Numerical Analysis and Scientific Computing Seminar

Filtering techniques for eigenvalue problems

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Abstract: The solution of large symmetric eigenvalue problems is central to applications ranging from electronic structure calculations to the study of vibrations in mechanical systems. A few of these applications require the computation of a large number of eigenvalues and associated eigenvectors. For example, when dealing with excited states in quantum mechanics, it is not uncommon to seek a few tens of thousands of eigenvalues of matrices of sizes in the tens of millions. In such situations it is imperative to resort to 'spectrum slicing' strategies, i.e., strategies that extract slices of the spectrum independently. The presentation will discuss a few techniques in this category, namely those based on a combination of filtering (polynomial, rational) and standard projection methods (Lanczos, subspace iteration). Filtering consists of computing eigenvalues and vectors of a matrix of the form $B = f(A)$, where f is typically a polynomial or rational function. With the mapping f the wanted eigenvalues of the original matrix are transformed in such a way that they become easier to extract. This particular area blends ideas from approximation theory with standard matrix algorithms. The presentation will emphasize rational filtering and will discuss some recent work on nonlinear eigenvalue problems.

Friday, February 22, 2019, 2:00 pm
Mathematics and Science Center: W301

Mathematics
Emory University