

Article

Numerical Solution of Nonlinear Problems with Multiple Roots Using Derivative-Free Algorithms

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Abstract: In the study of systems' dynamics the presence of symmetry dramatically reduces the complexity, while in chemistry, symmetry plays a central role in the analysis of the structure, bonding, and spectroscopy of molecules. In a more general context, the principle of equivalence, a principle of local symmetry, dictated the dynamics of gravity, of space-time itself. In certain instances, especially in the presence of symmetry, we end up having to deal with an equation with multiple roots. A variety of optimal methods have been proposed in the literature for multiple roots with known multiplicity, all of which need derivative evaluations in the formulations. However, in the literature, optimal methods without derivatives are few. Motivated by this feature, here we present a novel optimal family of fourth-order methods for multiple roots with known multiplicity, which do not use any derivative. The scheme of the new iterative family consists of two steps, namely Traub-Steffensen and Traub-Steffensen-like iterations with weight factor. According to the Kung-Traub hypothesis, the new algorithms satisfy the optimality criterion. Taylor's series expansion is used to examine order of convergence. We also demonstrate the application of new algorithms to real-life problems, i.e., Van der Waals problem, Manning problem, Planck law radiation problem, and Kepler's problem. Furthermore, the performance comparisons have shown that the given derivative-free algorithms are competitive with existing optimal fourth-order algorithms that require derivative information.

Keywords: multiple roots; convergence; nonlinear equations; derivative-free method

MSC: 49M15; 65H05; 41A25



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1. Introduction

Simple systems often embed a good amount of symmetry. Take for instance the characteristic polynomial (ChP) of hydrocarbons [1]. Considering 3 cases here, propane (ChP is $x^3 - 2x$), normal butane (ChP is $x^4 - 3x^2 + x$) and isobutane (ChP is $x^4 - 3x^2$), one should easily notice that the highest symmetry is in isobutane. At the same time, isobutane is the one having multiple roots in the characteristic polynomial. Same symmetry is responsible for the presence of the multiple roots in the ChP of 2,2,4,4-Tetramethylpentane (ChP is $x^9 - 8x^7 + 15x^5$, see a_{-25} in [2]). One should notice that, in the selected cases, the multiple root is banal ($x = 0$); however, in general, in more complex cases, the multiple root is not any more banal.

Much research has been conducted on the solution of nonlinear equations and systems of nonlinear equations. There are numerous publications on the topic, including those given in reference [3–10], and Traub's book [11] has a whole chapter devoted to

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