-52, p. 410].

- The function $(x - x_j, \mathbf{A}(x - x_j))$ can be used as a measure of the "goodness" of x_j as an estimate of x [HeSt-52, p. 413].

Various convergence characteristics

Example using [GuSt-00], $n = 48$.



Outline

1. CG and Gauss Quadrature
2. Construction of estimates in CG and PCG
3. Estimates in finite precision arithmetic
4. Rounding error analysis
5. Numerical experiments
6. Conclusions

1. CG and Gauss Quadrature

CG and Gauss Quadrature

$$Ax = b\,,\; x_0 \quad \longrightarrow \quad \int_\zeta^\xi f(\lambda)\, d\omega(\lambda)$$

$$\uparrow \qquad\qquad\qquad\qquad \uparrow$$

$$T_j\, y_j = \|r_0\|\, e_1 \quad \longleftrightarrow \quad \sum_{i=1}^{j} \omega_i^{(j)} f\left(\theta_i^{(j)}\right)$$

$$x_j = x_0 + Q_j y_j$$

$$\omega^{(j)} \longrightarrow \omega(\lambda)$$

CG and Gauss Quadrature

At any iteration step j, CG represents the matrix formulation of the j-point Gauss quadrature of the Riemann-Stieltjes integral determined by A and r_0,

$$\int_{\zeta}^{\xi} f(\lambda)\, d\omega(\lambda) \;=\; \sum_{i=1}^{j} \omega_i^{(j)} f(\theta_i^{(j)}) \;+\; R_j(f)\,.$$

For $f(\lambda) \equiv \lambda^{-1}$ the formula takes the form

$$\frac{\|x - x_0\|_{\mathbf{A}}^2}{\|r_0\|^2} \;=\; j\text{-th Gauss quadrature} \;+\; \frac{\|x - x_j\|_{\mathbf{A}}^2}{\|r_0\|^2}\,.$$

This was a base for CG error estimation in [DaGoNa-78, GoFi-93, GoMe-94, GoSt-94, GoMe-97, . . .] .

Equivalent formulas

- **Continued fractions** [GoMe-94, GoSt-94, GoMe-97]

$$\|r_0\|^2 \, C_n \;=\; \|r_0\|^2 \, C_j \;+\; \|x - x_j\|_{\mathbf{A}}^2 \,.$$

- **Warnick** [Wa-00]

$$r_0^T (x - x_0) \;=\; r_0^T (x_j - x_0) + \|x - x_j\|_{\mathbf{A}}^2 \,.$$

- **Hestenes and Stiefel** [HeSt-52, De-93, StTi-02]

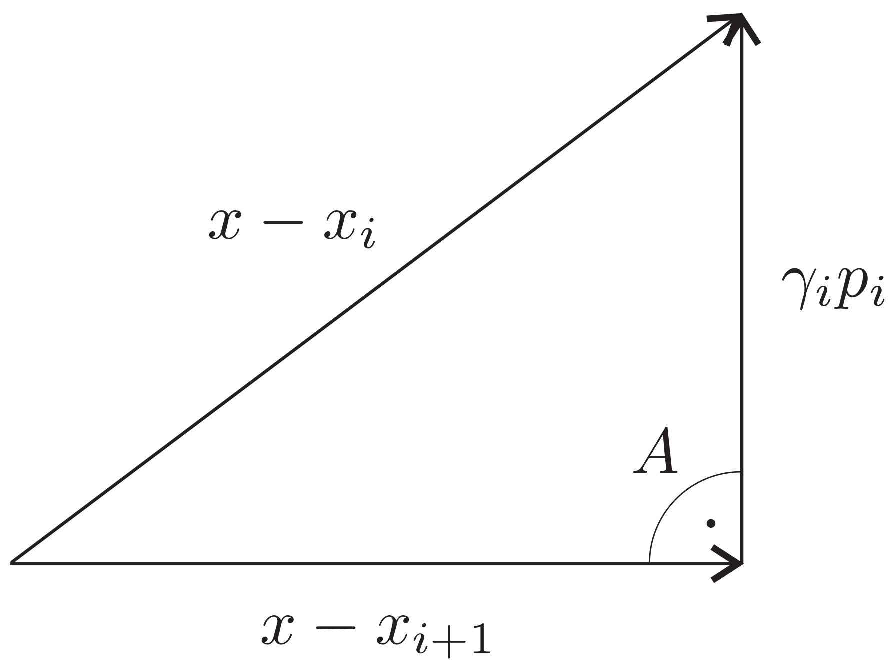
$$\|x - x_0\|_{\mathbf{A}}^2 \;=\; \sum_{i=0}^{j-1} \gamma_i \|r_i\|^2 + \|x - x_j\|_{\mathbf{A}}^2 .$$

The last formula is derived purely algebraically!

Local $\mathbf{A}$-orthogonality

Standard derivation of this formula uses global $\mathbf{A}$-orthogonality among direction vectors [AxKa-01, p. 274], [Ar-04, p. 8].

It follows, however, from the local $\mathbf{A}$-orthogonality and Pythagorean theorem,



Hestenes and Stiefel formula (derivation)

Using local orthogonality between r_{i+1} and p_i,

$$\|x - x_i\|_{\mathbf{A}}^2 - \|x - x_{i+1}\|_{\mathbf{A}}^2 = \gamma_i \|r_i\|^2 .$$

Then

$$\begin{aligned} \|x - x_0\|_{\mathbf{A}}^2 - \|x - x_j\|_{\mathbf{A}}^2 &= \sum_{i=0}^{j-1} \left(\|x - x_i\|_{\mathbf{A}}^2 - \|x - x_{i+1}\|_{\mathbf{A}}^2 \right) \\ &= \sum_{i=0}^{j-1} \gamma_i \|r_i\|^2 . \end{aligned}$$

The approach to derivation of this formula is very important for its justification in finite precision arithmetic.

2. Construction of estimates in CG and PCG

Construction of estimate in CG

Idea: Consider, for example,

$$\|x - x_j\|_{\mathbf{A}}^2 \;=\; \|r_0\|^2 \,[C_n - C_j]\;.$$

Run d extra steps. Subtracting identity for $\|x - x_{j+d}\|_A^2$ gives

$$\|x - x_j\|_{\mathbf{A}}^2 \;=\; \underbrace{\|r_0\|^2 \,[C_{j+d} - C_j]}_{EST^2} + \|x - x_{j+d}\|_{\mathbf{A}}^2\;.$$

When $\|x - x_j\|_{\mathbf{A}}^2 \gg \|x - x_{j+d}\|_{\mathbf{A}}^2$, we have a tight (lower) bound [GoSt-94, GoMe-97].

Mathematically equivalent estimates

- **Continued fractions** [GoSt-94, GoMe-97]

$$\eta_{j,d} = \|r_0\|^2 \left[C_{j+d} - C_j\right],$$

- **Warnick** [Wa-00]

$$\mu_{j,d} = r_0^T (x_{j+d} - x_j),$$

- **Hestenes and Stiefel** [HeSt-52]

$$\nu_{j,d} = \sum_{i=j}^{j+d-1} \gamma_i \|r_i\|^2 .$$

Construction of estimate in PCG

The $\mathbf{A}$-norm of the error can be estimated similarly as in ordinary CG.

- Extension of the Gauss Quadrature formulas based on continued fractions was published in [Me-99].

- Extension of the HS estimate: use the HS formula for $\hat{\mathbf{A}}\hat{x} = \hat{b}$ and substitution $\hat{\mathbf{A}} = \mathbf{L}^{-1}\mathbf{A}\mathbf{L}^{-T}$, $\hat{x}_j = \mathbf{L}^T x_j$, $\hat{\gamma}_i = \gamma_i$, $\hat{r}_i = \mathbf{L}^{-1} r_i$ [De-93, AxKa-01, StTi-04, Ar-04]

$$\underbrace{\|\hat{x} - \hat{x}_j\|^2_{\hat{\mathbf{A}}}}_{\|x - x_j\|^2_{\mathbf{A}}} = \sum_{i=j}^{j+d-1} \underbrace{\hat{\gamma}_i \, \|\hat{r}_i\|^2}_{\gamma_i \, (r_i, s_i)} + \underbrace{\|\hat{x} - \hat{x}_{j+d}\|^2_{\hat{\mathbf{A}}}}_{\|x - x_{j+d}\|^2_{\mathbf{A}}} .$$

In many problems it is convenient to use a stopping criterion that relates the relative $\mathbf{A}$-norm of the error to a discretization error, see [Ar-04].

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

To estimate the relative $\mathbf{A}$-norm of the error we use the identities

$$\begin{aligned} \|x - x_j\|_{\mathbf{A}}^2 &= \nu_{j,d} + \|x - x_{j+d}\|_{\mathbf{A}}^2 , \\ \|x\|_{\mathbf{A}}^2 &= \underbrace{\nu_{0,j+d} + 2b^T x_0 - \|x_0\|_{\mathbf{A}}^2}_{\xi_{j+d}} + \|x - x_{j+d}\|_{\mathbf{A}}^2 . \end{aligned}$$

Define

$$\varrho_{j,d} \equiv \frac{\nu_{j,d}}{\xi_{j+d}} .$$

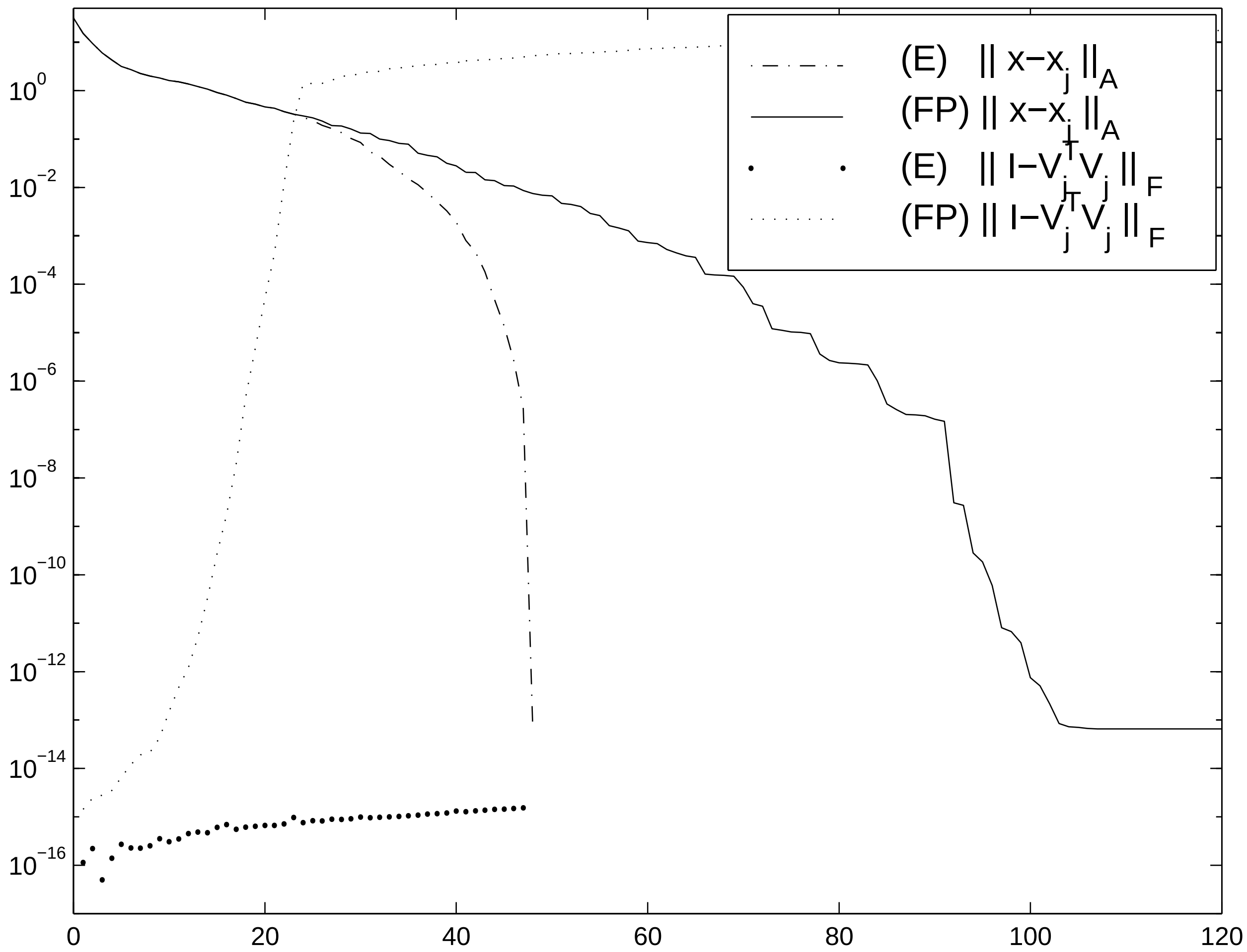
If $\|x\|_{\mathbf{A}} \geq \|x - x_0\|_{\mathbf{A}}$ then $\varrho_{j,d} > 0$ and

$$\varrho_{j,d} = \frac{\|x - x_j\|_{\mathbf{A}}^2 - \|x - x_{j+d}\|_{\mathbf{A}}^2}{\|x\|_{\mathbf{A}}^2 - \|x - x_{j+d}\|_{\mathbf{A}}^2} \leq \frac{\|x - x_j\|_{\mathbf{A}}^2}{\|x\|_{\mathbf{A}}^2} .$$

3. Estimates in finite precision arithmetic

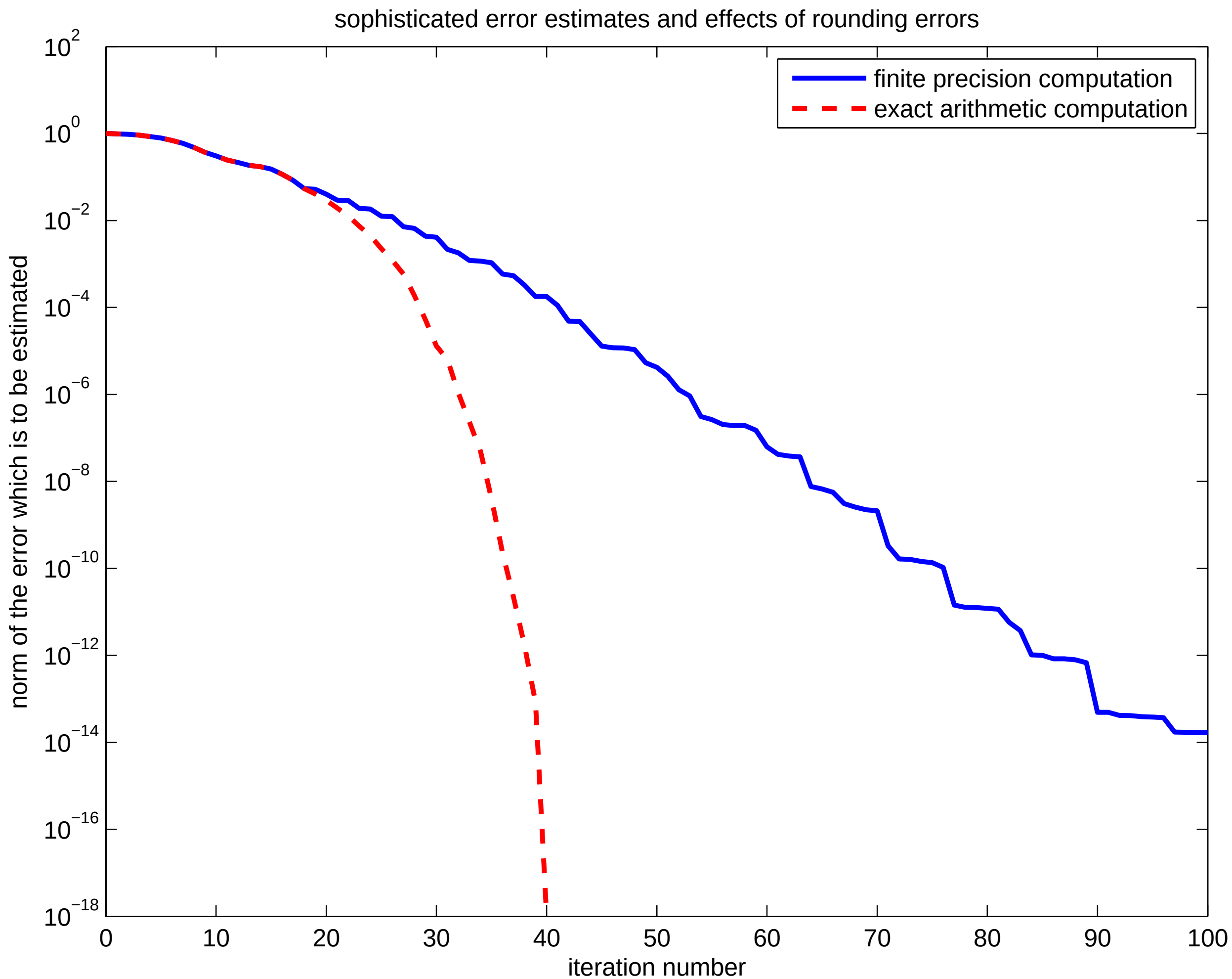
CG behavior in finite precision arithmetic

orthogonality is lost, convergence is delayed!



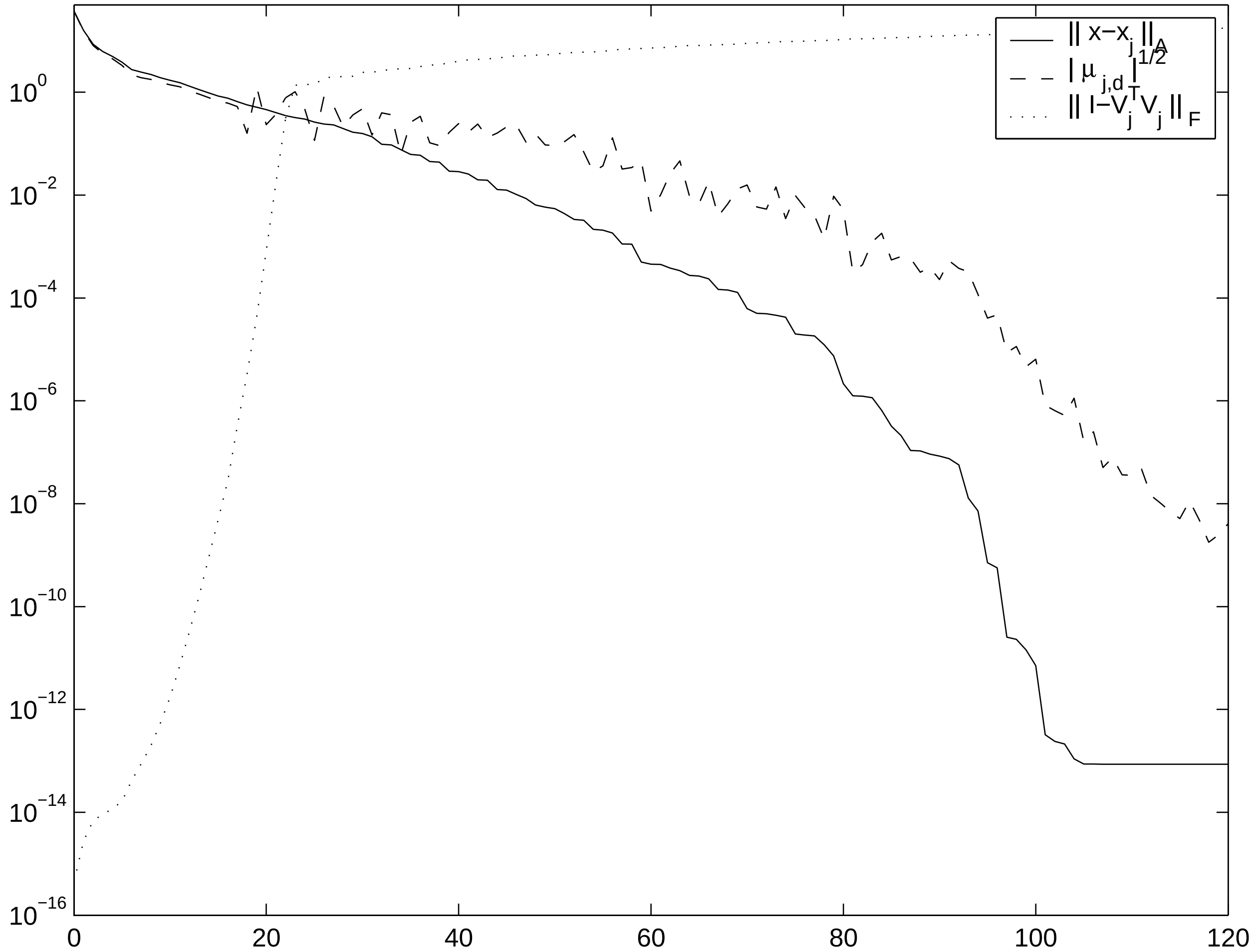
A principal, often overlooked, problem

Are estimates derived assuming exact arithmetic applicable in finite precision computations?



Estimates need not work

The identity $\|x - x_j\|_{\mathbf{A}}^2 = EST^2 + \|x - x_{j+d}\|_{\mathbf{A}}^2$ need not hold during the finite precision CG computations. An example: $\mu_{j,d} = r_0^T(x_{j+d} - x_j)$ does not work!



4. Rounding error analysis

Rounding error analysis

Without a proper rounding error analysis, there is no justification whatsoever that the proposed estimates work in finite precision arithmetic.

Do the estimates give good information in practical computations?

estimate	CG	PCG	
$\eta_{j,d}$ (continued fractions)	**yes***	**yes?**	[GoSt-94, GoMe-97, Me-99]
$\mu_{j,d}$ (Warnick)	**no**	**no**	[StTi-02]
$\nu_{j,d}$ (Hestenes and Stiefel)	**yes**	**yes**	[StTi-02, StTi-04]

*Based on [GrSt-92], [Gr-89], $\sqrt{\varepsilon}$ **limit.**

Hestenes and Stiefel estimate (CG)

[StTi-02]: Rounding error analysis based on

- detailed investigation of preserving local orthogonality in CG,
- results [Pa-71, Pa-76, Pa-80], [Gr-89, Gr-97].

Theorem:

Let $\varepsilon\,\kappa(\mathbf{A}) \ll 1$. Then the CG approximate solutions computed in finite precision arithmetic satisfy

$$\begin{aligned} \|x - x_j\|_{\mathbf{A}}^2 - \|x - x_{j+d}\|_{\mathbf{A}}^2 &= \nu_{j,d} + \|x - x_j\|_{\mathbf{A}}\, E_{j,d} + \mathcal{O}(\varepsilon^2), \\ |E_{j,d}| &\approx \left(\sqrt{\kappa(A)}\right)\, \varepsilon\, \|x - x_0\|_{\mathbf{A}}\,. \end{aligned}$$

Hestenes and Stiefel estimate (PCG)

[StTi-04]: Analysis based on:

- rounding error analysis from [StTi-02],
- solving of

$$\mathbf{M} s_{j+1} = r_{j+1}$$

enjoys perfect normwise backward stability [Hi-96, p. 206].

Similar result as for CG: Until $\|x - x_j\|_{\mathbf{A}}$ reaches a level close to $\varepsilon \, \|x - x_0\|_{\mathbf{A}}$, the estimate

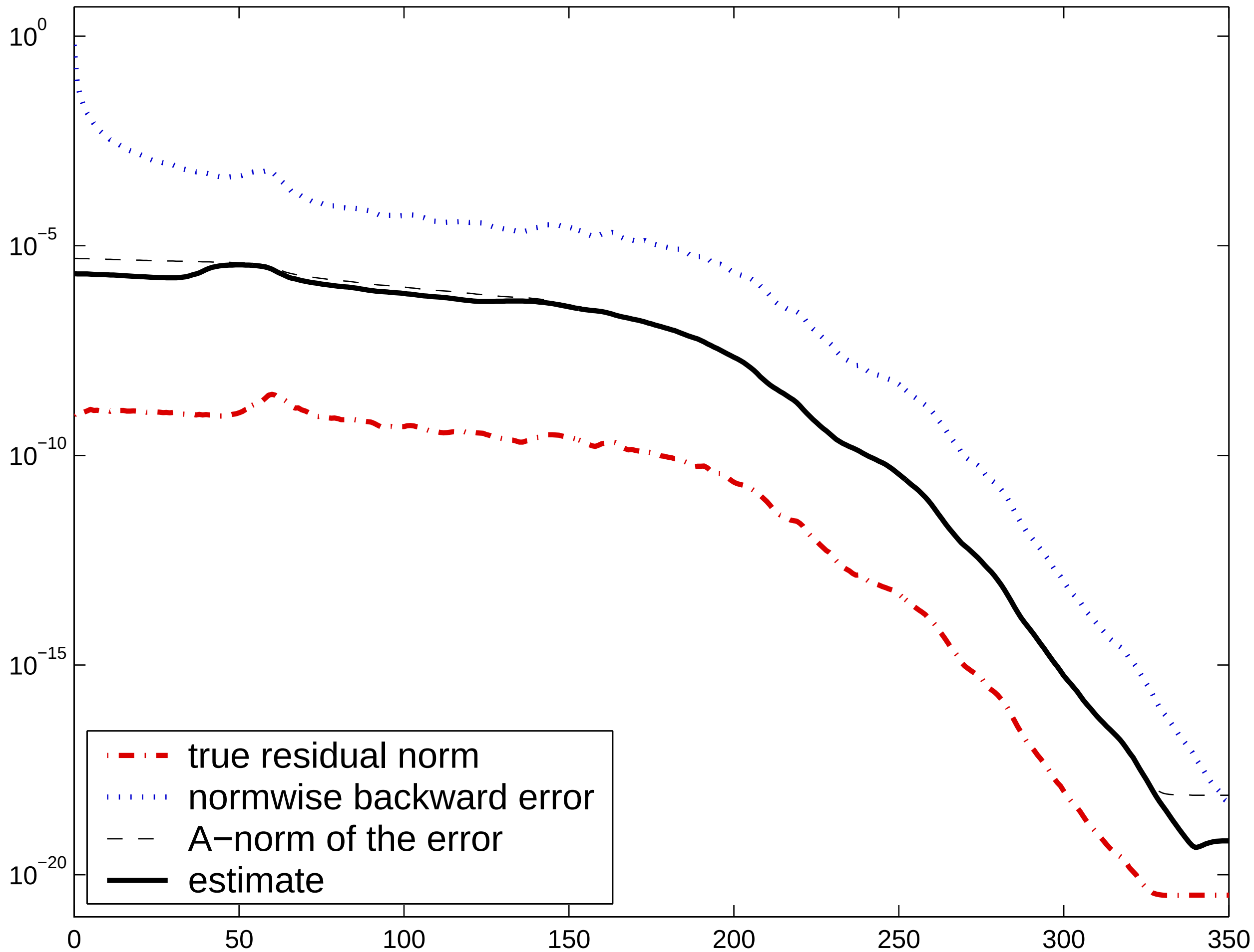
$$\nu_{j,d} = \sum_{i=j}^{j+d-1} \gamma_i (r_i, s_i)$$

must work.

5. Numerical Experiments

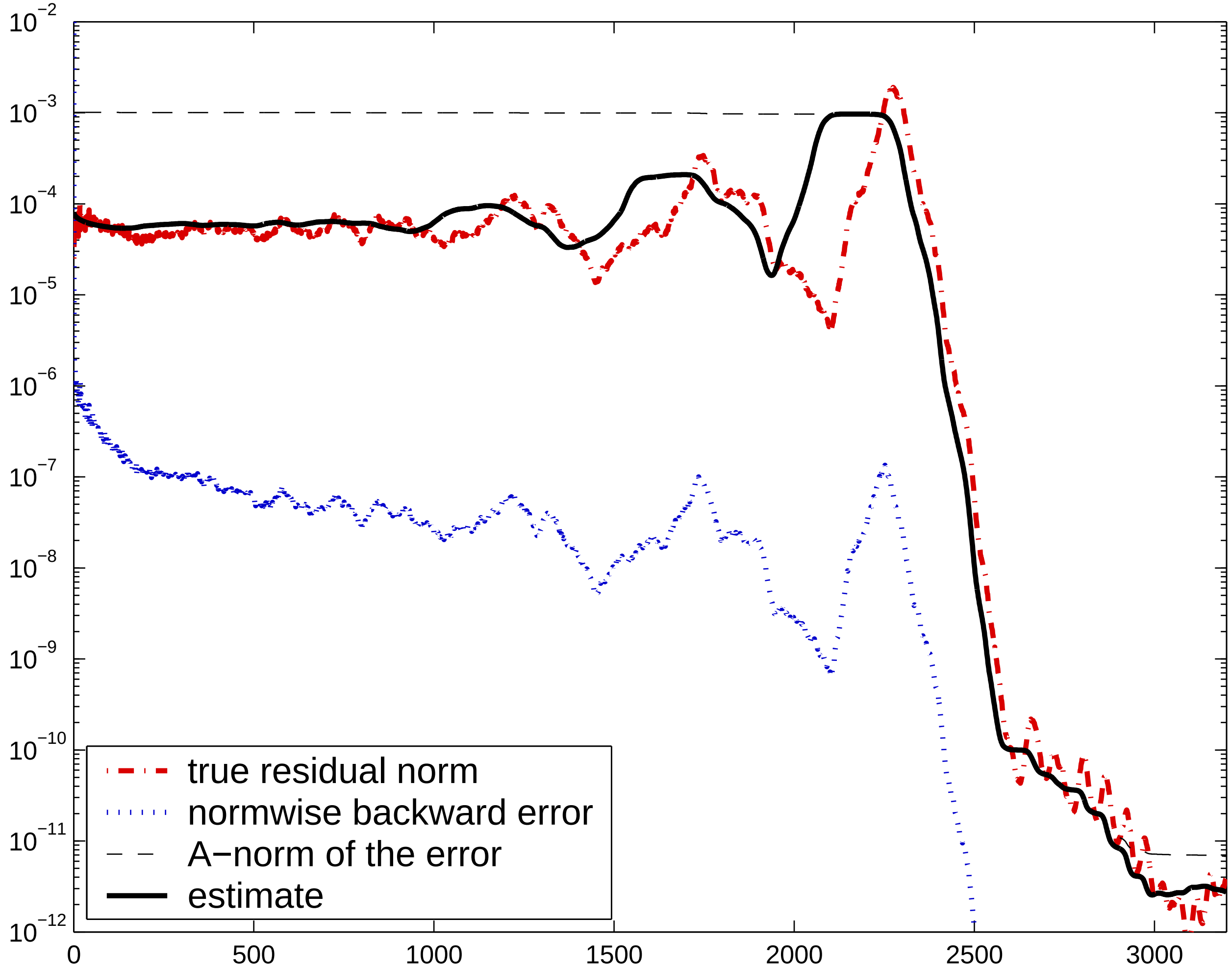
Estimating the $\mathbf{A}$-norm of the error

P. Benner: Large-Scale Control Problems, optimal cooling of steel profiles,
PCG, $\kappa(\mathbf{A}) = 9.7e+04\,,\ n = 5177\,,\ d = 4\,,\ \mathbf{L} = \text{cholinc}(\mathbf{A}, 0)\,.$



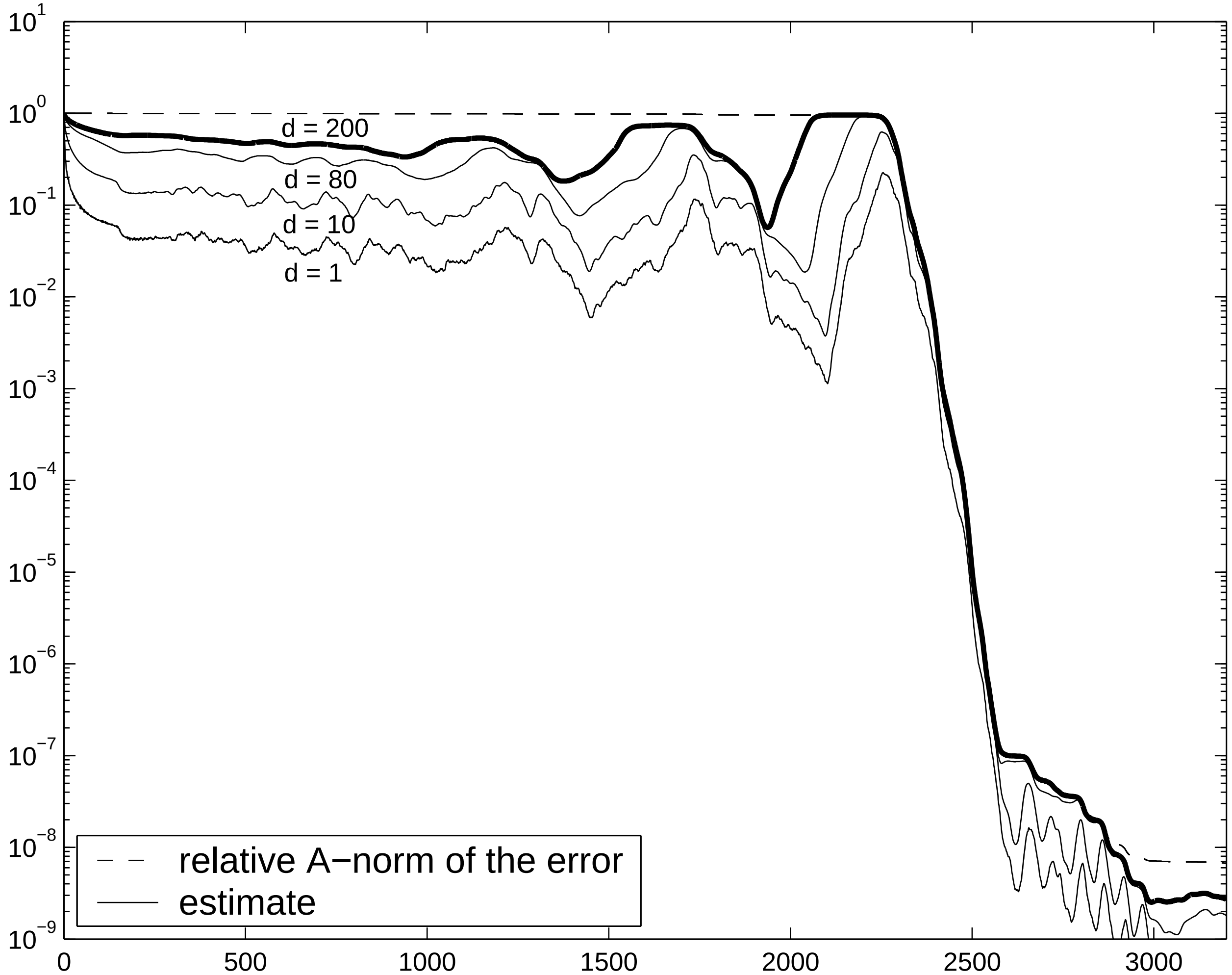
Estimating the $\mathbf{A}$-norm of the error

R. Kouhia: Cylindrical shell (Matrix Market), matrix s3dkt3m2,
PCG, $\kappa(\mathbf{A}) = 3.62e+11$, $n = 90499$, $d = 200$, $\mathbf{L} =$ cholinc($\mathbf{A}, 0$).



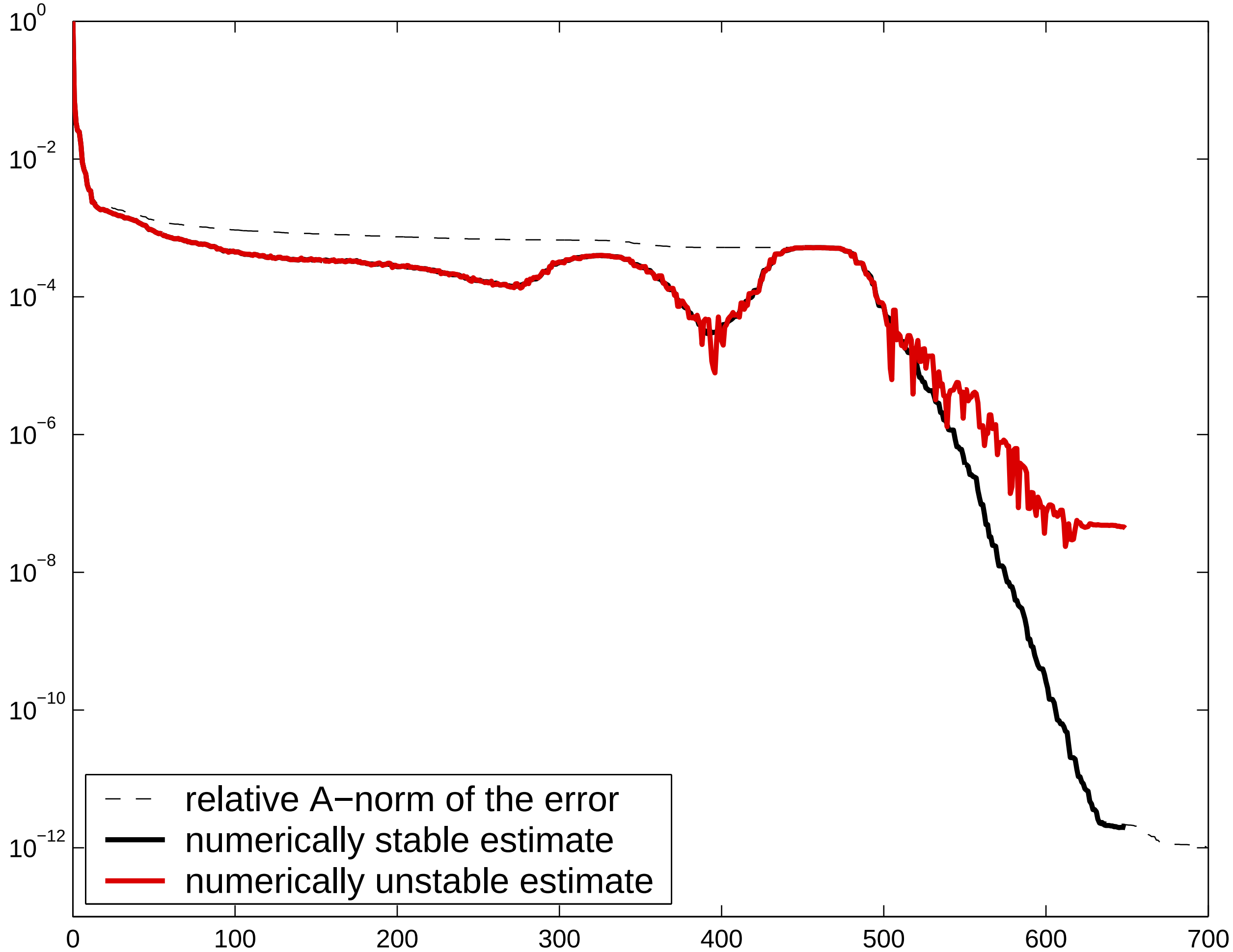
Estimating the relative $\mathbf{A}$-norm of the error

R. Kouhia: Cylindrical shell (Matrix Market), matrix s3dkt3m2,
PCG, $\kappa(\mathbf{A}) = 3.62e+11$, $n = 90499$, $d = 200$, $\mathbf{L} =$ cholinc$(\mathbf{A}, 0)$.



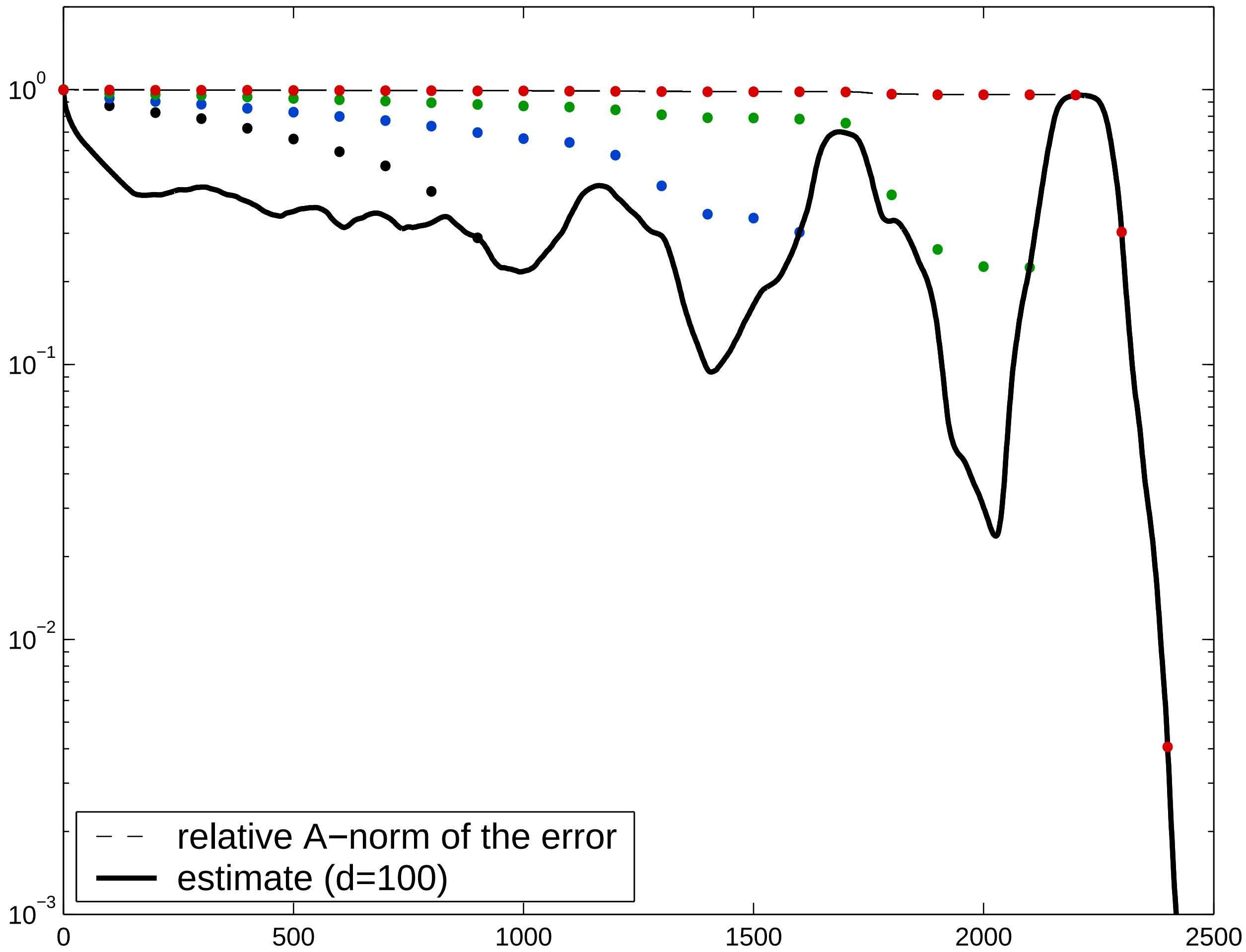
Estimating the relative $\mathbf{A}$-norm of the error

R. Kouhia: Cylindrical shell (Matrix Market), matrix s3rmt3m3,
PCG, $\kappa(\mathbf{A}) = 2.40e+10$, $n = 5357$, $d = 50$, $\mathbf{L} =$ cholinc($\mathbf{A}, 1e-5$).



Reconstruction of the convergence curve

R. Kouhia: Cylindrical shell (Matrix Market), matrix s3dkt3m2,
PCG, $\kappa(\mathbf{A}) = 3.62e+11$, $n = 90499$, $d = 100$, $\mathbf{L} =$ cholinc($\mathbf{A}, 0$) .



6. Conclusions

- Various formulas (based on Gauss quadrature) are mathematically equivalent to the formulas present (but somehow hidden) in the original Hestenes and Stiefel paper.

- Hestenes and Stiefel estimate is very simple, it can be computed almost for free and it has been proved numerically stable.

- We suggest to incorporate the estimates $\nu_{j,d}^{1/2}$ and $\varrho_{j,d}^{1/2}$ into any software realizations of the CG and PCG methods.

- The estimates are tight if the $\mathbf{A}$-norm of the error reasonably decreases.

Open problem: The adaptive choice of the parameter d.

More details can be found in

Strakoš, Z. and Tichý, P., On error estimation in the Conjugate Gradient method and why it works in finite precision computations, Electronic Trans. Numer. Anal. (ETNA), 13: pp. 56-80, (2002).

Strakoš, Z. and Tichý, P., Simple estimation of the $\mathbf{A}$-norm of the error in the Preconditioned Conjugate Gradients, BIT Numerical Mathematics, 45: pp. 789-817, (2005).

`http://www.cs.cas.cz/~strakos`,
`http://www.cs.cas.cz/~tichy`

Meurant, G. and Strakoš, Z., The Lanczos and conjugate gradient methods in finite precision arithmetic, Acta Numerica, 15 (to appear in 2006).

Thank you for your kind attention!