Energy and variance optimization of many-body wave functions

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We present a simple, robust and efficient method for varying the parameters in a many-body wave function, both for continuum and lattice problems, to optimize the expectation value of the energy[1]. The method is compared to what is currently the most popular method for optimizing many-body wave functions, namely minimization of the variance of the local energy[2]. The variance minimization method is far more efficient than *straightforward* energy minimization because for a sufficiently flexible variational wave function, it is possible to lower the energy on the finite set of Monte Carlo (MC) configurations on which the optimization is performed, while in fact raising the true expectation value of the energy. On the other hand, if the variance of the local energy is minimized, each term in the sum over MC configurations is bounded from below by zero and the problem is far less severe[2]. Our new energy optimization method gets around this problem by adding terms to the straightforward expression for the Hessian that are zero when the integrals are performed exactly, but that cancel much of the statistical fluctuations for a finite Monte Carlo sample. With the additional terms, the Hessian is written as a sum of covariances resulting in much reduced fluctuations. In case the wave function parameters are linear in the exponent, part of the Hessian can be written as a tri-covariance, as also pointed out by Sorella[3], making it apparent that further cancellations of fluctuations occur. The optimization of Jastrow parameters converges in two Monte Carlo steps if a sufficiently large sample is used, but, it is more computationally efficient to first do 2 or 3 iterations with small samples followed by a single large-sample iteration. The estimated gain in efficiency increases with system size, ranging from 3 orders of magnitude for small molecules to 5 orders of magnitude for the larger molecules we used as test cases.

[1] C. J. Umrigar and Claudia Filippi, Phys. Rev. Lett. **94**, 150201-1 (2005).

[2] C. J. Umrigar, K.G. Wilson and J. W. Wilkins, Phys. Rev. Lett. **60**, 1719 (1988).

[3] S. Sorella, cond-mat/0502553.