Optimization Problems with Orthogonality Constraints -- from Feasible to Infeasible

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Abstract: To construct a parallel approach for solving optimization problems with orthogonality constraints is usually regarded as an extremely difficult mission, due to the low scalability of the orthogonalization procedure. However, such demand is particularly huge in some application domains such as material computation. In this talk, we introduce several efficient algorithms including feasible and infeasible methods. Such methods have much lower computational complexity and can also benefit from parallel computing since they are full of BLAS3 operations. In the infeasible algorithm based on a modified augmented Lagrange method, the orthogonalization procedure is only invoked once as the last step. Consequently, the main parts of the proposed algorithms can be parallelized naturally. We establish global subsequence convergence results for our proposed algorithms. Worst-case complexity and local convergence rate are also studied under some mild assumptions. Numerical experiments, including tests under parallel environment, illustrate that our new algorithms attain good performances and high scalability in solving discretized Kohn-Sham total energy minimization problems.