

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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The Numerical Solution of Nonlinear Problems Christopher T. H. Baker, Chris Phillips, 1981 Newton Methods for Nonlinear Problems Peter Deufhard, 2011-09-18 This book deals with the efficient numerical solution of challenging nonlinear problems in science and engineering both in finite dimension algebraic systems and in infinite dimension ordinary and partial differential equations Its focus is on local and global Newton methods for direct problems or Gauss Newton methods for inverse problems The term affine invariance means that the presented algorithms and their convergence analysis are invariant under one out of four subclasses of affine transformations of the problem to be solved Compared to traditional textbooks the distinguishing affine invariance approach leads to shorter theorems and proofs and permits the construction of fully adaptive algorithms Lots of numerical illustrations comparison tables and exercises make the text useful in computational mathematics classes At the same time the book opens many directions for possible future research

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Table of Contents Numerical Solution Of Nonlinear Problems

1. Understanding the eBook Numerical Solution Of Nonlinear Problems
 - The Rise of Digital Reading Numerical Solution Of Nonlinear Problems
 - Advantages of eBooks Over Traditional Books
2. Identifying Numerical Solution Of Nonlinear Problems
 - Exploring Different Genres
 - Considering Fiction vs. Non-Fiction
 - Determining Your Reading Goals
3. Choosing the Right eBook Platform
 - Popular eBook Platforms
 - Features to Look for in an Numerical Solution Of Nonlinear Problems
 - User-Friendly Interface
4. Exploring eBook Recommendations from Numerical Solution Of Nonlinear Problems
 - Personalized Recommendations
 - Numerical Solution Of Nonlinear Problems User Reviews and Ratings
 - Numerical Solution Of Nonlinear Problems and Bestseller Lists
5. Accessing Numerical Solution Of Nonlinear Problems Free and Paid eBooks

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 - Numerical Solution Of Nonlinear Problems Budget-Friendly Options
6. Navigating Numerical Solution Of Nonlinear Problems eBook Formats
 - ePub, PDF, MOBI, and More
 - Numerical Solution Of Nonlinear Problems Compatibility with Devices
 - Numerical Solution Of Nonlinear Problems Enhanced eBook Features
 7. Enhancing Your Reading Experience
 - Adjustable Fonts and Text Sizes of Numerical Solution Of Nonlinear Problems
 - Highlighting and Note-Taking Numerical Solution Of Nonlinear Problems
 - Interactive Elements Numerical Solution Of Nonlinear Problems
 8. Staying Engaged with Numerical Solution Of Nonlinear Problems
 - Joining Online Reading Communities
 - Participating in Virtual Book Clubs
 - Following Authors and Publishers Numerical Solution Of Nonlinear Problems
 9. Balancing eBooks and Physical Books Numerical Solution Of Nonlinear Problems
 - Benefits of a Digital Library
 - Creating a Diverse Reading Collection Numerical Solution Of Nonlinear Problems
 10. Overcoming Reading Challenges
 - Dealing with Digital Eye Strain
 - Minimizing Distractions
 - Managing Screen Time
 11. Cultivating a Reading Routine Numerical Solution Of Nonlinear Problems
 - Setting Reading Goals Numerical Solution Of Nonlinear Problems
 - Carving Out Dedicated Reading Time
 12. Sourcing Reliable Information of Numerical Solution Of Nonlinear Problems
 - Fact-Checking eBook Content of Numerical Solution Of Nonlinear Problems
 - Distinguishing Credible Sources
 13. Promoting Lifelong Learning
 - Utilizing eBooks for Skill Development

- Exploring Educational eBooks

14. Embracing eBook Trends

- Integration of Multimedia Elements
- Interactive and Gamified eBooks

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