Quasi-Newton algorithms for the eigenvector-dependent nonlinear eigenproblem

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We consider the problem of computing eigenpair solutions (λ, v) to the problem:

$$\begin{aligned} A(v)v &= \lambda v, \\ c^T v &= 1, \end{aligned} \tag{1}$$

where $A : \mathbb{R}^n \to \mathbb{R}^{n\times n}$ is a nonlinear function of v. This class of eigenvalue problems with an eigenvector-dependent nonlinearity arises in quantum mechanics when we are interested in computing the ground states of bosons using the Gross-Pitaevskii equation[1]. They also commonly occur in electronic structure calculations in quantum chemistry[3] and trace ratio optimization problems in linear discriminant analysis for dimension reduction[2]. In this work, we take a Quasi-Newton approach to the problem by viewing (1) as a structured nonlinear system of equations. We characterize several Quasi-Newton methods theoretically and computationally. The linearly convergent self-consistent field (SCF) iteration which is a very common algorithm for this problem is shown to be equivalent to one of these methods. More precisely, we show how the SCF iteration can be derived using a modified Jacobian depending on the iterate in the next step, i.e., it is an implicit Quasi-Newton method. We illustrate the properties of the proposed methods with simulation examples and one of these methods exhibits quadratic convergence with a faster convergence rate than the standard Newton method.

References

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