

An Algorithm That Localizes and Counts the Zeros of a C^2 -Function

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Abstract. We describe an algorithm that localizes the zeros of a given real C^2 -function f on an interval $[a, b]$. The algorithm generates a sequence of subintervals which contain a single zero of f . In particular, the exact number of zeros of f on $[a, b]$ can be determined in this way. Apart from f , the only additional input of the algorithm is an upper and a lower bound for f'' . We also show how the intervals determined by the algorithm can be further refined until they are contained in the basin of attraction of the Newton method for the corresponding zero.

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1. Introduction

A fundamental task, both in pure and in numerical analysis, is to localize and to count the zeros of a given function f in a certain region. For example the Argument Principle and Rouché's theorem for holomorphic functions allow to determine the number of zeros of f , counted with their multiplicity, in a bounded domain of \mathbb{C} with sufficiently regular boundary (see, e.g., [5] for an overview of methods used for analytic functions). In real analysis Sturm's theorem, a refinement of Descartes' Sign Rule and the Fourier-Budan theorem, allows to count the exact number of roots of a polynomial p with simple roots on a real interval (see, e.g., [3, 9, 10]). Several attempts have been made to transfer the method of Sturm to trigonometric polynomials: see [1, 7, 8]. The mentioned methods are restricted to holomorphic functions and polynomials, respectively. If we consider a function f which is merely continuous, the theorem of Bolzano yields the information that f has at least one zero on an interval $[a, b]$ if f has opposite signs at its endpoints. An iterative method to enclose all real zeros of a real function in an interval of minimal length has been discussed in [6]. Only recently, a method which counts the zeros of a function f under only mild regularity conditions on an interval

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$[a, b]$ has been proposed in [4]. In particular, if an L^∞ -bound on the second derivative of

$$\frac{f'^2 - f f''}{f^2 + f'^2}$$

is known, then the number of zeros of f can be computed by evaluating f , f' and f'' on a fine enough grid. In the present paper, we would like to present an algorithm which works for functions $f \in C^2([a, b])$ and which only requires an upper and a lower bound for f'' (see Section 3). The termination proof will be given in Section 4. This algorithm can in particular be used as a preconditioner for other algorithms like Newton's or Aitken's method to compute the zeros numerically (see Section 5). But first we need a refinement of Bolzano's theorem.

2. Refinement of Bolzano's theorem

We start from the following elementary observation:

Lemma 2.1. *Let $f, g \in C^2([a, b])$ be functions with $f(a) = g(a)$, $f(b) = g(b)$ and $f'' \leq g''$ on $[a, b]$. Then, we have $f \geq g$ on $[a, b]$.*

Proof. Let $h := g - f$. Then we have $h(a) = h(b) = 0$ and $h'' \geq 0$ on $[a, b]$. Hence, h is convex and therefore we conclude $h \leq 0$ on $[a, b]$. \square

Now we want to formulate a criterion which ensures that a function $f \in C^2([a, b])$ does *not* have a zero. To do so, we will use Lemma 2.1 with a comparison function g of constant second derivative. First, we note the following:

Lemma 2.2. *Let $g : [a, b] \rightarrow \mathbb{R}$ be the unique function g with $g(a) = \alpha$, $g(b) = \beta$ and $g'' = \gamma$ on $[a, b]$. Then we have*

$$\min g = \begin{cases} \frac{1}{2} \left(\alpha + \beta - \frac{\gamma}{4}(b-a)^2 - \frac{(\beta - \alpha)^2}{\gamma(b-a)^2} \right), & \text{if } \gamma(b-a)^2 > 2|\beta - \alpha|, \\ \min\{\alpha, \beta\}, & \text{otherwise.} \end{cases} \quad (2.1)$$

Proof. The proof is an elementary calculation. \square

As a consequence of Lemma 2.2 we now get:

Corollary 2.1. *Let $f \in C^2([a, b])$ be a function with $f(a) = \alpha > 0$, $f(b) = \beta > 0$ and $f'' \leq \gamma$ on $[a, b]$. If*

$$\gamma(b-a)^2 \leq 2|\beta - \alpha| \quad \text{or} \quad 4(\alpha + \beta) > \gamma(b-a)^2 + \frac{4}{\gamma} \left(\frac{\beta - \alpha}{b-a} \right)^2,$$

then f has no zero on $[a, b]$.