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# Verified Error Bounds for Double Roots of Nonlinear Equations

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**Abstract**— It is well known that it is an ill-posed problem to decide whether a function has a multiple root. For example, an arbitrarily small perturbation of a real polynomial may change a double real root into two distinct real or complex roots. In this paper we describe a computational method for the verified computation of a complex disc to contain exactly 2 roots of a univariate nonlinear function. The function may be given by some program. Computational results using INTLAB, the Matlab toolbox for reliable computing, demonstrate properties and limits of the method.

## 1. Introduction

It is well known that to decide whether a univariate polynomial has a multiple root is an ill-posed problem: An arbitrary small perturbation of a polynomial coefficient may change the answer from yes to no. In particular a real double root may change into two simple (real or complex) roots.

Therefore it is hardly possible to verify that a polynomial or a nonlinear function has a double root if not the entire computation is performed without any rounding error, i.e. using methods from Computer Algebra.

Let a suitably smooth nonlinear function $f : \mathbb{K} \to \mathbb{K}$ for $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$ be given with a numerically double root $\tilde{x}$. In a recent paper [8] we dealt with the problem as follows. We calculated an inclusion $X \in \mathbb{IK}$ such that a slightly perturbed function $g$ has a *true* double (or $k$-fold) root within $X$. Similar methods have been described in [1].

For real or complex polynomials we solved the problem in [7] in a different way. We presented ten methods to calculate a complex disc containing exactly or at least $k$ roots of the original polynomial. In the present paper we summarize how to treat the problem in the same way for double roots of general nonlinear functions. In a subsequent full paper methods for $k$-fold roots will be presented.

There is not much literature on this problem. In [3] Neumaier gives a sufficient criterion, namely that

$$|\Re\mathrm{e}\,\frac{f^{(k)}(z)}{k!}| > \sum_{i=0}^{k-1} |\frac{f^{(i)}(\tilde{z})}{i!}|\, r^{i-k} \qquad (1)$$

is satisfied for all $z$ in the disc $D(\tilde{z}, r)$. Under this condition he proves that $f$ has exactly $k$ roots in $D$. In our formulation we can omit the $(k-1)$-st summand on the right of (1), which is the first derivative in case of double roots, and we can derive a direct method for the inclusion. Moreover, we give a constructive scheme how to find a suitable disc $D$.

In [2] a general method for systems of nonlinear equations is described based on the topological degree. However, sometimes significant computational effort is needed.

## 2. Inclusion of 2 roots

Let a function $f : D_0 \to \mathbb{C}$ being analytic in the open disc $D_0$ be given. We suppose some $\tilde{x} \in D_0$ to be given such that $\tilde{x}$ is a numerically double root, i.e.

$$f(\tilde{x}) \approx 0 \approx f'(\tilde{x})\,. \qquad (2)$$

We first give a sufficient criterion for a certain disc $Y$ near $\tilde{x}$ to contain (at least) 2 roots of $f$.

The analytic function admits for $z, \tilde{z} \in D_0$ the Taylor expansion

$$f(z) = \sum_{\nu=0}^{\infty} c_\nu (z - \tilde{z})^\nu\,, \qquad (3)$$

where $c_\nu = \frac{1}{\nu!} f^{(\nu)}(\tilde{z})$ denote the Taylor coefficients. Let $X \subset D_0$ denote a real interval or complex closed disc near $\tilde{x}$ such that $f'(\hat{x}) = 0$ for some $\hat{x} \in X$. The assumption (2) implies that it is likely that there is a *simple* root of $f'$ near $\tilde{x}$, so that the corresponding $X$ can be computed by well-known verification routines [5]. Such a routine is implemented as Algorithm `verifynlss` in INTLAB, the Matlab toolbox for reliable computing ([6], see `http://www.ti3.tu-harburg.de/rump`).

We aim to prove that some closed disc $Y \subset D_0$ with $X \subseteq Y$ contains at least 2 roots of $f$.

We expand $f$ with respect to $\hat{x}$ and split the series into

$$\begin{aligned} f(y) &= f(\hat{x}) + \left(\tfrac{1}{2} f''(\hat{x}) + \textstyle\sum_{\nu=3}^{\infty} c_\nu (y-\hat{x})^{\nu-3}\right)(y-\hat{x})^2 \\ &=: f(\hat{x}) + g(y)(y-\hat{x})^2\,. \end{aligned} \qquad (4)$$

Note that $g$ is holomorphic in $D_0$, and that $c_1 = 0$ by assumption. Later we will see how to estimate $g(Y)$; for the moment we assume that an inclusion interval $G$ with $\{g(y) : y \in Y\} \subseteq G$ is known and $0 \notin G$. With this we can state the following theorem.

**Theorem 1** *Let holomorphic $f : D_0 \to \mathbb{C}$ in the open disc $D_0$ be given, and closed discs $X, Y \subset D_0$ with $X \subseteq Y$. Assume there exists $\hat{x} \in X$ with $f'(\hat{x}) = 0$. Define $g(y)$ as in (4) and let $G \in \mathbb{IC}$ be a complex interval with $g(y) \in G$ for all $y \in Y$. Assume $0 \notin G$, and define the two functions $N_{1,2} : Y \to \mathbb{C}$ by*

$$N_{1,2}(y) := \hat{x} \pm \sqrt{-f(\hat{x})/g(y)}\,. \tag{5}$$

*Assume*

$$N_\nu(Y) \subseteq Y \quad \text{for} \;\; \nu = 1, 2\,. \tag{6}$$

*Then, counting multiplicities, the function $f$ has at least two roots in $Y$.*

Proof. Since $g(y) \neq 0$ for $y \in Y$ both $N_{1,2}$ are continuous functions. Complex intervals are non-empty, convex, closed and bounded, so Brouwer's Fixed Point Theorem and (6) imply the existence of $y_{1,2} \in Y$ with $N_\nu(y_\nu) = 0$ or

$$(y_\nu - \hat{x})^2 = -f(\hat{x})/g(y_\nu) \quad \text{for} \;\; \nu = 1, 2\,. \tag{7}$$

Now (4) implies

$$0 = f(\hat{x}) + g(y_\nu)(y_\nu - \hat{x})^2 = f(y_\nu) \quad \text{for} \;\; \nu = 1, 2\,. \tag{8}$$

If $y_1 \neq y_2$, the assertion follows. If $y_1 = y_2$, then (5) implies $f(\hat{x}) = 0 = f'(\hat{x})$, so that $y_1 = y_2$ is a double root of f. The theorem is proved. □

The main assumption to check in Theorem 1 is (6). This, however, can be performed directly by interval evaluation noting that for all $x \in X$ and for all $y \in Y$

$$N_{1,2}(y) \in X \pm \sqrt{-f(X)/g(Y)}\,. \tag{9}$$

Concerning the computation of $g(Y)$ one can show that

$$g(Y) \subseteq X + \{z \in \mathbb{C} : |z| \leq \frac{1}{2} diam(Y)^2 |f''(Y)|\}\,.$$

Note that the diameter of this inclusion is proportional to the square of the diameter of $Y$, so in general we may expect a good quality.

Theorem 1 proves existence of at least 2 roots of $f$ in $Y$. It remains the problem to find a suitable inclusion interval $Y$. Note that necessarily the inclusion interval is complex: If the assumptions of Theorem 1 are satisfied for some function $f$, they are by continuity satisfied for a suitably small perturbation of $f$ as well. But an arbitrary small perturbation of $f$ may move a double real root into two complex roots.

Since $\hat{x} \in X$ is necessary by assumption, a starting interval may be $Y^0 := X$. However, the sensitivity of a double root is $\varepsilon^{1/2}$ for an $\varepsilon$-perturbation of the coefficients. But the quality of the inclusion $X$ of the *simple* root of $f'$ can be expected to be nearly machine precision.

The functions $N_\nu$ in (5) represent a Newton step. Thus a suitable candidate for a first inclusion interval is $Y^{(0)} := X \pm \sqrt{-f(X)/g(X)}$ in (9). This already defines an iteration scheme, where $Y^{m+1} \subset \mathrm{int}(Y^m)$ verifies the conditions of Theorem 1.

Table 1: Radius of inclusion for nearby root.

| e | rad(Y) | iter |
|---|---|---|
| $10^{-1}$ | $1.74 \cdot 10^{-7}$ | 1 |
| $10^{-2}$ | $5.59 \cdot 10^{-7}$ | 1 |
| $10^{-3}$ | $1.93 \cdot 10^{-6}$ | 1 |
| $10^{-4}$ | $5.71 \cdot 10^{-6}$ | 1 |
| $10^{-5}$ | $1.71 \cdot 10^{-5}$ | 1 |
| $10^{-6}$ | failed | 5 |

However, it is superior for such an interval iteration to slightly "blow-up" the intervals. This process is called "epsilon-inflation". The term was coined in [4] and the process was analyzed over there. Thus we define the iteration as follows:

$$\begin{aligned}
&Y := X \\
&\text{repeat} \\
&\quad Z := Y \circ \epsilon \\
&\quad Y := X \pm \sqrt{-f(X)/g(Y)} \\
&\text{until } Y \subset \mathrm{int}(Z)
\end{aligned} \tag{10}$$

Here $Y \circ \epsilon$ denotes a slight relative and absolute inflation. We use $Z := Y \cdot (1 \pm 10^{15}) \pm 10^{-324}$, where the constants are adapted to IEEE 754 double precision with relative precision $10^{-16}$.

## 3. Computational results

We briefly report some computational result. Consider

$$f(x) := (3x-2)^2 sin(x) = (9xsin(x) - 12sin(x))x + 4sin(x)\,. \tag{11}$$

The expansions are generated by the symbolic toolbox of Matlab. First we use the method described in [8]. It is satisfied that a function

$$\tilde{f}(x) := f(x) + \varepsilon \qquad \text{with} \qquad |\varepsilon| < 1.3 \cdot 10^{-31} \tag{12}$$

has a precise double root in the interval

$$X1 := [0.66666666666666, 0.66666666666667]\,. \tag{13}$$

Using Theorem 1 it is verified that two roots of the original function $f$ are enclosed in

$$X2 := \{z \in \mathbb{C} : |z - 0.66666666666667| < 10^{-14}\}\,. \tag{14}$$

Next we test the influence of the nearness of another root to a multiple root. Consider $f(x) := (3x-2)^2 sin(x)(x - \frac{2}{3} + e)$ for different values of $e := 10^{-k}$. There is a double root $\frac{2}{3}$ and a nearby simple root $\frac{2}{3} - e$. An increase of the radius and thus decrease of accuracy can be observed in Table 1 when another root approaches the cluster.

This effect becomes worse when two clusters are near each other. Consider $f(x) := (3x-2)^2 sin(x)(x - \frac{2}{3} + e)^2$

Table 2: Radius of inclusion for nearby double root.

| e | rad(Y) | iter |
|---|---|---|
| $10^{-1}$ | $1.16 \cdot 10^{-6}$ | 1 |
| $10^{-2}$ | $1.30 \cdot 10^{-5}$ | 1 |
| $9 \cdot 10^{-3}$ | $1.29 \cdot 10^{-6}$ | 1 |
| $8 \cdot 10^{-3}$ | $1.67 \cdot 10^{-5}$ | 1 |
| $7 \cdot 10^{-3}$ | $1.60 \cdot 10^{-5}$ | 1 |
| $6 \cdot 10^{-3}$ | $2.10 \cdot 10^{-5}$ | 1 |
| $5 \cdot 10^{-3}$ | $2.39 \cdot 10^{-5}$ | 1 |
| $4 \cdot 10^{-3}$ | $2.90 \cdot 10^{-5}$ | 1 |
| $3 \cdot 10^{-3}$ | $3.63 \cdot 10^{-5}$ | 3 |
| $2 \cdot 10^{-3}$ | failed | 5 |

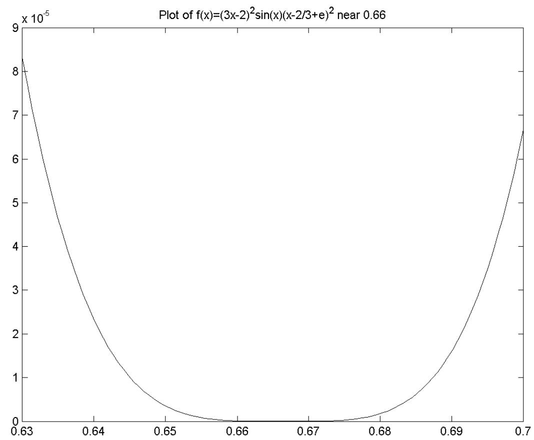


Figure 1: Plot near first and second double root.

for different values of $e$. There is a double root $\frac{2}{3}$ and a nearby double root $\frac{2}{3} - e$. For the inclusion, as before, we used the expanded version of this function, which is in this case $f(x) = 81 \sin(x) x^4 - 216 \sin(x) x^3 + 54 \sin(x) x^3 e + 216 \sin(x) x^2 - 108 \sin(x) x^2 e + 9 \sin(x) x^2 e^2 - 96 \sin(x) x + 72 \sin(x) xe - 12 \sin(x) xe^2 + 16 \sin(x) - 16 \sin(x) e + 4 \sin(x) e^2$. As can be seen in Table 2 the inclusion fails when the difference between the two clusters becomes 0.002 or smaller.

One may ask, why the algorithm fails for the distance 0.002. In Figure 1 we display the function plot near both triple roots. As can be seen it seems not easy to separate the two clusters numerically. In Figure 2 we show the behavior of the function near the individual double roots. Here it becomes clear that we basically see roundoff errors because of the numerical instability. Concerning the lengthy expression of the function we expect some overestimation due to interval arithmetic. In that sense the achieved results seem not bad.

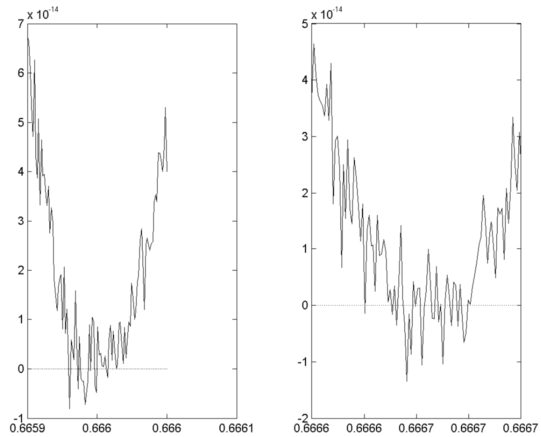


Figure 2: Individual plots near first and second double root.

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