A review of quadrature-based bounds of the error norms in CG

Gérard MEURANT

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To set the notation, A symmetric of order n

Lanczos algorithm

input A, v
$\beta_0 = 0, \; v_0 = 0$
$v_1 = v/\|v\|$
for $k = 1, \ldots$ **do**
  $w = Av_k - \beta_{k-1} v_{k-1}$
  $\alpha_k = v_k^T w$
  $w = w - \alpha_k v_k$
  $\beta_k = \|w\|$
  $v_{k+1} = w/\beta_k$
end for

It generates tridiagonal matrices T_k, $k = 1, \ldots, n$ with coefficients α_i, β_i

A symmetric positive definite, $Ax = b$

CG algorithm

input A, b, x_0

$r_0 = b - Ax_0$

$p_0 = r_0$

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

$\gamma_{k-1} = \frac{r_{k-1}^T r_{k-1}}{p_{k-1}^T A p_{k-1}}$

$x_k = x_{k-1} + \gamma_{k-1} p_{k-1}$

$r_k = r_{k-1} - \gamma_{k-1} A p_{k-1}$

$\delta_k = \frac{r_k^T r_k}{r_{k-1}^T r_{k-1}}$

$p_k = r_k + \delta_k p_{k-1}$

end for

Relations between CG and Lanczos

$$T_k = L_k D_k L_k^T$$

with

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

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

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

M.R. Hestenes and E. Stiefel, *Methods of conjugate gradients for solving linear systems*, J. Nat. Bur. Standards, v 49 n 6 (1952), pp. 409–436

Hestenes and Stiefel "error function" was the A-norm of the error

$$\|\varepsilon_k\|_A \equiv (\varepsilon_k^T A \varepsilon_k)^{1/2}$$

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

Note that

$$\|\varepsilon_k\|_A^2 = r_k^T A^{-1} r_k, \quad \|\varepsilon_k\|^2 = r_k^T A^{-2} r_k$$

H-S also noticed the connection of CG with orthogonal polynomials and Riemann-Stieltjes integrals

Let

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

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

This result was used by Gene Golub and his collaborators to compute approximations of quadratic forms $u^T f(A) v$ with several different applications by using Gauss quadrature rules

G. Dahlquist, S.C. Eisenstat, and G.H. Golub, Bounds for the error of linear systems of equations using the theory of moments, J. Math. Anal. Appl., 37, pp. 151-166, 1972

G. Dahlquist, G.H. Golub, and S.G. Nash Bounds for the error in linear systems, in R. Hettich, ed., Proceedings of the workshop on semi-infinite programming, pp. 154-172, Berlin, 1978 Springer

B. Fischer and G.H. Golub, On the error computation for polynomial based iteration methods, in A. Greenbaum and M. Luskin, eds., Recent advances in iterative methods, pp. 59-67, 1994, Springer

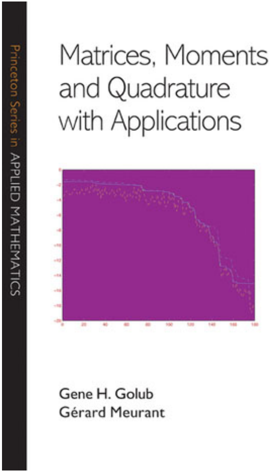
G.H. Golub and Z. Strakoš, Estimates in quadratic formulas, Numer. Algorithms, 8(2), pp. 241-268, 1994

G.H. Golub and G. Meurant, Matrices, moments and quadrature, in D.F. Griffiths and G.A. Watson, eds., Numerical Analysis 1993, volume 303 of Pitman Research Notes in Mathematics, pp. 105-156, Longman Sci. Tech., 1994

G.H. Golub and G. Meurant, Matrices, moments and quadrature II or how to compute the norm of the error in iterative methods, BIT, 37(3), pp. 687-705, 1997

G. Meurant, The computation of bounds for the norm of the error in the conjugate gradient algorithm, Numer. Algorithms, 16, pp. 77-87, 1997

The computation of $u^T f(A) v$ and applications are summarized in the book published by Princeton University Press in 2010



For CG we used the relation

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

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

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

or

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

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

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

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

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

Since we don't know $\|\varepsilon_0\|_A^2$, we use

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

where d is a positive integer smaller than k

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

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

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

Subtracting

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

we obtain

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

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

$$(\widehat{T}_{k+1}^{-1})_{1,1} - (T_{k-d}^{-1})_{1,1} = (\widehat{T}_{k+1}^{-1})_{1,1} - (T_k^{-1})_{1,1} + Q_{k-d,d}$$

with the Gauss lower bound

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

We have to find $\alpha_{k+1}^{(\mu)}$ such that μ is an eigenvalue of the extended tridiagonal matrix

$$\widehat{T}_{k+1}^{(\mu)} = \begin{pmatrix} \alpha_1 & \beta_1 & & & \\ \beta_1 & \ddots & \ddots & & \\ & \ddots & \ddots & \beta_{k-1} & \\ & & \beta_{k-1} & \alpha_k & \beta_k \\ & & & \beta_k & \alpha_{k+1}^{(\mu)} \end{pmatrix}$$

where the α_j's and β_j's are the Lanczos coefficients
It is known that

$$\alpha_{k+1}^{(\mu)} = \mu + \xi_k^{(\mu)}$$

where $\xi_k^{(\mu)}$ is the last component of the solution of

$$(T_k - \mu I)\xi^{(\mu)} = \beta_k^2 e_k$$

This is computed with the LDL^T factorization of $T_k - \mu I$

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. Meurant, 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. Meurant 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

It was also proved that

$$\gamma_k \|r_k\|^2 < \|\varepsilon_k\|_A^2 < \gamma_k^{(\mu)} \|r_k\|^2 < \left(\frac{\phi_k}{\mu}\right) \|r_k\|^2$$

with $\phi_k = \|r_k\|^2 / \|p_k\|^2$ and

$$\phi_k = \frac{\phi_{k-1}}{\phi_{k-1} + \delta_k}, \qquad \phi_0 = 1$$

CGQ

input $A,\ b,\ x_0,\ \mu,\ \eta,\ d$

$r_0 = b - Ax_0,\ p_0 = r_0,\ g_0^{(\mu)} = \frac{\|r_0\|^2}{\mu},\ g_0^{(\eta)} = \frac{\|r_0\|^2}{\eta}$

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

$$\gamma_{k-1} = \frac{r_{k-1}^T r_{k-1}}{p_{k-1}^T A p_{k-1}}$$

$$x_k = x_{k-1} + \gamma_{k-1} p_{k-1},\ r_k = r_{k-1} - \gamma_{k-1} A p_{k-1}$$

$$\delta_k = \frac{r_k^T r_k}{r_{k-1}^T r_{k-1}}$$

$$p_k = r_k + \delta_k p_{k-1}$$

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

$$\Delta_{k-1}^{(\mu)} = g_{k-1}^{(\mu)} - g_{k-1}\,, \qquad g_k^{(\mu)} = \frac{\|r_k\|^2 \Delta_{k-1}^{(\mu)}}{\mu \Delta_{k-1}^{(\mu)} + \|r_k\|^2}$$

$$\Delta_{k-1}^{(\eta)} = g_{k-1}^{(\eta)} - g_{k-1}\,, \qquad g_k^{(\eta)} = \frac{\|r_k\|^2 \Delta_{k-1}^{(\eta)}}{\eta \Delta_{k-1}^{(\eta)} + \|r_k\|^2}$$

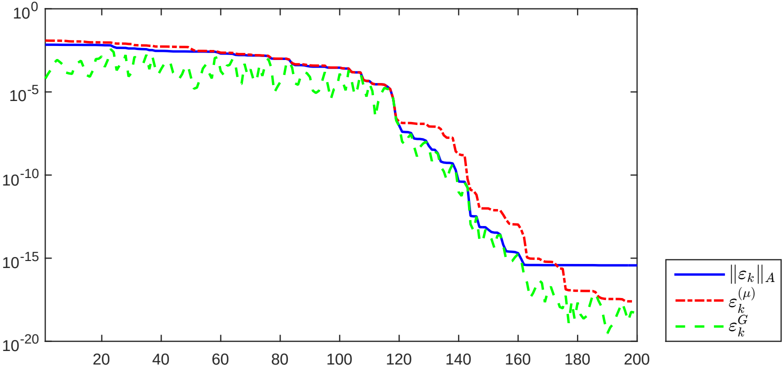
$$Q_{k-d,d} = \sum_{j=k-d}^{k-1} g_j, \quad \varepsilon_{k-d}^{G} = \sqrt{Q_{k-d,d}}$$

$$\varepsilon_{k-d}^{(\mu)} = \sqrt{Q_{k-d,d} + g_k^{(\mu)}}, \quad \varepsilon_{k-d}^{(\eta)} = \sqrt{Q_{k-d,d} + g_k^{(\eta)}}$$

end for

bcsstk01

$\mu = (1 - 10^{-8})\lambda_1 = 3417.267528494$, whence
$\lambda_1 = 3417.267562666$, $d = 1$



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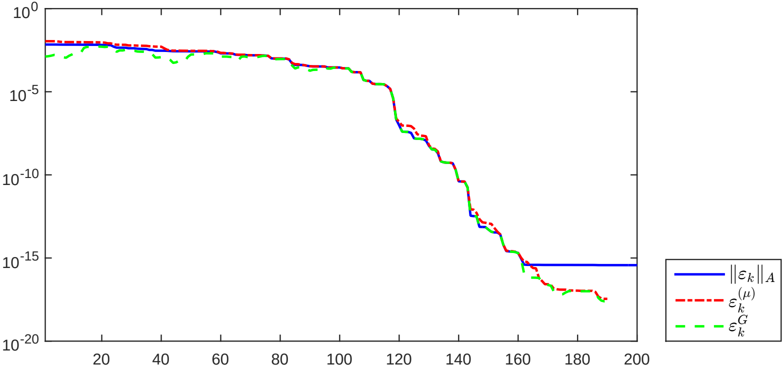
Same μ, $d = 10$



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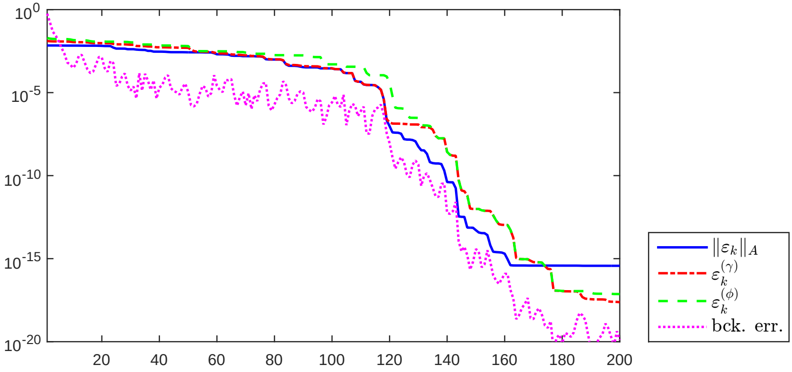
Same μ, other bounds



How to choose d?

An algorithm for choosing the delay for the Gauss lower bound is described in

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

to obtain

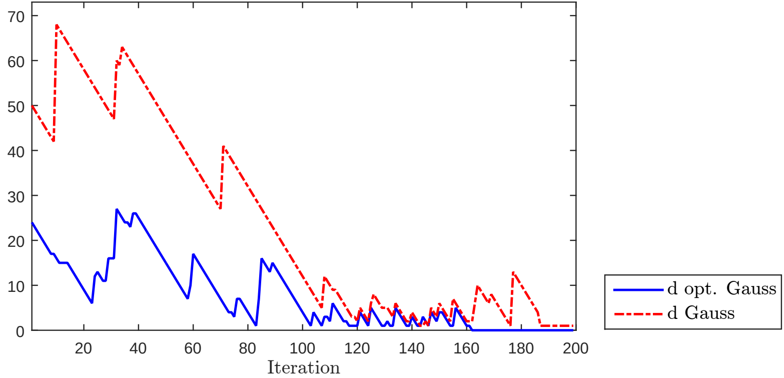
$$\frac{\|\varepsilon_{k-d}\|_A^2 - Q_{k-d,d}}{\|\varepsilon_{k-d}\|_A^2} \leq \tau$$

with

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

bcsstk01

$\tau = 0.25$



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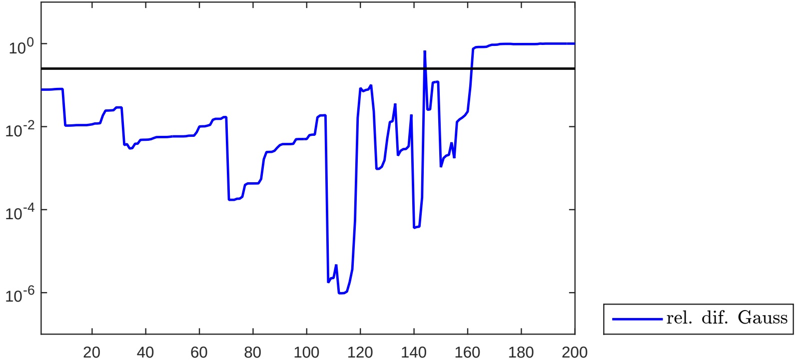
$\tau = 0.25$



The Gauss-Radau problem

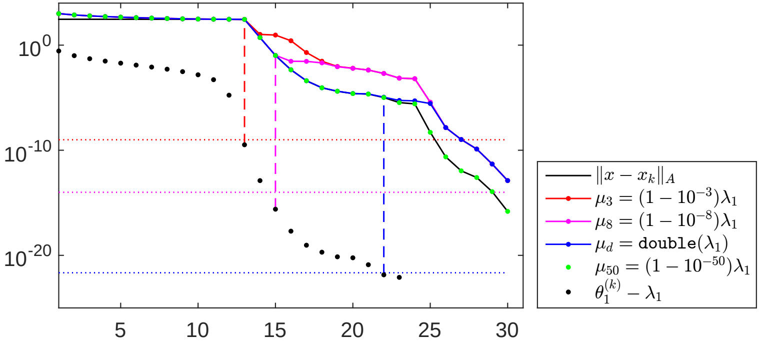
To study why the Gauss-Radau bound is not tight even when μ is close to λ_1, we set up a model problem of order 30 and we run CG in extended precision with `digits=128`

G. Meurant and P. Tichý, The behaviour of the Gauss-Radau upper bound of the A-norm of the error for the conjugate gradient algorithm, in preparation

The problem does not come from rounding errors

Model problem

$\theta_1^{(k)}$ is the smallest Ritz value



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

We have a theoretical explanation for that phenomenon

One remedy is to increase the delay for Gauss-Radau

We are currently working on an adaptative algorithm to do so

Other papers on error estimation:

C. Brezinski, Error estimates for the solution of linear systems, SIAM J. Sci. Comput., 21, pp. 764-781, 1999

D. Calvetti, S. Morigi, L. Reichel, and F. Sgallari, Computable error bounds and estimates for the conjugate gradient method, Numer. Algorithms, 25, pp. 79-88, 2000

Z. Strakoš and P. Tichý, Error estimation in preconditioned conjugate gradients, BIT Numerical Mathematics, 45, pp. 789-817, 2005

A. Frommer, K. Kahl, T. Lippert, and H. Rittich, 2-norm error bounds and estimates for Lanczos approximations to linear systems and rational matrix functions, SIAM J. Matrix Anal. Appl., 34(3), pp. 1046-1065, 2013

R. Estrin, D. Orban, and M.A. Saunders, Euclidean-norm error bounds for SYMMLQ and CG, SIAM J. Matrix Anal. Appl., 40(1), pp. 235-253, 2019

E. Hallman Sharp 2-norm error bounds for LSQR and the conjugate gradient method, SIAM J. Matrix Anal. Appl., 41(3), pp. 1183-1207, 2020