Efficient Estimation of the A-norm of the Error in the Preconditioned Conjugate Gradient Method

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Abstract

Discretization of mathematical models of real-world problems often leads to large and sparse (possibly structured) systems of linear algebraic equations. All steps of mathematical modeling (mathematical description of reality in the form of a mathematical model, its discretization and numerical solution of the discretized problem) are subject to errors (errors of the model, discretization errors and computational errors, the last being often composed of two parts – truncation errors and errors due to roundoff). An output of the solution process must therefore be confronted with its possible errors through *verification and validation*. While verification addresses the question – whether and how accurately the obtained (approximate) solution conforms to the mathematical model, validation deals with the more general question – to which extent the whole modeling process represents the modeled reality (for a recent discussion of these fundamental topics we refer to [4, 9]). It is desirable that the errors of the model, discretization errors and computational errors are in some balance.

When the linear algebraic systems arising from mathematical modeling are very large, preconditioned iterative methods become competitive with the purely direct methods. Iterative methods can in very large scale computations exploit a fundamental advantage over direct methods – they can increase effectiveness of the whole solution process by stopping the iteration when the desired accuracy (as compared, e.g., to the discretization error) is reached (cf. [1, 2]). This requires, however, a cheap and reliable evaluation of convergence, which is the essential ingredience for choosing proper stopping criteria.

In this contribution we consider a system of linear algebraic equations

$$Ax = b$$

where A is a symmetric positive definite n by n matrix and b is n-dimensional vector (for simplicity of notation we consider A, b real; all results can trivially be extended to the Hermitian positive definite systems in the complex case). For such systems the preconditioned conjugate gradient method [7, 8, 13, 10] represents in most large scale cases a good choice. A goal of this contribution is to summarize and discuss evaluation of convergence in the preconditioned

conjugate gradient method. In particular, we will focus on estimating the A-norm of the error.

Estimating the A-norm of the error in the conjugate gradient method was subject of many papers, reports and subsections in the books. History and various aspects of estimating the A-norm of the error in the unpreconditioned conjugate gradient method were thoroughly described in [11]. The formulas presented in [11] were published (in some form) previously, e.g. in [7, 5] and [3]. The original contribution of [11] consists, to our opinion, in providing *theoretical justification for practical use of the error estimates* and in putting different estimates in the proper context. The subsequent paper [12] extends the results from [11] to the preconditioned conjugate gradient method. In particular, as in [11], we take into consideration effects of finite precision arithmetic, which can in preconditioned conjugate gradient computations be very substantial. In order to be widely used, practical error estimators need a proper justification including a thorough analysis of rounding error effects (for a related discussion, see [11, 12] and also [6]).

After summarizing fundamentals of the conjugate gradient method and of several possible ways of convergence evaluation, we present a simple estimate for the A-norm of the error in the preconditioned conjugate gradient method. We then describe results of numerical stability analysis and illustrate the effectivity and possible drawbacks of the proposed estimate on numerical experiments.

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