Dissertation Defense

Localization Phenomena in Matrix Functions: Theory and Algorithms

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Abstract

Many physical phenomena are characterized by strong *localization*, that is, rapid decay outside a small spatial or temporal region. Frequently, such localization can be expressed as decay in the entries of a function $f(A)$ of an appropriate sparse or banded matrix A that encodes a description of the system. Important examples include the decay in the entries of the density matrix for non-metallic systems in quantum chemistry (a function of the Hamiltonian), and the decay behavior of the inverse of a banded symmetric positive definite matrix. Localization phenomena are of fundamental importance in physical theory and in computation, because they open up the possibility of approximating relevant matrix functions in $O(n)$ time, where n is a measure of the size of the system.

In this talk we give a brief background on matrix functions and their importance in scientific applications. We will review the existing results on decay in matrix functions. Next, we present our main results that generalize and unify several previous bounds known in the literature for special classes of functions and matrices, such as the inverse, the resolvent, and the exponential. The theory can be used to determine the bandwidth or sparsity pattern outside which the entries of $f(A)$ are guaranteed to be so small that they can be neglected without exceeding a prescribed error tolerance. We discuss sufficient conditions for the possibility of $O(n)$ approximations to given accuracy in terms of the possible singularities of f and the spectral properties of the matrices involved. Finally, numerical experiments illustrating the promising behavior of the proposed approximation schemes will be presented.

Advisor: Michele Benzi

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