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The rate of multiplicity of the roots of nonlinear equations and its application to iterative methods

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ABSTRACT

Nonsimple roots of nonlinear equations present some challenges for classic iterative methods, such as instability or slow, if any, convergence. As a consequence, they require a greater computational cost, depending on the knowledge of the order of multiplicity of the roots. In this paper, we introduce dimensionless function, called *rate of multiplicity*, which estimates the order of multiplicity of the roots, as a dynamic global concept, in order to accelerate iterative processes. This rate works not only with integer but also fractional order of multiplicity and even with poles (negative order of multiplicity).

1. Introduction

Classic high order iterative methods for solving nonlinear equations in Banach spaces, such as Newton's, do not behave in an optimal way when they look for multiple roots. In fact, convergence of most of these methods (second order Newton's, third order Halley-like, and higher order ones), decay to first order when they approximate multiple roots [18]. This behavior leads to pathologies which range from minor troubles (greater computational cost), to severe difficulties (no convergence at all). Knowledge of the order of multiplicity of the roots makes it easier to deal with these difficulties.

Anomalous behavior of iterative methods when dealing with multiple roots is a well known fact at least since 19th century, when Schröder [17] devised a modification of Newton's method in order to preserve second order of convergence. More recently, Traub [18], Rall [16], Van de Vel [19] and many other authors studied this topic, proposing different ways to deal with nonsimple roots.

In [18], the author points out a link between the speed of convergence of Newton's method and the order of multiplicity of the sought root. There, he introduces an acceleration method based on extrapolation for Newton's method. Similar processes are introduced in [7,11,12,16], among others. Good surveys, including comparison of the performances of the algorithms when solving polynomial equations appear in [4,11].

On the other side, many equations arising from different topics such as complex variable, statistics (Lévy distributions), fractional calculus, with applications to economics, fractional diffusion or image processing, among others, have roots with noninteger multiplicity.

Fractional multiplicity provides computational challenges: typical methods to estimate the order of multiplicity become unstable, (those based on difference schemes, for example). A small error for this estimation may produce a loss of speed and accuracy in the process.

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Another context in which multiplicity becomes an important issue is that of poles, that is, negative multiplicity. Location of poles is often present in complex variable problems, and they must be carefully tracked due to the singularities they generate.

Convergence of nonlinear iterative methods, such as Newton's, does not behave uniformly for all the starting points: any given function has a stability region, where the optimal order of convergence is reached. Stability regions are included in, but they are not always equal to, the convergence domain, that is, there are intervals, where these methods converge but the order is not optimal. Thus, a method can evolve as slow as a first order method when the iterates are far from the root (in a similar way as if it were a multiple root), and with a high order convergence when iterates are close to the root (as in the presence of a simple root). Hence, by considering the multiplicity of the roots related to the stability region, it can be considered not as a static (constant) concept, as in classical analysis, but as a dynamic concept, like a function, depending on the distance to the root, and the derivatives of the nonlinear equation.

In this paper, we introduce the function *rate of multiplicity* of a root, related to the dynamic behavior of the iteration. This rate does not only analyze the theoretical properties of the function but it can also be used as an accelerator of the iteration. Though indicators, as defined in [4] based on [3] are closely related to first order rates of multiplicity, our definition is more general and can be used for accelerating higher order methods (such as Halley's and similar third order ones, or even higher than third order). Besides, they are useful for noninteger orders of multiplicity.

We will show examples connecting this rate to well known methods, and we will devise some new ones. The evaluation of the rate is more robust and stable than other older techniques. Furthermore, this will be a dimensionless function, hence scale invariant. Furthermore, dimensionless operators are easily adapted to general vector spaces such as systems of equations or Banach spaces.

This paper is organized as follows: in the next section we compare two different concepts of multiplicity, studying their properties. In Section 3 we review some methods for nonsimple roots. In Section 4 we introduce the rate of multiplicity with applications to iterative methods, which will be illustrated through examples in Section 5. Finally, we will draw conclusions in Section 6.

2. Multiplicity of the roots of a function

We begin by reminding the definition of multiplicity of the roots of functions. Although the results we present here can be generalized to complex domains, throughout this paper, we will consider $f(x)$ a real and continuous function defined in an interval $V \subset \mathbb{R}$. Besides, we assume x^* is an isolated root or pole of $f(x)$, that is, there exists an $\delta > 0$ such that x^* is the only root and pole in $[x^* - \delta, x^* + \delta] \subset V$.

Definition 1. x^* is a root of **order of multiplicity at least** m if there exist two constants $C > 0$, and $\varepsilon > 0$ such that $\left|\frac{f(x)}{(x-x^*)^m}\right| \le C$, for all $|x - x^*| < \varepsilon$.

The *exact* order of multiplicity is defined as the supreme of the orders of multiplicity, as follows:

Definition 2. x^* is a root of **exact order of multiplicity** m if there exist constants $C \ge c > 0$ and $\varepsilon > 0$ such that $c \le \left|\frac{f(x)}{(x-x^*)^m}\right| \le C$, for all $|x - x^*| < \varepsilon$.

If $f(x)$ is differentiable around x^*, the multiplicity is a positive integer or a rational $r = \frac{j}{2k+1}$ for j and k integers. In other cases, $f(x)$ must be complex valued at one side of x^* [19]. When multiplicity is positive and integer, these definitions, based on differentiability, are often useful:

Definition 3. $x^* \in \mathbb{R}$ is a root of $f(x) \in \mathcal{C}^m$ of **order of multiplicity at least** m if $f(x^*) = f'(x^*) = \cdots = f^{(m-1)}(x^*) = 0$.

And the corresponding,

Definition 4. x^* is a root of $f(x) \in \mathcal{C}^m$ **exact order of multiplicity** m if its multiplicity is at least m and $f^{(m)}(x^*) \neq 0$.

Both Definitions 2 and 4 are equivalent when $f(x)$ is differentiable and the order of multiplicity is a positive integer, but Definition 2 is more general and it allows noninteger or even negative orders of mutiplicity. The natural setting for these multiplicities is that of complex variable or fractional analysis but, under the required restrictions, such as considering one sided convergence, or Lipschitz continuity around x^*, it is possible to work in real domains.

Though in many mathematical models the equations are differentiable and, hence, their roots have a positive integer order of multiplicity, there are more and more practical models where noninteger (fractional) orders of multiplicities arise.

Due to nondifferentiability at x^* when its order of multiplicity is noninteger or negative, numerical approximation of these orders are challenging problems. Troubles arise from complex variable (negative multiplicities are related to poles in integer complex functions), and for noninteger orders we get additional problems from the fact that one important step of most extrapolation methods is rounding to the nearest integer.

In this paper we will deal with both, integer and fractional multiplicities. Therefore, we will define an algebra of orders of multiplicities as follows:

Theorem 1. *Let $f(x)$ be a differentiable function, and x^* an isolated root of real multiplicity m # 0 (not necessarily integer or positive). Then, these properties are verified:*