

APPROXIMATION OF THE TRACE OF MATRIX FUNCTIONS BASED ON DECAY BOUNDS

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The computation of the trace of functions of sparse matrices is an important task in numerous applications. Since we assume A to be large and sparse, it is not possible to compute $f(A)$ and extract the diagonal entries. Commonly, for sparse matrices A , the matrix $f(A)$ exhibits a rapid decay away from the sparsity pattern of A , such that many entries of $f(A)$ are very small in magnitude. Based on this observation, we present a method for approximating the trace of $f(A)$. The method requires decay bounds for the entries of $f(A)$ and graph coloring algorithms and then computes just a few bilinear forms to determine an approximation of the trace of $f(A)$. The algorithm is compared to a stochastic trace estimator and the effectiveness of this approach is shown in numerical experiments.