High Accuracy Variational Slater-Jastrow Wave Functions from the Stochastic Gradient Algorithm

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Key to producing reliable variational wave functions for use on their own or as starting points for more accurate techniques is the ability to optimize large sets of variational parameters at relatively low cost. In this work, we present a technique that combines our previous method for producing second-quantized Jastrow-type wave functions with the Stochastic Gradient Approximation to optimize Slater-Jastrow wave functions containing thousands of parameters. We demonstrate that our technique yields variational energies that are within .1% of exact answers for the 4x4 repulsive Hubbard. We then employ our method to study correlated phenomena such as charge and spin density waves exhibited in Hubbard models far larger than those typically accessible using projection techniques such as Constrained Path Monte Carlo. Lastly, we present preliminary results for several small molecules to demonstrate the method's flexibility. We find this technique to be surprisingly accurate given the comparitively few parameters it employs. Our method paves the way toward performing predictive simulations of large lattice models, materials, and molecules at significantly reduced cost.