Strakoš, Zdeněk; Tichý, Petr

On Estimation of the A-norm of the Error in CG and PCG

We concentrate on the preconditioned conjugate gradient method and describe a simple and numerically well-justified way of estimation of the A-norm of the error. In this way this note represents an extension of [5] and its aim is to mediate the analytic results from [5] to practical users of the preconditioned conjugate gradient method.

1. Introduction

In this paper we consider a system of linear algebraic equations $Ax = b$ where A is a Hermitian positive definite n by n matrix and b n-dimensional vector (both real or complex). When A is large and sparse, as in matrices arising from FEM discretization of 3-D problems, iterative methods become competitive alternatives to direct solvers. For Hermitian positive definite systems, the conjugate gradient (CG) method [4] with a proper (typically problem–inspired) preconditioning represents in most cases a good choice. A goal of this paper is to present a simple way of estimating the A-norm of the error in the preconditioned conjugate gradient (PCG) method.

Estimating the A-norm of the error in CG and PCG has been studied by many authors. History and various aspects of this topic are thoroughly described in [5]. Though the formulas emphasized in [5] were published (in some form) previously, e.g. in [4], [2] or [1], our contribution is, to our opinion, novel in providing *theoretical justification* for practical use of the error estimates in computations affected by rounding errors. The presented note extends the results from [5] to PCG. A need for writing it can perhaps be seen from a comparison with [1, Section 6]. The last paper thoroughly and extensively examines estimating error norms in PCG. However, all derivations in [1, Section 6] assume exact arithmetic, no loss of orthogonality is considered there and the results are based on exploiting the finite termination property, i.e., on getting the exact solution in a finite number of steps (which does not exceed the dimension of the problem). These assumptions are clearly, in general, violated in practical computations. In order to be widely used, a practical error estimator needs to be properly justified (for a more detailed discussion see [5] and also [3]).

2. Estimation of the A-norm of the error

The standard version of the PCG method is given by the formulas

given x_0, $r_0 = b - Ax_0$, $s_0 = M^{-1}r_0$, $p_0 = s_0$,
for $j = 0, 1, \ldots$

$$\gamma_j = \frac{(r_j, s_j)}{(p_j, Ap_j)}, \quad x_{j+1} = x_j + \gamma_j \, p_j, \quad r_{j+1} = r_j - \gamma_j \, Ap_j, \quad s_{j+1} = M^{-1} r_{j+1},$$

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

end for.

The preconditioner $M = LL^T$ is chosen so that a linear system with the matrix M is easy to solve, while the matrix $L^{-1}AL^{-T}$ ensures fast convergence of PCG. This goal is fulfilled, e.g., when $L^{-1}AL^{-T}$ is well conditioned (approximates the identity matrix) or has properly clustered eigenvalues (*the positions* as well as *the diameters* of the clusters are important). An estimator for the A-norm of the error is then formulated in a very simple way. Following [5], we get fundamental identity for decrease of the A-norm of the error in d consecutive steps

$$\|x - x_j\|_A^2 \;=\; \sum_{i=j}^{j+d-1} \gamma_i \, (r_i, s_i) \;+\; \|x - x_{j+d}\|_A^2 \,. \tag{1}$$

Assuming a reasonable decrease of the A-norm of the error in the steps $j+1$ through $j+d$, the square root of

$$\nu_{j,d} \equiv \sum_{i=j}^{j+d-1} \gamma_i \, (r_i, s_i) \tag{2}$$

gives a tight lower bound for the A-norm of the jth error of PCG applied to the system $Ax = b$. Please notice that (similarly as in the ordinary CG) the quantities γ_i and (r_i, s_i) are at our disposal during the PCG iterations.

3. Numerical stability of the estimate

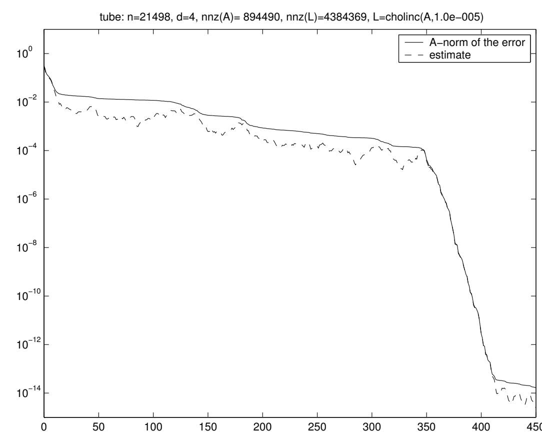
Numerical stability analysis of the estimate (2) must answer a question to which extent the identity (1) holds for quantities computed *in finite precision arithmetic* (characterized by machine precision ε). Please notice that this question if fundamentally different from its trivial part examining the error in computing $\nu_{j,d}$ from (2) using γ_i and (r_i, s_i). In order to justify the estimate (2), we have to derive the identity for the computed quantities analogous to (1) without using any assumption which does not hold in finite precision computations. In particular, we can not use any assumption about orthogonality or finite termination. A complicated analysis published in [6], see also [5], shows that the computed quantities satisfy

$$\|x - x_j\|_A^2 - \|x - x_{j+d}\|_A^2 \;=\; \nu_{j,d} + \nu_{j,d}\, E_{j,d}^{(1)} \;+\; \|x - x_j\|_A\, E_{j,d}^{(2)} + O(\varepsilon^2), \tag{3}$$

where the terms $E_{j,d}^{(1)}$ and $E_{j,d}^{(2)}$ are small (for their quantification see [6]). This formula can be interpreted in a following way: until $\|x - x_j\|_A$ reaches a level close to $\varepsilon\|x - x_0\|_A$, the estimate $\nu_{j,d}$ must work.

4. Numerical Experiment

To illustrate the quality and also the drawbacks of the estimate (2), we use a problem of the size $n = 21498$ arised from cylindrical shell modeling, given at the R. Kouhia's homepage `http://www.hut.fi/~kouhia/`. Experiment was performed in MATLAB 6.5 on a PC with machine precision $\varepsilon \sim 10^{-16}$. We set $x_0 = 0$, determined L simply by the MATLAB command `cholinc(A, 1e–5)`, and used a fixed value $d = 4$. The figure demonstrates that if the A-norm of the error (solid line) decreases rapidly (iterations $350-400$), we can not visually distinguish this quantity from its estimate (dashed line). On the other hand, if the convergence is slow (iterations $1-350$) (2) may underestimate the actual A-norm of the error. Still, the behaviour of the estimate offers a good information about convergence. We emphasize that this example represents *an illustration*, and neither the preconditioner nor the estimate (parameter d) has been tuned for this specific problem.



Acknowledgements

Z. Strakoš is supported by GA CR under grant 201/02/0595, and P. Tichý is supported by the Emmy Noether-Programm of the Deutsche Forschungsgemeinschaft. The authors thank to R. Kouhia and M. Tůma for their valuable help.

5. References

1 O. Axelsson and I. Kaporin, Error norm estimation and stopping criteria in preconditioned Conjugate Gradient iterations, Numerical Linear Algebra with Applications, 8 (2001), pp. 265–286.
2 P. Deuflhard, Cascadic conjugate gradient methods for elliptic partial differential equations: Algorithm and numerical results, Contemporary Mathematics, 180 (1994), pp. 29–42.
3 G. H. Golub and Z. Strakoš, Estimates in quadratic formulas, Numerical Algorithms, 8 (1994), pp. 241–268.
4 M. R. Hestenes and E. Stiefel, Methods of conjugate gradients for solving linear systems, J. Res. Nat. Bureau Standarts, 49 (1952), pp. 409–435.
5 Z. Strakoš and P. Tichý, On Error Estimation in the Conjugate Gradient Method and Why It Works In Finite Precision Computations, Electronic Transaction on Numerical Algebra (ETNA), Volume 13, pp. 56-80, 2002.
6 Z. Strakoš and P. Tichý, Simple estimation of the A-norm of the error in the preconditioned conjugate gradient method, Technical report No. 892, ICS AS CR, Prague, Czech Republic, 2003.

Zdeněk Strakoš, Institute of Computer Science AS CR, Pod vodárenskou věží 2, 182 07 Prague 8, Czech Republic, `strakos@cs.cas.cz`
Petr Tichý, Institute of Mathematics, Technical University of Berlin, Strasse des 17. Juni, 106 23 Berlin, Germany, `tichy@math.tu-berlin.de`