# How to control the accuracy of error estimates in CG?

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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** $A$, $b$

$r_0 = p_0 = b$

**for** $k = 0, \ldots$ until convergence **do**

$$\left.\begin{aligned} \alpha_k &= \tfrac{r_k^T r_k}{p_k^T A p_k} \\ x_{k+1} &= x_k + \alpha_k p_k \\ r_{k+1} &= r_k - \alpha_k A p_k \\ \beta_{k+1} &= \tfrac{r_{k+1}^T r_{k+1}}{r_k^T r_k} \\ p_{k+1} &= r_{k+1} + \beta_{k+1} p_k \end{aligned}\right\} \quad \texttt{cgiter(k)}$$

**end for**

$$\varepsilon_k \;\equiv\; \|x - x_k\|_A^2 = \min_{y \in \mathcal{K}_k} \|x - y\|_A^2$$

# How to measure quality of approximation?

. . . it depends on what problem we solve.

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

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

- **using error estimates,**
  – estimate of the $A$-norm of the error,
  – estimate of the Euclidean norm of the error.

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

# Estimating the $A$-norm of the error in CG

$$\varepsilon_k \equiv \|x - x_k\|_A^2$$

- **Estimating errors** using quadrature approach:

  [Dahlquist, Golub, Nash 1978], [Golub, Meurant 1994], [Golub, Strakoš 1994], [Golub, Meurant, 1997], [Calvetti et al. 2000], [Strakoš, T. 2002], [Meurant, T. 2013, 2019]

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

  [Golub, Strakoš 1994], [Strakoš, T. 2002, 2005, 2011]

- An important role in **stopping criteria**:

  [Deuflhard 1994], [Arioli 2004], [Jiránek, Strakoš, Vohralík 2006], [Papež, Vohralík 2022]

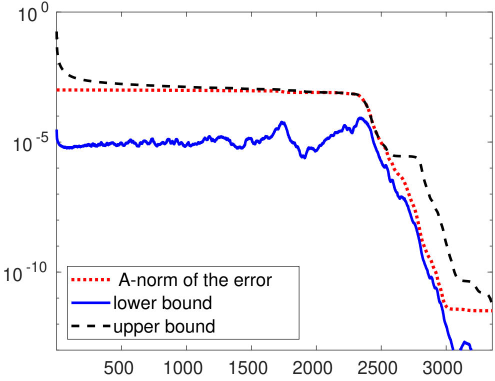
- How to **improve** and **control** the accuracy?

# Basic bounds

# Estimating $\|x - x_k\|_A^2$

Given $\mu \leq \lambda_{\min}$,

$$\alpha_k \|r_k\|^2 < \varepsilon_k < \alpha_k^{(\mu)} \|r_k\|^2$$



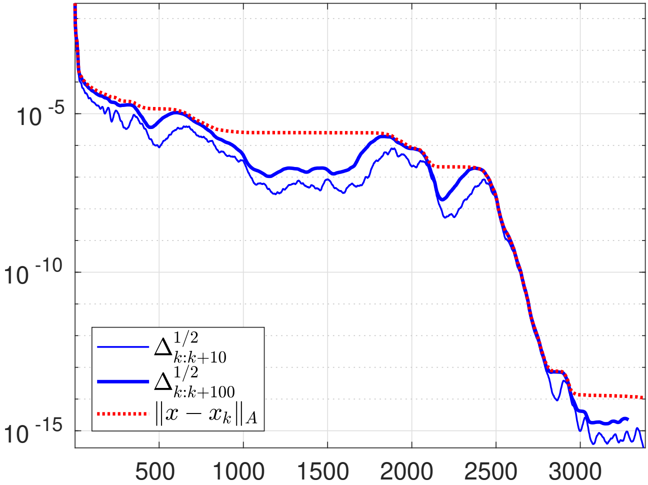
# How to improve the accuracy of the estimates?

$$\varepsilon_k \;=\; \underbrace{\sum_{j=k}^{\ell-1} \alpha_j \|r_j\|^2}_{\Delta_{k:\ell-1}} \;+\; \varepsilon_\ell$$

[Golub, Strakoš 1994, Golub, Meurant 1997, Strakoš, T. 2002, 2005]

## $\ell = k + d$ with a constant $d$

s3dkq4m2, $n = 90449$, `ichol`




A need to **determine $d$ adaptively**.

# Prescribing the accuracy of the estimate

$$\varepsilon_k \; = \; \Delta_{k:\ell-1} \; + \; \varepsilon_\ell$$

Ideally, we would like to determine $\ell > k$ such that

$$\frac{\varepsilon_k - \Delta_{k:\ell-1}}{\varepsilon_k} \; = \; \frac{\varepsilon_\ell}{\varepsilon_k} \; \leq \; \tau \, ,$$

where $\tau \in (0, 1)$ is a given tolerance. Then

$$\Delta_{k:\ell-1} \; < \; \varepsilon_k \; \leq \; \frac{\Delta_{k:\ell-1}}{1 - \tau} \, .$$

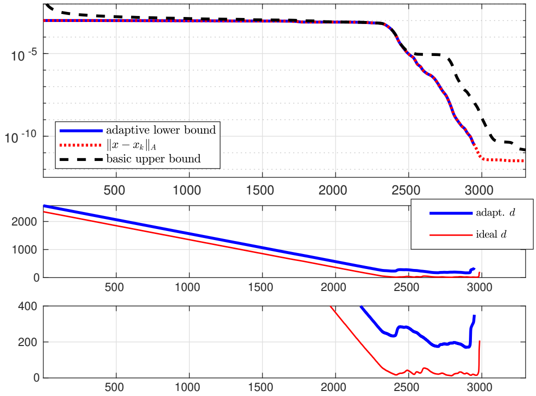
The delay $\ell - k$ should be as small as possible.

## Find $\ell$ such that

$$\frac{\varepsilon_k - \Delta_{k:\ell-1}}{\varepsilon_k} = \frac{\varepsilon_\ell}{\varepsilon_k} \leq \tau$$

# Using the upper bound

$$\frac{\varepsilon_\ell}{\varepsilon_k} \leq \frac{\alpha_\ell^{(\mu)} \|r_\ell\|^2}{\Delta_{k:\ell-1}} \leq \tau$$




Safe, but requires $\mu$ and, moreover, $\ell - k$ is far from being optimal!

# Heuristic strategy

## Learn from the history

It holds that [Meurant, Papež, T. 2021]

$$\Delta_j < \varepsilon_j < \kappa(A)\,\Delta_j\,.$$

Idea $\rightarrow$ find $S_\ell$ such that

$$\varepsilon_\ell \approx S_\ell\,\Delta_\ell.$$

Define

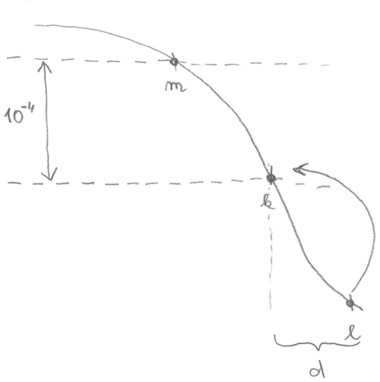
$$S_\ell \equiv \max_{m \leq j < \ell} \widetilde{S}_j, \quad \widetilde{S}_j \equiv \frac{\Delta_{j:\ell}}{\Delta_j} \approx \frac{\varepsilon_j}{\Delta_j}\,.$$

Approximate

$$\frac{\varepsilon_\ell}{\varepsilon_k} \approx \frac{S_\ell \Delta_\ell}{\Delta_{k:\ell-1}} \leq \tau\,.$$

# How far to go into history?

## Learn from the latest significant decrease




$$\varepsilon_k = \Delta_{k:\ell-1} + \varepsilon_\ell$$

- find $m$ such that

$$\frac{\varepsilon_k}{\varepsilon_m} \approx \frac{\Delta_{k:\ell}}{\Delta_{m:\ell}} \leq 10^{-4}$$

- define

$$S_\ell = \max_{m \leq j < \ell} \widetilde{S}_j$$

- test

$$\frac{S_\ell \Delta_\ell}{\Delta_{k:\ell-1}} \leq \tau$$

# Estimating $\varepsilon_k$ with a prescribed accuracy

[Meurant, Papež, T. 2021]

```
input A, b, τ
r_0 = p_0 = b, k = 0
cgiter(0)
for ℓ = 1, ..., do
    cgiter(ℓ)
    compute Δ_{k:ℓ-1} and Δ_ℓ
    determine S_ℓ
    while ℓ > k and (S_ℓ Δ_ℓ)/(Δ_{k:ℓ-1}) ≤ τ do
        accept Δ_{k:ℓ}
        k = k + 1
    end while
end for
```

Preconditioned CG $\rightarrow$ $\varepsilon_k = \sum_{j=k}^{\ell-1} \hat{\alpha}_j \, z_j^T r_j + \varepsilon_\ell$

```
function [x,estim,delay] = pcga(A,b,tau,maxit,L,x)
r = b - A * x;
z = L\r; z = L'\z; p = z;
rr = z' * r;
k = 1;

for ell = 1:maxit+1

    RR    = rr;                          % ... begin cgiter(ell)
    Ap    = A * p;
    alpha = RR/(p' * Ap);
    x     = x + alpha * p;
    r     = r - alpha * Ap;
    z     = L \ r; z = L' \ z;
    rr    = z' * r;
    beta  = rr / RR;
    p     = z + beta * p;                % ... end cgiter(ell)

    Delta(ell) = alpha * RR;
    history(ell) = 0; history = history + Delta(ell);

    if ell > 1                           % ... adaptive choice of the delay
        S = findS(history,Delta,k);
        num = S * Delta(ell);
        den = sum(Delta(k:ell-1));
        while (ell > k) && (num/den <= tau)
            delay(k) = ell-k;
            estim(k) = den;
            k = k + 1;
            den = sum(Delta(k:ell-1));
        end
    end
end
end % of function

function [S] = findS(history,Delta,k)
ind = find((history(k)./history) <= 1e-4, 1, 'last');
if isempty(ind), ind = 1; end
S = max(history(ind:end-1)./Delta(ind:end-1));
end
```

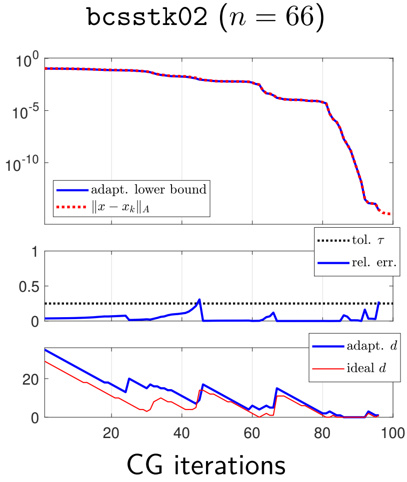
# Numerical experiments

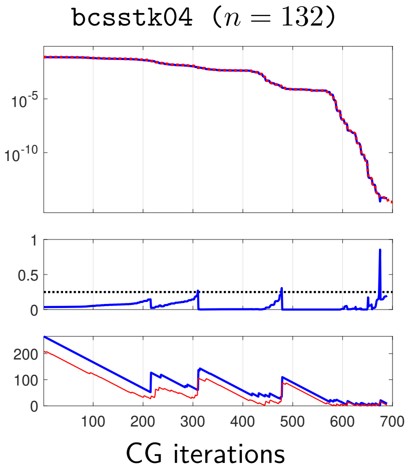
# Test problems

## SuiteSparse Matrix collection

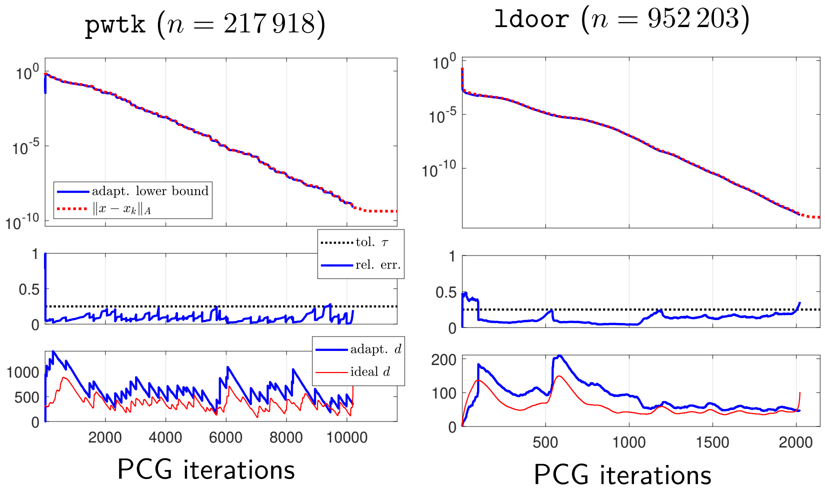
| name | size | rhs $b$ | $M = LL^T$ |
|---|---|---|---|
| bcsstk02 | 66 | equal components | — |
| bcsstk04 | 132 | equal components | — |
| bcsstk09 | 1083 | equal components | ict(1e-3, 1e-2) |
| s3dkt3m2 | 90 449 | comes with the matrix | ict(1e-5, 1e-2) |
| s3dkq4m2 | 90 449 | $\text{rand}(-1, 1)$ | ict(1e-5, 1e-2) |
| pwtk | 217 918 | $\text{rand}(-1, 1)$ | ict(1e-5, 1e-1) |
| af_shell3 | 504 855 | $\text{rand}(-1, 1)$ | zero-fill |
| tmt_sym | 726 713 | $\text{rand}(-1, 1)$ | zero-fill |
| ldoor | 952 203 | $\text{rand}(-1, 1)$ | zero-fill |

# Problems without preconditioning



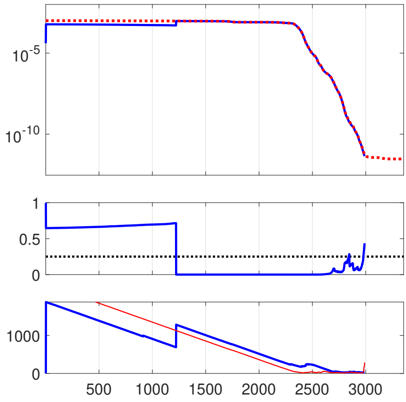



# Problems with preconditioning



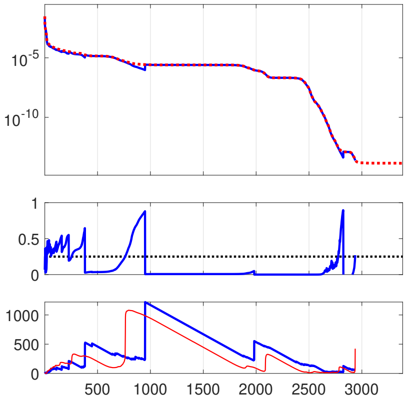
# Difficult problems

s3dkt3m2 ($n = 90\,449$)




PCG iterations

s3dkq4m2 ($n = 90\,449$)




PCG iterations

# Conclusions

- One can **improve** the accuracy of estimates of $\varepsilon_k$ using the information from the forthcoming CG iterations.
- We can **control** the accuracy of the estimates using:
  - Gauss-Radau **upper bound** $\rightarrow$ safe, far from being optimal.
  - A **heuristic strategy** $\rightarrow$ robust, reliable, often almost optimal.
- Generalization is possible for other CG-like methods.

# Related papers

G. Meurant, J. Papež, and P. Tichý,

[Accurate error estimation in CG, Numer. Algorithms, 88 (2021), pp. 1337-1359.]

- G. H. Golub and Z. Strakoš, [Estimates in quadratic formulas, Numer. Algorithms, 8 (1994), pp. 241–268.]
- G. Meurant and P. Tichý, [Approximating the extreme Ritz values and upper bounds in CG, Numer. Algorithms, 82 (2019), pp. 937-968]
- 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!**

# Delay of the Gauss-Radau upper bound?

Work in progress ...