Haw-ren Fang Two Classes of Multisecant Methods for Nonlinear Acceleration

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Many applications in science and engineering lead to models which require solving large-scale fixed point problems, or equivalently, systems of nonlinear equations. Several successful techniques for handling such problems are based on quasi-Newton methods that implicitly update the approximate Jacobian or inverse Jacobian to satisfy a certain secant condition.

We present two classes of multisecant methods which allows to take into account a variable number of secant equations at each iteration. The first is the Broyden-like class, of which Broyden's family is a subclass, and Anderson mixing is a particular member. The second class is that of the nonlinear Eirola-Nevanlinnatype methods.

This work was motivated by a problem in electronic structure calculations, whereby a fixed point iteration, known as the self-consistent field (SCF) iteration, is accelerated by various strategies termed 'mixing'.