On solving the Rachford-Rice equation with higher order methods

The Rachford-Rice equation calculates the amounts and compositions of two equilibrium phases at constant K-factors. This single variable equation is a perfect candidate for applying higher order iteration methods because the additional cost for evaluating the derivatives with order higher than two is relatively low. This study compares the performance of Householder's high order iterations up to order seven. In addition, a method to improve the initial estimate is proposed for the situation where the Rachford-Rice function shows abrupt change close to the asymptotes and overshooting happens. The proposed method can largely reduce repeated use of the bisection adjustment in the subsequent iterations. The comparison shows that the Householder's iteration with order three or four gives the best performance on average.

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