Analysis of self-consistent field and direct minimization algorithms for electronic structure

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Numerous algorithms exist to solve the Kohn-Sham equations of electronic structure. They are either based on the direct minimization of the energy under constraints or based on fixed point iterations to solve a self-consistent formulation of the problem. It is not clearly understood which class of algorithms is more efficient and robust in which situation. We propose in this poster a first approach to the understanding of the intrinsic differences between two simple algorithms of each class: a damped self-consistent field algorithm and a projected gradient descent. We perform a local analysis and derive explicit convergence rates, confirmed by numerical experiments.