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An estimator for the diagonal of a matrix. (English) Zbl 1123.65026

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Summary: A number of applications require to compute an approximation of the diagonal of a matrix when this matrix is not explicitly available but matrix-vector products with it are easy to evaluate. In some cases, it is the trace of the matrix rather than the diagonal that is needed. This paper describes methods for estimating diagonals and traces of matrices in these situations. The goal is to obtain a good estimate of the diagonal by applying only a small number of matrix-vector products, using selected vectors.

We begin by considering the use of random test vectors and then explore special vectors obtained from Hadamard matrices. The methods are tested in the context of computational materials science to estimate the diagonal of the density matrix which holds the charge densities. Numerical experiments indicate that the diagonal estimator may offer an alternative method that in some cases can greatly reduce computational costs in electronic structures calculations.

MSC:

65F30 Other matrix algorithms (MSC2010)
15A15 Determinants, permanents, traces, other special matrix functions

Keywords:

Stochastic estimator; Hadamard matrices; Grassmannian spaces; Electronic structure calculations; Density functional theory; diagonals; traces; matrix-vector products; numerical experiments

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