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On an application of symbolic computation and computer graphics to root-finders: The case of multiple roots of unknown multiplicity

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ABSTRACT

The contemporary powerful mathematical software enables a new approach to handling and manipulating complex mathematical expressions and other mathematical objects. Particularly, the use of symbolic computation leads to new contribution to constructing and analyzing numerical algorithms for solving very difficult problems in applied mathematics and other scientific disciplines. In this paper we are concerned with the problem of determining multiple zeros when the multiplicity is not known in advance, a task that is seldom considered in literature. By the use of computer algebra system *Mathematica*, we employ symbolic computation through several programs to construct and investigate algorithms which both determine a sought zero and its multiplicity. Applying a recurrent formula for generating iterative methods of higher order for solving nonlinear equations, we construct iterative methods that serve (i) for approximating a multiple zero of a given function f when the order of multiplicity is unknown and, simultaneously, (ii) for finding exact order of multiplicity. In particular, we state useful cubically convergent iterative sequences that find the exact multiplicity in a few iteration steps. Such approach, combined with a rapidly convergent method for multiple zeros, provides the construction of efficient composite algorithms for finding multiple zeros of very high accuracy. The properties of the proposed algorithms are illustrated by several numerical examples and basins of attraction.

1. Introduction

The development of digital computers, circa 1970, has enabled easy and successful computations in many scientific disciplines such as engineering disciplines, physics, chemistry, communication, biology, education, astronomy, geology, banking, business, insurance, health care, social science, as well as many other fields of human activities. In this paper we pay our attention to applied mathematics, in particular, to the construction of algorithms in numerical analysis, and a specific application of computers—symbolic computation. In the course of the development of numerical methods, it turned out in the last quarter of the 20th century that further development of new algorithms of higher efficiency and greater accuracy was not possible due to the lack of fast hardware and advanced software. At the beginning of the 21st century the rapid development of computer power and accessibility, computer multi-precision arithmetics and symbolic

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computation enabled the construction, testing and analysis of very efficient numerical algorithms, even "confirmation analytically derived results" [1]. Simply, symbolic computation replaced lengthy hand derivations and manipulation with computer-based derivation and manipulation.

Symbolic computation, employed in solving mathematical problems, is concerned with software for handling and manipulating mathematical expressions and other mathematical objects. It is important to emphasize that these expressions contain variables in general form such as $f(a, b, c, \ldots)$, where a, b, c are not numerical values and f may or may not be given explicitly. Various manipulations (automatic simplification of expressions, differentiation, indefinite integration, polynomial decomposition, polynomial factorization, etc.) treat these variables as symbols (hence the name *symbolic computation*) and provide *exact* computation. It is superfluous to emphasize that, in the case of complex and lengthy expressions, symbolic computation is the only tool for solving given problems; their solution and analysis would not be possible by a classic "paper-and-pencil" fashion. Note that software applications that execute symbolic computation are most frequently called *computer algebra systems* (shorter CAS) although some authors make distinction between "symbolic computation" and "computer algebra", see, e.g., [2]. For more details on symbolic computation and its applications see the book [3].

As mentioned in [4], "newer generation of mathematicians and computer scientists can really take advantage of computer aided research supported by the modern CAS". Among the major general purposes CAS are certainly Mathematica and Maple, although Axiom, GAP, Maxima, Sage and SymPy are very useful within their symbolic functionality. All of these CAS are available of the platforms Windows, Mac OS X and Linux (with the exception of Sage which works in Windows as "virtual machine"). All of these computational packages perform sophisticated mathematical operations.

In this paper we present a class of iterative methods for the determination of multiple zeros of functions when the multiplicity is not known in advance. One should say that there is a vast literature concerned with iterative methods for finding multiple zeros were developed, see. e.g., [5–13]. However, in most papers one assumes that the order of multiplicity is known. Procedures for the determination of exact value of multiplicity m and sufficiently close initial approximation x_0 were very seldom discussed in the literature. The knowledge of multiplicity m and a good initial approximation x_0 are two very important tasks and should be a composite part of any root-finder. The latter task was considered in some recent papers and books, see, for instance, [14–18].

Here we are concerned with generating iterative methods of higher order for solving nonlinear equations. More precisely, we study iterative methods for finding a multiple zero of a given function f when the order of multiplicity is unknown (Section 2). At the same time, we develop iterative methods for approximating multiplicity and prove their cubic convergence (Sections 3 and 4). Such approach, combined with fourth order two-point method for multiple zeros proposed in [7], provides the construction of an efficient algorithm for finding multiple zeros of very high accuracy, which is presented in Section 5. Throughout the text it is assumed that order of multiplicity is a positive integer. The case of fractional order is discussed in Section 7 and demonstrated on a numerical example.

It is worth noting that numerical experiments and the study of computational efficiency of considered root-finding methods based on convergence order and computational costs (see [19, p. 12]) are not often sufficient to give a real estimation of the quality of these methods and, consequently, their proper ranking. For this reason, a powerful tool for comparison and analysis of root-finding algorithms, using basins of attraction, is presented in Section 6 for six examples. This approach gives a much better insight into visualization in approximating function zeros, especially in regard to areas of convergence. The mentioned tools provide considerably better understanding of iterative processes.

Properties of the presented iterative methods are demonstrated on numerical examples in Section 7. Our main tools in developing and analyzing these methods are symbolic computation realized through several programs (implemented in computer algebra system *Mathematica*) and dynamic study by plotting basins of attraction for four methods and seven polynomials.

2. Generator of root-finders

Approximating zeros of a given scalar function f belongs to the most important problems appearing not only in applied mathematics but also in many disciplines of physics, finance, engineering branches, and so on. Solution of the mentioned task often requires from the user to combine numerical analysis and computing science, first of all symbolic computation (assuming, of course, the use of necessary computer hardware). During the last three centuries, many one-point methods were stated, such as Newton's, Halley's, Laguerre's, Chebyshev's method. Particular attention is due to the so-called the Traub–Schröder basic sequence (often called Schröder's family of the first kind, see [19,20]) and the Schröder–König sequence or Schröder's family of the second kind [20]. Both families explicitly depend on f and its $n-1$ derivatives and have the order at most n. The latter of these families will be considered in this section.

Let f be a given function with isolated zero α in some interval. If α is a zero of multiplicity m, then we have the representation $f(x) = (x-\alpha)^m p(x),\ p(\alpha) \neq 0$. An iterative method for approximating a single (simple or multiple zero) α will be written in the form $x_{k+1} = g(x_k)$, assuming that the initial approximation x_0 is known. The applied iterative method will produce the sequence $\{x_k\}$ that converges to the zero α if x_0 is reasonably close to α. Iterative methods for finding multiple zeros usually require the knowledge of order of multiplicity m, otherwise, many of them will converge only *linearly*. In this paper we mainly consider a class of methods for finding multiple zeros which do not require the multiplicity but their order of convergence is higher than 1.

We start with the following assertion proved in [21].