

DECAY BOUNDS AND $O(n)$ ALGORITHMS FOR APPROXIMATING FUNCTIONS OF SPARSE MATRICES*

MICHELE BENZI[†] AND NADER RAZOUK[†]

Dedicated to Gene Golub on the occasion of his 75th birthday

Abstract. We establish decay bounds for the entries of $f(A)$, where A is a sparse (in particular, banded) $n \times n$ diagonalizable matrix and f is smooth on a subset of the complex plane containing the spectrum of A . Combined with techniques from approximation theory, the bounds are used to compute sparse (or banded) approximations to $f(A)$, resulting in algorithms that under appropriate conditions have linear complexity in the matrix dimension. Applications to various types of problems are discussed and illustrated by numerical examples.

Key words. Matrix functions, sparse and banded matrices, decay rates, linear time algorithms, Chebyshev polynomials, Faber polynomials, density matrix, trace, determinant

AMS subject classifications. Primary 65F10, 65F30. Secondary 15A.

*Received March 12, 2007. Accepted for publication May 10, 2007. Recommended by A. Wathen. Work supported by National Science Foundation grant DMS-0511336.

[†]Department of Mathematics and Computer Science, Emory University, Atlanta, Georgia 30322, USA ({benzi,nrazouk}@mathcs.emory.edu).