

Applications of trace estimation techniques in numerical linear algebra

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A well-known technique used in statistical methods is to estimate the trace of some matrix function via sampling. For example, one can estimate the trace of $\exp(A)$ by computing $w = \exp(A)v$ for many vectors v , and the mean of the inner products of v and w will yield an approximation of the trace under some conditions. This basic technique has found uses in areas as diverse as physics, statistics, machine learning, and numerical linear algebra. A closely related problem is that of estimating the diagonal of $f(A)$ which has important applications in quantum mechanics. Thus, when $f(t)$ is a step function, and A is a Hamiltonian, then the diagonal of $f(A)$ represents the charge density of the system. We first discuss these applications and recent work in this area and will put in contrast random sampling versus probing techniques. Then the presentation will focus on the important problem of computing spectral densities and its application to ‘spectrum slicing’, or the technique of dividing the spectrum into subintervals.