ON ERROR ESTIMATION IN THE CONJUGATE GRADIENT METHOD AND WHY IT WORKS IN FINITE PRECISION COMPUTATIONS *

ZDENĚK STRAKOŠ[†] AND PETR TICHÝ[*]

Abstract. In their paper published in 1952, Hestenes and Stiefel considered the conjugate gradient (CG) method an iterative method which terminates in at most n steps if no rounding errors are encountered [p. 410]. , They also proved identities for the A-norm and the Euclidean norm of the error which could justify the stopping criteria [Theorems 6:1 and 6:3, p. 416]. , The idea of estimating errors in iterative methods, and in the CG method in particular, was independently (of these results) promoted by Golub; the problem was linked to Gauss quadrature and to its modifications [7], [8]. A comprehensive summary of this approach was given in [15], [16]. During the last decade several papers developed error bounds algebraically without using Gauss quadrature. However, we have not found any reference to the corresponding results in [24]. All the existing bounds assume exact arithmetic. Still they seem to be in a striking agreement with finite precision numerical experiments, though in finite precision computations they estimate quantities which can be orders of magnitude different from their exact precision counterparts! For the lower bounds obtained from Gauss quadrature formulas this nontrivial phenomenon was explained, with some limitations, in [17].

In our paper we show that the lower bound for the A-norm of the error based on Gauss quadrature ([15], [17], [16]) is mathematically equivalent to the original formula of Hestenes and Stiefel [24]. We will compare existing bounds and we will demonstrate necessity of a proper rounding error analysis: we present an example of the well-known bound which can fail in finite precision arithmetic. We will analyse the simplest bound based on [24, Theorem 6:1], and prove that it is numerically stable. Though we concentrate mostly on the lower bound for the A-norm of the error, we describe also an estimate for the Euclidean norm of the error based on [24, Theorem 6:3]. Our results are illustrated by numerical experiments.

Key words. conjugate gradient method, Gauss quadrature, evaluation of convergence, error bounds, finite precision arithmetic, rounding errors, loss of orthogonality.

AMS subject classifications. 15A06, 65F10, 65F25, 65G50.