

# Direct minimization of electronic structure calculations with Householder reflections

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We consider a minimization scheme based on the Householder transport operator for the Grassman manifold, where a point on the manifold is represented by a  $m \times n$  matrix with orthonormal columns. In particular, we consider the case where  $m \gg n$  and present a method with asymptotic complexity  $mn^2$ . To avoid explicit parametrization of the manifold we use Householder transforms to move on the manifold, and present a formulation for simultaneous Householder reflections for S-orthonormal columns. We compare a quasi-Newton and nonlinear conjugate gradient implementation adapted to the manifold with a projected nonlinear conjugate gradient method, and demonstrate that the convergence rate is significantly improved if the manifold is taken into account when designing the optimization procedure.

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