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Extending hierarchical probing for computing the trace of matrix inverses. (English)
Zbl 1442.65057

The problem of this paper is to estimate the diagonal or the trace of \( f(A) \), where \( A \) is a large sparse (symmetric) matrix and \( f \) can be approximated by a polynomial of degree \( n \). The structure of \( A \) is caught by a colored graph (no connected vertices share the same color). The diagonal elements are estimated by solving systems with random right-hand sides selected based on the coloring of the graph. A 0-1 probing vector is used for each color. Coloring for \( A^n \) corresponds to distance-\( n \) coloring of \( A \). It is important to apply hierarchical probing, which means that vertices in different distance-\( n \) color groups should not be in the same distance-(\( n + 1 \)) color group. This idea of a binary multilevel hierarchy was already worked out for matrices with a toroidal lattice structure in a previous paper: [A. Stathopoulos et al., SIAM J. Sci. Comput. 35, No. 5, S299–S322 (2013; Zbl 1281.65072)]. This is generalized in the present paper, first for higher dimensional lattices and for a vector of arbitrary dimension lengths (which need not be a powers-of-two, but there should be a common prime factor) and eventually the hierarchical probing idea is generalized to work for any undirected graph structure. The authors work through successive steps to introduce the ideas that are summarized in the form of formal algorithms. The number of colors is not optimal but the variance reduction is close to classical probing, while considerably reducing memory and computational time.

Reviewer: Adhemar Bultheel (Leuven)

MSC:

65F15 Numerical computation of eigenvalues and eigenvectors of matrices
65F50 Computational methods for sparse matrices
05C50 Graphs and linear algebra (matrices, eigenvalues, etc.)
05C15 Coloring of graphs and hypergraphs
05B20 Combinatorial aspects of matrices (incidence, Hadamard, etc.)
81V05 Strong interaction, including quantum chromodynamics
15A15 Determinants, permanents, traces, other special matrix functions

Keywords:
probing; trace of the inverse; sparse matrix; lattice QCD

Full Text: DOI

References:

[8] D. Goldfarb and Ph. L. Tont, Optimal estimation of Jacobian and Hessian matrices that arise in finite difference calculations,


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