Approximating spectral densities of large matrices: old and new

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Abstract: In physics, it is sometimes desirable to compute the so-called Density Of States (DOS), also known as the spectral density, of a Hermitian matrix $A$. The spectral density can be viewed as a probability density distribution that measures the likelihood of finding eigenvalues near some point on the real line. The most straightforward way to obtain this density is to compute all eigenvalues. But this approach is generally costly and wasteful, especially for matrices of large dimension. In many cases, the only affordable operation is matrix-vector multiplication. In this talk I will define the problem of estimating the spectral density carefully, and discuss a few known algorithms based on stochastic sampling, in particular, those using the kernel polynomial method and the Lanczos method, for estimating the spectral density. The accuracy of stochastic algorithms converge as $O(1/\sqrt{N_v})$, where $N_v$ is the number of stochastic vectors. I will also talk about recent progresses of stochastic estimation of spectral densities with convergence rate much faster than $O(1/\sqrt{N_v})$ using a relatively high degree of polynomials and modest choice of $N_v$. (Joint work with Yousef Saad and Chao Yang)

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