A review of quadrature-based error bounds in the conjugate gradient algorithm

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Paris, May 2024

Joint work with Petr Tichý and Jan Papež

Lanczos algorithm

A symmetric of order n

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input A, v
β_0 = 0, v_0 = 0
v_1 = v/‖v‖
for k = 1, ... do
    w = A v_k − β_{k−1} v_{k−1}
    α_k = v_k^T w
    w = w − α_k v_k
    β_k = ‖w‖
    v_{k+1} = w/β_k
end for
```

It generates tridiagonal matrices T_k, $k = 1, \ldots, n$ with coefficients $(\beta_{i-1}, \alpha_i, \beta_i)$

CG algorithm

Solve $Ax = b$ with A symmetric positive definite

input A, b, x_0

$r_0 = b - Ax_0$

$p_0 = r_0$

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

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

end for

$$\varepsilon_k = \|x - x_k\|_A^2 = r_k^T A^{-1} r_k = \min_{y \in x_0 + \mathcal{K}_k(A, r_0)} \|x - y\|_A^2$$

Relations between CG and Lanczos

$$T_k = L_k D_k L_k^T$$

with

$$L_k \equiv \begin{pmatrix} 1 & & & \\ \sqrt{\delta_1} & \ddots & & \\ & \ddots & \ddots & \\ & & \sqrt{\delta_{k-1}} & 1 \end{pmatrix}, \qquad D_k \equiv \begin{pmatrix} \gamma_0^{-1} & & & \\ & \ddots & & \\ & & \ddots & \\ & & & \gamma_{k-1}^{-1} \end{pmatrix}$$

$$\beta_k = \frac{\sqrt{\delta_k}}{\gamma_{k-1}}, \quad \alpha_k = \frac{1}{\gamma_{k-1}} + \frac{\delta_{k-1}}{\gamma_{k-2}}, \quad \delta_0 = 0, \quad \gamma_{-1} = 1$$

$$v_{j+1} = (-1)^j \frac{r_j}{\|r_j\|}, \qquad j = 0, \dots, k$$

Quality of the approximation?

- 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
  - bounds on the A-norm of the error
  - bounds on the ℓ_2 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."

Let

$$A = U \Lambda U^T, \qquad U U^T = U^T U = I$$

with $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$, w be a given unit norm vector,

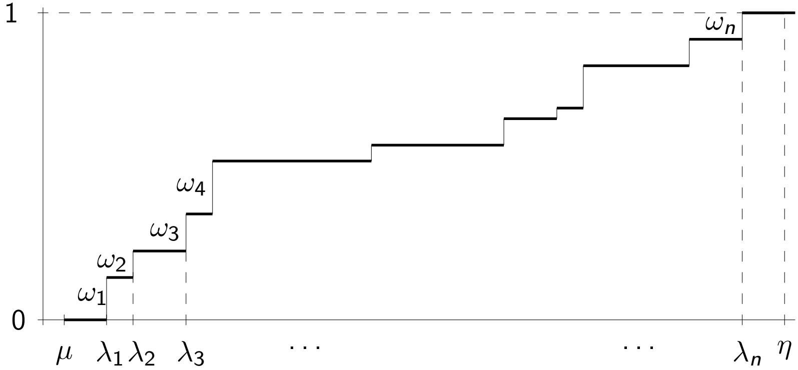
$$\omega_i \equiv (w, u_i)^2 \qquad \text{so that} \qquad \sum_{i=1}^{n} \omega_i = 1$$

and the stepwise constant distribution function

$$\omega(\lambda) \equiv \begin{cases} 0 & \text{for} \quad \lambda < \lambda_1 \,, \\ \sum_{j=1}^{i} \omega_j & \text{for} \quad \lambda_i \le \lambda < \lambda_{i+1} \,, \quad 1 \le i \le n-1 \,, \\ 1 & \text{for} \quad \lambda_n \le \lambda \end{cases}$$

$$\int_{\mu}^{\eta} f(\lambda) \, d\omega(\lambda) = \sum_{i=1}^{n} \omega_i f(\lambda_i) \; = \; w^T f(A) w$$

Choosing $w = r_k / \|r_k\|$ and $f(\lambda) = 1/\lambda$, it is clear that $r_k^T A^{-1} r_k$ can be written as a Riemann-Stieltjes integral


1
0
ω_1
ω_2
ω_3
ω_4
ω_n
μ
λ_1
λ_2
λ_3
$\cdots$
$\cdots$
λ_n
η

For CG we used the relation

$$\varepsilon_k = \|r_0\|^2 \left[(T_n^{-1} e_1, e_1) - (T_k^{-1} e_1, e_1) \right]$$

It was shown by Z. Strakoš and P. Tichý that this relation holds in finite precision arithmetic up to a small perturbation term

It can also be written as

$$\varepsilon_0 = \sum_{j=0}^{k-1} \gamma_j \|r_j\|^2 + \varepsilon_k$$

or

$$\left(T_n^{-1}\right)_{1,1} = \left(T_k^{-1}\right)_{1,1} + \mathcal{R}_k^{(G)}[\lambda^{-1}]$$

$$\left(T_n^{-1}\right)_{1,1} = \frac{\varepsilon_0}{\|r_0\|^2} = \int_{\mu}^{\eta} \lambda^{-1} \, d\omega(\lambda)$$

$\left(T_k^{-1}\right)_{1,1}$ is the Gauss quadrature approximation of the integral and the remainder is

$$\mathcal{R}_k^{(G)}\left[\lambda^{-1}\right] = \frac{\varepsilon_k}{\|r_0\|^2}$$

The nodes of the Gauss quadrature rule are the eigenvalues of T_k

Since we don't know ε_0, we use

$$\varepsilon_{k-d} - \varepsilon_k = \sum_{j=k-d}^{k-1} \gamma_j \|r_j\|^2$$

where the delay d is a positive integer smaller than k

The right-hand side is a lower bound of the A-norm squared at iteration $\ell = k - d$

The simplest lower bound at iteration $k-1$ is $\gamma_{k-1}\|r_{k-1}\|^2$

To obtain an upper bound of the A-norm we use a Gauss-Radau quadrature rule with a fixed node $\mu \le \lambda_1$

$$\varepsilon_0 = \|r_0\|^2 (\widehat{T}_{k+1}^{-1})_{1,1} + \widehat{\mathcal{R}}_{k+1}[\lambda^{-1}]$$

Subtracting

$$\varepsilon_0 = \|r_0\|^2 (T_{k-d}^{-1})_{1,1} + \varepsilon_{k-d}$$

we obtain

$$\varepsilon_{k-d} = \|r_0\|^2 [\,(\widehat{T}_{k+1}^{-1})_{1,1} - (T_{k-d}^{-1})_{1,1}\,] + \widehat{\mathcal{R}}_{k+1}[\lambda^{-1}]$$

The difference in the right-hand side can be written as

$$(\widehat{T}_{k+1}^{-1})_{1,1} - (T_{k-d}^{-1})_{1,1} = (\widehat{T}_{k+1}^{-1})_{1,1} - (T_{k}^{-1})_{1,1} + \Delta_{\ell:k-1}$$

with the Gauss lower bound

$$\Delta_{\ell:k-1} = \sum_{j=\ell}^{k-1} \gamma_j \|r_j\|^2$$

with $\ell = k - d$

The matrix $\widehat{T}_{k+1}$ is equal to T_{k+1}, except that α_{k+1} is replaced with $\alpha_{k+1}^{(\mu)}$ computed such that $\widehat{T}_{k+1}$ has μ as an eigenvalue (that is, it is a prescribed node the the quadrature rule)

Then, we can use the Sherman-Morrison for the difference $(\widehat{T}_{k+1}^{-1})_{1,1} - (T_k^{-1})_{1,1}$
This gives the CGQL algorithm in G.H. Golub and G. M., 1997

CG coeffs $\rightarrow$ Lanczos coeffs $\rightarrow$ Gauss-Radau upper bound

Can we compute the upper bound directly from the CG coefficients?

We look for a coefficient $\gamma_k^{(\mu)}$ such that

$$T_{k+1}^{(\mu)} = L_{k+1} \begin{pmatrix} D_k & \\ & \left(\gamma_k^{(\mu)}\right)^{-1} \end{pmatrix} L_{k+1}^T$$

such that μ is an eigenvalue

This problem was solved in

G. M. and P. Tichý, On computing quadrature-based bounds for the A-norm of the error in conjugate gradients, Numer. Algorithms, 62(2), pp. 163-191, 2013

$$\gamma_{j+1}^{(\mu)} = \frac{\gamma_j^{(\mu)} - \gamma_j}{\mu(\gamma_j^{(\mu)} - \gamma_j) + \delta_{j+1}}, \qquad \gamma_0^{(\mu)} = \frac{1}{\mu}$$

This leads to the CGQ algorithm

CGQ algorithm

input A, b, x_0, μ, d

$r_0 = b - Ax_0, \quad p_0 = r_0$

$\gamma_0^{(\mu)} = 1/\mu, \quad \Delta_0^{(\mu)} = \gamma_0^{(\mu)} \|r_0\|^2$

$\varphi_0^{(\mu)} = \sqrt{\Delta_0^{(\mu)}}$

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

  `cgiter`(k)

  $\Delta_{k-1} = \gamma_{k-1} \|r_{k-1}\|^2$

  $\gamma_k^{(\mu)} = \frac{\gamma_{k-1}^{(\mu)} - \gamma_{k-1}}{\mu(\gamma_{k-1}^{(\mu)} - \gamma_{k-1}) + \delta_k}, \quad \Delta_k^{(\mu)} = \gamma_k^{(\mu)} \|r_k\|^2$

  $\ell = k - d$

  $\varphi_{k-1} = \sqrt{\Delta_{k-1}}, \quad \varphi_{\ell:k-1} = \sqrt{\Delta_{\ell:k-1}}$

  $\varphi_k^{(\mu)} = \sqrt{\Delta_k^{(\mu)}}, \quad \varphi_{\ell:k}^{(\mu)} = \sqrt{\Delta_{\ell:k-1} + \Delta_k^{(\mu)}},$

end for

Choice of the delay

How to choose d (or ℓ)?

A heuristic algorithm for choosing the delay for the Gauss lower bound is described in

G. M., J. Papež, and P. Tichý, Accurate error estimation in CG, Numer. Algorithms, 88(3), pp. 1337-1359, 2021

to obtain

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

with

$$\Delta_{\ell:k-1} = \sum_{j=\ell}^{k-1} \gamma_j \|r_j\|^2$$

Choice of the delay for Gauss-Radau

$$\Delta_{\ell:k}^{(\mu)} \equiv \Delta_{\ell:k-1} + \Delta_k^{(\mu)}.$$

As for the Gauss lower bound, we would like to find an index $\ell < k$ such that the relative error of the Gauss-Radau upper is small enough,

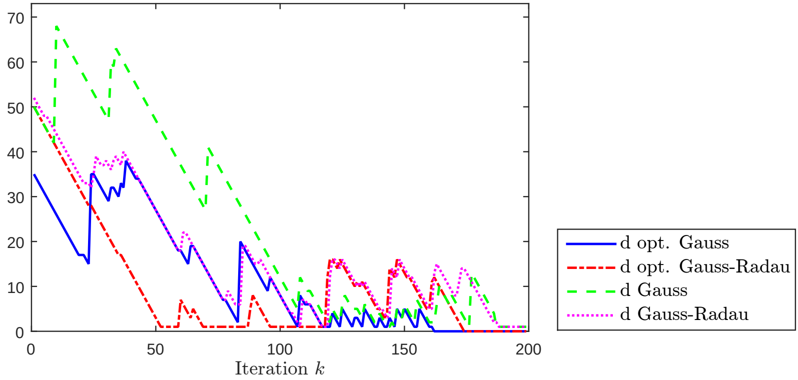
$$\frac{\Delta_{\ell:k}^{(\mu)} - \varepsilon_\ell}{\varepsilon_\ell} \leq \tau$$

Since

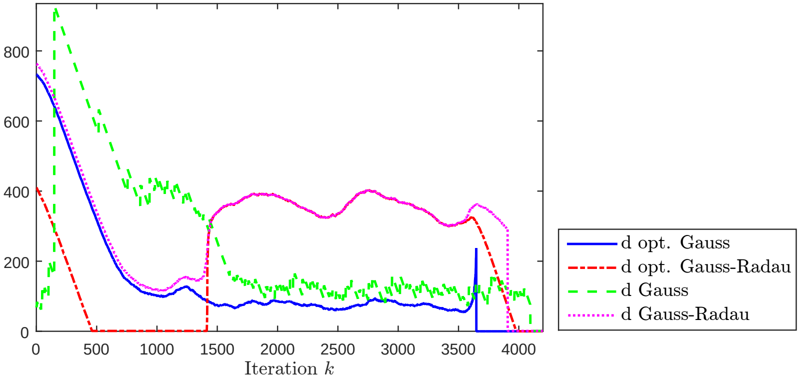
$$\frac{\Delta_{\ell:k}^{(\mu)} - \varepsilon_\ell}{\varepsilon_\ell} < \frac{\Delta_{\ell:k}^{(\mu)} - \Delta_{\ell:k-1}}{\Delta_{\ell:k-1}} = \frac{\Delta_k^{(\mu)}}{\Delta_{\ell:k-1}},$$

we can require ℓ, satisfying $\ell < k$, to be the largest integer such that

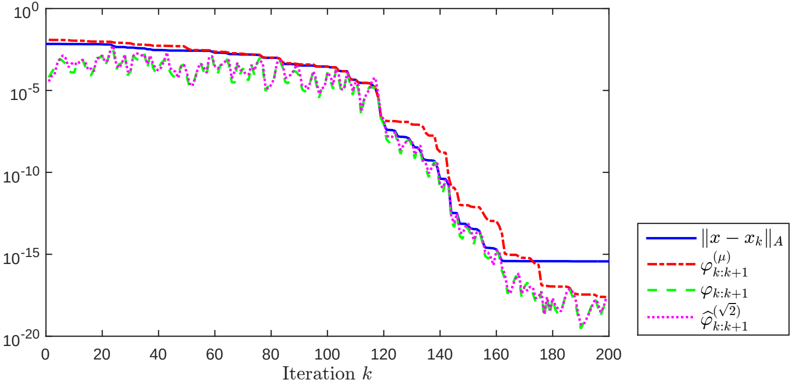
$$\frac{\Delta_k^{(\mu)}}{\Delta_{\ell:k-1}} \leq \tau$$



bcsstk01, optimal and computed delays for Gauss and Gauss-Radau, $\tau = 0.25$

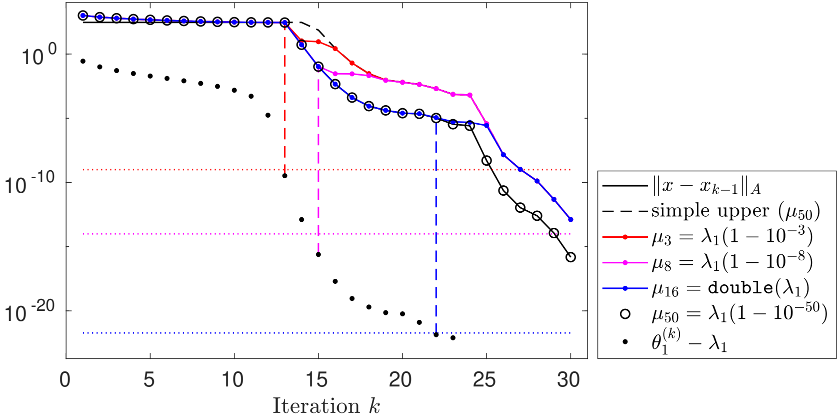


1138_bus, optimal and computed delays for Gauss and Gauss-Radau, $\tau = 0.25$



bcsstk01, A-norm of the error and bounds or estimates, $d = 1$

Problem with the Gauss-Radau upper bound



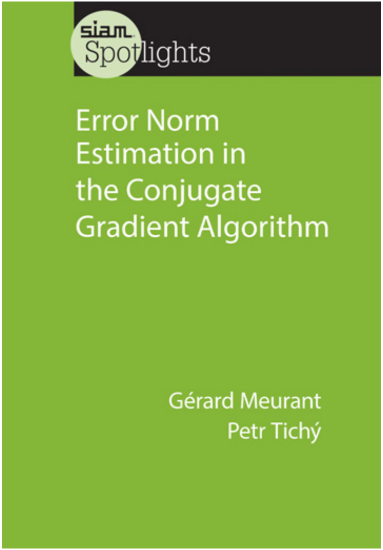
`Model problem`, A-norm of the error and Gauss-Radau upper bounds

The problem starts when $\theta_1^{(k)} - \lambda_1 \approx \lambda_1 - \mu$

A theoretical explanation for that phenomenon is given in G. M. and P. Tichý, The behaviour of the Gauss-Radau upper bound of the error norm in CG, Numer. Algorithms, 94(2), pp. 847-876, 2023

One remedy is to increase the delay for Gauss-Radau

For details


siam Spotlights
Error Norm Estimation in the Conjugate Gradient Algorithm
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