Variance reduction techniques for computing the trace of the inverse of a matrix

by Andreas Stathopoulos
College of William and Mary

Abstract. The computation of the trace of the inverse of a large matrix appears in many statistics, machine learning, and quantum mechanics applications. Our driving application comes from Lattice Quantum Chromodynamics (LQCD). To solve the problem, practitioners typically use a variant of the Monte Carlo method that requires the solution of a linear system at each step. The variance of this estimator equals the squared Frobenious norm of the matrix inverse, excluding its diagonal.

In this talk, we present some variance reduction techniques we developed that try to approximate the off-diagonal elements of the matrix inverse based either on structural or on spectral information. Our first approach, Hierarchical Probing, produces a sequence of Hadamard vectors that hierarchically annihilate elements of the matrix inverse whose vertices in the lattice are increasingly farther from each other. Our second approach is to deflate the smallest singular triplets. Contrary to low rank matrix approximations, the above deflation may actually increase variance. We provide an analysis and derive criteria on when to expect improvement.