# Verified computation of a dise containing exactly $k$ roots of a univariate nonlinear function 

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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 $k$ 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.


Key Words : nonlinear equations, double roots, multiple roots, verification, error bounds, INTLAB

## 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 $f: \mathbb{K} \rightarrow \mathbb{K}$ for $\mathbb{K} \in\{\mathbb{R}, \mathbb{C}\}$ be given with a numerically $k$-fold root $\tilde{x}$. In a recent paper [10] we dealt with the problem as follows. We calculated an inclusion $X \in \mathbb{K} \mathbb{K}$ such that a slightly perturbed function $g$ has a true $k$-fold root within $X$. Moreover, an inclusion of the amount of the perturbation is calculated. In this paper we also demonstrated a similar method for double roots of a system of nonlinear equations.

For real or complex polynomials we solved the problem in [9] 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 treat the problem in the same way for general nonlinear functions.

There is not much literature on this problem. In [5] Neumaier gives a similar sufficient criterion, namely that

$$
\begin{equation*}
\left|\mathfrak{R e} \frac{f^{(k)}(z)}{k!}\right|>\sum_{i=0}^{k-1}\left|\frac{f^{(i)}(\tilde{z})}{i!}\right| r^{i-k} \tag{1}
\end{equation*}
$$

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), and we present sharper expressions for the left hand side in (14), (15) and (25). Moreover, we give a constructive scheme how to find a suitable disc $D$.

In [3] 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 $f: D_{0} \rightarrow \mathbb{C}$ 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. $\left|f^{\prime \prime}(\tilde{x})\right| \gg 0$ and

$$
\begin{equation*}
f(\tilde{x}) \approx 0 \approx f^{\prime}(\tilde{x}) \tag{2}
\end{equation*}
$$

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

$$
\begin{equation*}
f(z)=\sum_{v=0}^{\infty} c_{\nu}(z-\tilde{z})^{v} \tag{3}
\end{equation*}
$$

where $c_{v}=\frac{1}{v!} f^{(v)}(\tilde{z})$ denote the Taylor coefficients. Let $X \subset D_{0}$ denote a real interval or complex closed disc near $\tilde{x}$ such that $f^{\prime}(\hat{x})=0$ for some $\hat{x} \in X$. The assumption (2) implies that it is likely that there is a simple root of $f^{\prime}$ near $\tilde{x}$, so that the corresponding $X$ can be computed by well-known verification routines [7]. Such a routine is implemented as Algorithm verifynlss in INTLAB, the Matlab toolbox for reliable computing ([8], 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

$$
\begin{align*}
f(y) & =f(\hat{x})+\left(\frac{1}{2} f^{\prime \prime}(\hat{x})+\sum_{v=3}^{\infty} c_{v}(y-\hat{x})^{v-2}\right)(y-\hat{x})^{2}  \tag{4}\\
& =: f(\hat{x})+g(y)(y-\hat{x})^{2} .
\end{align*}
$$

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 $f: D_{0} \rightarrow \mathbb{C}$ 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 $f^{\prime}(\hat{x})=0$. Define $g(y)$ as in (4) and let $G \in \mathbb{I C}$ be a complex interval with $g(y) \in G$ for all $y \in Y$. Assume $0 \notin G$, and define the two functions $N_{1,2}: Y \rightarrow \mathbb{C}$ by

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

Assume

$$
\begin{equation*}
N_{v}(Y) \subseteq Y \quad \text { for } \quad v=1,2 \tag{6}
\end{equation*}
$$

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 $N_{v}\left(y_{v}\right)=y_{v}$ or

$$
\begin{equation*}
\left(y_{v}-\hat{x}\right)^{2}=-f(\hat{x}) / g\left(y_{v}\right) \text { for } v=1,2 . \tag{7}
\end{equation*}
$$

Now (4) implies

$$
\begin{equation*}
0=f(\hat{x})+g\left(y_{v}\right)\left(y_{v}-\hat{x}\right)^{2}=f\left(y_{v}\right) \quad \text { for } v=1,2 . \tag{8}
\end{equation*}
$$

If $y_{1} \neq y_{2}$, the assertion follows. If $y_{1}=y_{2}$, then (5) implies $f(\hat{x})=0$, so that $\hat{x}$ is a double root of $f$. The theorem is proved.

Theorem 1 proves existence of at least 2 roots of $f$ in $Y$. In the next section we show how to verify existence of exactly $k$ roots of a function in a disc $Y$.

## 3. Inclusion of exactly $k$ roots

Let again a function $f: D_{0} \rightarrow \mathbb{C}$ analytic in the open disc $D_{0}$ be given. Now we suppose some $\tilde{x} \in D_{0}$ be given such that $\tilde{x}$ is a numerically $k$-fold zero, i.e.

$$
\begin{equation*}
f^{(v)}(\tilde{x}) \approx 0 \text { for } 0 \leq v<k \tag{9}
\end{equation*}
$$

Note that this is not a mathematical assumption to be verified. As in the previous section we will give a sufficient criterion for a certain disc $D$ near $\tilde{x}$ to contain exactly $k$ roots of $f$. If the derivatives are too large in absolute value, then it is less likely that the criterion is satisfied. All assertions are true for any $\tilde{x} \in D_{0}$.

As before the analytic function admits for $z, \tilde{z} \in D_{0}$ the Taylor expansion (3). Now let $X \subset D_{0}$ denote a real interval or complex closed disc near $\tilde{x}$ such that $f^{(k-1)}(\hat{x})=0$ for some $\hat{x} \in X$. The assumptions imply that likely there is a simple root $\hat{x}$ of $f^{(k-1)}$ near $\tilde{x}$, and the corresponding $X$ can be computed as before by Algorithm verifynlss in INTLAB ([8].

Now we aim to prove that some closed disc $Y \subset D_{0}$ with $X \subseteq Y$ contains exactly $k$ roots of $f$.
We expand $f$ with respect to $\hat{x}$ and split the series into

$$
\begin{equation*}
f(y)=q(y)+g(y)(y-\hat{x})^{k} \quad \text { and } \quad g(y)=c_{k}+e(y) \tag{10}
\end{equation*}
$$

with

$$
\begin{equation*}
q(y)=\sum_{\nu=0}^{k-2} c_{\nu}(y-\hat{x})^{\nu} \quad \text { and } \quad e(y)=\sum_{\nu=k+1}^{\infty} c_{\nu}(y-\hat{x})^{v-k} . \tag{11}
\end{equation*}
$$

Note that $g$ is holomorphic in $D_{0}$, and that $c_{k-1}=0$ by assumption. The minimum of $|g(y)|$ on $Y$ can be estimated by the maximum of the remainder term $|e(y)|$. This is possible by the following version of a complex Mean Value Theorem due to Darboux ${ }^{1}$.

Theorem 2 Let holomorphic $f: D_{0} \rightarrow \mathbb{C}$ in the open disc $D_{0}$ be given and $a, b \in D_{0}$. Then for $1 \leq p \leq k+1$ there exists $0 \leq \Theta \leq 1$ and $\omega \in \mathbb{C},|\omega| \leq 1$ such that for $h:=b-a$ and $\xi:=a+\Theta(b-a)$

$$
\begin{equation*}
f(b)=\sum_{v=0}^{k} \frac{h^{v}}{v!} f^{(v)}(a)+\omega \frac{h^{k+1}}{k!} \frac{(1-\Theta)^{k-p+1}}{p} f^{(k+1)}(\xi) . \tag{12}
\end{equation*}
$$

The following proof is due to F. Bünger [1]. For $a=b$ the assertion is trivial, so henceforth we assume $a \neq b$. We first set $\ell:=|b-a|$ and define a function $g:[0, \ell] \rightarrow a \underline{\cup} b$ by $g(t):=a+t \frac{b-a}{\ell}$. Then $\left|g^{\prime}(t)\right|=\frac{|b-a|}{\ell} \equiv 1$. For

$$
F(x):=\sum_{v=0}^{k} \frac{(b-x)^{v}}{v!} f^{(v)}(x)
$$

we obtain

$$
\begin{aligned}
F^{\prime}(x)=f^{\prime}(x)+\sum_{v=1}^{k} & -\frac{(b-x)^{v-1}}{(v-1)!} f^{(v)}(x)+\frac{(b-x)^{v}}{v!} f^{(v+1)}(x) \\
& =\frac{(b-x)^{k}}{k!} f^{(k+1)}(x)
\end{aligned}
$$

With this we obtain for $1 \leq p \leq k+1$

$$
\begin{aligned}
& |F(b)-F(a)|=|F(g(\ell))-F(g(0))|=\left|\int_{0}^{\ell}(F \circ g)^{\prime}(t) d t\right| \\
& \leq \int_{0}^{\ell}\left|F^{\prime}(g(t))\right|\left|g^{\prime}(t)\right| d t=\int_{0}^{\ell}\left|\frac{|b-g(t)|^{k}}{k!} \| f^{(k+1)}(g(t))\right| d t \\
& \quad=\int_{0}^{\ell} \frac{(\ell-t)^{k}}{k!p(\ell-t)^{p-1}}\left|f^{(k+1)}(g(t))\right| p(\ell-t)^{p-1} d t
\end{aligned}
$$

[^0]\[

$$
\begin{gathered}
\leq \frac{\left(\ell-t^{*}\right)^{k-p+1}}{k!p}\left|f^{(k+1)}\left(g\left(t^{*}\right)\right)\right| \int_{0}^{\ell}\left(-(\ell-t)^{p}\right)^{\prime} \\
\quad=\frac{\left(\ell-t^{*}\right)^{k-p+1} \ell^{p}}{k!p}\left|f^{(k+1)}\left(g\left(t^{*}\right)\right)\right|
\end{gathered}
$$
\]

for some $t^{*} \in[0, \ell]$, where we used $\left|g^{\prime}(t)\right| \equiv 1$ and $|b-g(t)|=\ell-t$. The last expression is equal to

$$
\frac{e^{k+1}(1-\Theta)^{k-p+1}}{k!p}\left|f^{(k+1)}(a+\Theta(b-a))\right|
$$

so that there exists complex $\omega$ with $|\omega| \leq 1$ and

$$
\begin{aligned}
& f(b)-f(a)-\sum_{v=1}^{k} \frac{(b-a)^{v}}{v!} f^{(v)}(a)=F(b)-F(a) \\
= & -\omega \frac{(b-a)^{k+1}}{k!} \frac{(1-\Theta)^{k-p+1}}{p}\left|f^{(k+1)}(a+\Theta(b-a))\right|
\end{aligned}
$$

Using interval arithmetic we can evaluate an inclusion of $c_{k}=\frac{1}{k!} f^{(k)}(\hat{x})$. In fact in the new version of INTLAB [8] there will be a Taylor toolbox which allows easy and fast computation of Taylor coefficients, approximately as well an inclusion for some real or complex interval argument.
Using Theorem 2 we can estimate the remainder term $e(y)$ as well. Note that there is some freedom to choose $p$. The choice $p=k+1$ gives the traditionally looking expansion

$$
f(b)=\sum_{v=0}^{k} \frac{h^{v}}{v!} f^{(v)}(a)+\omega \frac{h^{k+1}}{(k+1)!} f^{(k+1)}(\xi)
$$

so that we obtain

$$
\begin{equation*}
|e(y)| \leq \frac{|b-a|}{(k+1)!} \max _{z \in \partial Y}\left|f^{(k+1)}(z)\right| \quad \forall y \in Y \tag{13}
\end{equation*}
$$

For $p=k$ we may split the interval for $\Theta$ and obtain $|e(y)| \leq \max \left(\beta_{1}, \beta_{2}\right)$ with

$$
\begin{equation*}
\beta_{1}:=\frac{|b-a|}{k!} \max _{|y-x| \leq \frac{5}{2}}\left|f^{(k+1)}(y)\right| \tag{14}
\end{equation*}
$$

and

$$
\begin{equation*}
\beta_{2}:=\frac{|b-a|}{2 k!} \max _{|y-x| \leq r}\left|f^{(k+1)}(y)\right| \tag{15}
\end{equation*}
$$

where $r:=\max _{y \in Y}|y-\hat{x}|$. By the definition (10) this gives a computable lower bound for $|g(y)|$.
Let a polynomial $P(z) \in \mathbb{C}[z]$ with $P(z)=\sum_{v=0}^{n} p_{v} z^{\nu}$ be given with $p_{n} \neq 0$. The Cauchy polynomial $C(P)$ with respect to $P$ is defined by $C(P):=\left|p_{n} x^{n}\right|-\sum_{v=0}^{n-1}\left|p_{v}\right| x^{\nu} \in \mathbb{R}[x]$. By Descartes' rule of sign $C(P)$ has exactly one non-negative root, called the Cauchy-bound $\overline{C(P)}$. It is well known that the Cauchy bound is an upper bound for the absolute value of all (real and complex) roots of P :

$$
\begin{equation*}
P(z)=0 \Rightarrow|z| \leq \overline{C(P)} . \tag{16}
\end{equation*}
$$

In fact is the best upper bound taking only the absolute values $\left|p_{v}\right|$ into account. Note that the leading coefficient $p_{n}$ must be nonzero.

The Cauchy-bound can be defined for interval polynomials as well. For $\mathfrak{P}(z) \in \mathbb{K} \mathbb{K}[z]$ with $\mathfrak{P}(z)=\sum_{v=0}^{n} \mathfrak{p}_{v} z^{v}$ and $\mathfrak{p}_{v} \in \mathbb{I} \mathbb{K}$ define

$$
\begin{equation*}
C(\mathfrak{P}):=\operatorname{mig}\left(\mathfrak{p}_{n}\right) x^{n}-\sum_{v=0}^{n-1} \operatorname{mag}\left(\mathfrak{p}_{v}\right) x^{\nu} \in \mathbb{R}[x], \tag{17}
\end{equation*}
$$

where $\operatorname{mig}\left(\mathfrak{p}_{n}\right):=\min \left\{|\pi|: \pi \in \mathfrak{p}_{n}\right\}$ and $\operatorname{mag}\left(\mathfrak{p}_{v}\right):=\max \left\{|\pi|: \pi \in \mathfrak{p}_{v}\right\}$. Then the unique non-negative root $\overline{C(\mathcal{P})}$ of $C(\mathfrak{P})$ is a root bound for all polynomials $P \in \mathfrak{P}$ :

$$
\begin{equation*}
P \in \mathfrak{P} \text { and } P(z)=0 \Rightarrow|z| \leq \overline{C(\mathfrak{P})} \tag{18}
\end{equation*}
$$

The Cauchy-bound for real or complex interval polynomials is easily bounded from above by applying few Newton iterations on $C(\mathfrak{P})$ starting at some other traditional root bound. Note that the iteration converges quickly to $\overline{C(\mathfrak{P})}$.

With these definitions we can state our main result.
Theorem 3 Let holomorphic $f: D_{0} \rightarrow \mathbb{C}$ in the open disc $D_{0}$ and fixed $k \in \mathbb{N}$ be given, and closed discs $X, Y \subset D_{0}$ with $X \subseteq Y$. Assume there exists $\hat{x} \in X$ with $f^{(k-1)}(\hat{x})=0$. Define $g(y)$ as in (10), and let $G \in \mathbb{I} \mathbb{C}$ be a complex interval with $g(y) \in G$ for all $y \in Y$. Assume $0 \notin G$, and define the interval polynomial

$$
\begin{equation*}
\mathfrak{P}(z):=q(z)+G \cdot(z-\hat{x})^{k} \in \mathbb{I} \mathbb{C}[z] . \tag{19}
\end{equation*}
$$

Denote the closed complex disc with center $m$ and radius $r$ by $D(m ; r)$. Assume that the Cauchy-bound $\overline{C(\mathfrak{P})}$ for $\mathfrak{P}$ satisfies

$$
\begin{equation*}
D(\hat{x} ; \overline{C(\mathfrak{P})}) \subset \operatorname{int}(Y) . \tag{20}
\end{equation*}
$$

Then, counting multiplicities, there are exactly $k$ roots of the function $f$ in $D(\hat{x} ; \overline{C(\mathfrak{P})})$.
Proof. Define the parameterized set of polynomials

$$
\begin{equation*}
P_{y}(z):=q(z)+g(y)(z-\hat{x})^{k} \in \mathbb{C}[z] . \tag{21}
\end{equation*}
$$

Note that only the leading term depends on the parameter $y$. By definition (10) we have $f(y)=P_{y}(y)$. Moreover, $P_{y} \in \mathfrak{P}$ for all $y \in Y$, so that $g(y) \neq 0$ and (18) imply that $P_{y}(z)=0$ is only possible for $z \in D(\hat{x} ; \overline{C(\mathfrak{P})})$. Thus (20) implies for all $y \in Y$ that $P_{y}(z) \neq 0$ for all $z \in \partial Y$.

Next define

$$
\begin{equation*}
P_{y, t}(z):=t \cdot q(z)+g(y)(z-\hat{x})^{k} \tag{22}
\end{equation*}
$$

and the homotopy function

$$
\begin{equation*}
h_{t}(y):=P_{y, t}(y)=t \cdot q(y)+g(y)(y-\hat{x})^{k} . \tag{23}
\end{equation*}
$$

Since $q$ is a polynomial and $g$ is holomorphic, all functions $h_{t}$ are holomorphic as well. The definition of the Cauchy-bound implies

$$
\begin{equation*}
\overline{C\left(P_{y, t}\right)} \leq \overline{C\left(P_{y}\right)} \leq \overline{C(\mathfrak{P})} \tag{24}
\end{equation*}
$$

for all $t \in[0,1]$ and all $y \in Y$. Thus definition (23) implies that for all $t \in[0,1]$ we have $h_{t}(y) \neq 0$ for all $y \in \partial Y$. We conclude that all holomorphic functions $h_{t}$ must have the same number of roots in $Y$, in particular $h_{0}$ and $h_{1}$.

For $t=0$ we have $h_{0}(y)=g(y)(y-\hat{x})^{k}$ which has exactly $k$ roots in $Y$ because $g(y) \neq 0$ for all $y \in Y$. Hence

$$
h_{1}(y)=q(y)+g(y)(y-\hat{x})^{k}=P_{y}(y)=f(y)
$$

must have exactly $k$ roots in $Y$. By (24) for all $t \in[0,1]$ and all $y \in Y$, all roots of $P_{y, t}(z)$ lie in $D(\hat{x} ; \overline{C(\mathfrak{P})})$, so in particular the roots of $f$. This concludes the proof.

From a computational point of view the quality of the bound depends directly on the lower bound on $|g(Y)|$, so by (10) on the lower bound of $c_{k}=\frac{1}{k!} f^{(k)}(\hat{x}) \in \frac{1}{k!} f^{(k)}(X)$. The direct computation of $\frac{1}{k!} f^{(k)}(X)$ by interval arithmetic can be improved by observing

$$
\begin{equation*}
c_{k} \in \frac{1}{k!} f^{(k)}(\tilde{x})+\frac{1}{(k+1)!} f^{(k+1)}(X) \cdot(X-\tilde{x}) \tag{25}
\end{equation*}
$$

for any $\tilde{x} \in X$. A suitable choice is a point $\tilde{x}$ near the midpoint of $X$.
It remains the problem to find a suitable inclusion interval $Y$. Note that necessarily the inclusion interval is complex: If the assumptions of Theorem 3 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 $k$-fold root is $\varepsilon^{1 / k}$ for an $\varepsilon$-perturbation of the coefficients, which is seen as follows.

For analytic $f$ with $k$-fold root $\hat{x}$, define $\tilde{f}(x):=f(x)-\epsilon$ for some small $\epsilon$. This represents in some way the inevitable presence of rounding errors in numerical computations. By continuity, for small enough $\epsilon$ there is small $h$ with $\tilde{f}(\hat{x}+h)=0$, so that

$$
\begin{equation*}
0=-\epsilon+c_{k} h^{k}+O\left(h^{k+1}\right) \tag{26}
\end{equation*}
$$

using the Taylor expansion $f(\hat{x}+h)=\sum c_{\nu} f^{(v)}(\hat{x}) h^{\nu}$. Thus $h$, the sensitivity of the $k$-fold root $\hat{x}$ with respect to an $\epsilon$-perturbation of the original function, is of the order $\left(\epsilon / c_{k}\right)^{1 / k}$ for small $\epsilon$.

However, the quality of the inclusion $X$ of the simple root of $f^{(k-1)}$ can be expected to be nearly machine precision.

The polynomial in (19) depends on $Y$, denote it by $\mathfrak{P}_{Y}$. The main condition to check is (20). Thus a suitable candidate for a first inclusion interval is $Y^{1}:=D\left(\hat{x} ; \overline{C\left(\mathfrak{P}_{Y^{0}}\right)}\right)$. This already defines an iteration scheme, where $Y^{m+1} \subset \operatorname{int}\left(Y^{m}\right)$ verifies the conditions of Theorem 3.

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 [6] and the process was analyzed over there. Thus we define the iteration as follows:

$$
\begin{align*}
& Y:=X \\
& \text { repeat } \\
& \qquad Z:=Y \circ \epsilon  \tag{27}\\
& \qquad Y:=D\left(\hat{x} ; \overline{C\left(P_{Z}\right)}\right) \\
& \text { until } Y \subset \operatorname{int}(Z)
\end{align*}
$$

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

## 4. Computational Results

In this section we present some computational results. All computations are performed in IEEE 754 double precision which means a relative precision of $\varepsilon:=2^{-53} \approx 10^{-16}$.

First we expand $f_{k}(x):=(3 x-2)^{k} \sin (x)$ for different values of $k$. The function has a $k$-fold root $\hat{x}=\frac{2}{3}$. For example,

$$
f_{3}(x)=-8 \sin (x)+(36 \sin (x)+(-54 \sin (x)+27 \sin (x) x) x) x .
$$

The expansions are generated by the symbolic toolbox of Matlab [4]. In the following Table I we display the radius of the inclusion interval as well as the sensitivity $\varepsilon^{1 / k}$ of the $k$-fold root $\frac{1}{3}$ for different values of $k$, and the number of interval iterations in (27). The initial approximation $\tilde{x}=0.66$ is first improved by some Newton steps.

Table I. Radius of inclusion for different multiplicities.

| $k$ | $\operatorname{rad}(Y)$ | $\varepsilon^{1 / k}$ | iter |
| ---: | :---: | :---: | :---: |
| 1 | $4.44 \cdot 10^{-16}$ | $1.11 \cdot 10^{-16}$ | 1 |
| 2 | $2.19 \cdot 10^{-8}$ | $1.05 \cdot 10^{-8}$ | 1 |
| 3 | $9.48 \cdot 10^{-6}$ | $4.81 \cdot 10^{-6}$ | 1 |
| 4 | $1.82 \cdot 10^{-4}$ | $1.03 \cdot 10^{-4}$ | 1 |
| 5 | $1.06 \cdot 10^{-3}$ | $6.44 \cdot 10^{-4}$ | 1 |
| 10 | $4.02 \cdot 10^{-2}$ | $2.54 \cdot 10^{-2}$ | 1 |
| 15 | $1.39 \cdot 10^{-1}$ | $8.64 \cdot 10^{-2}$ | 1 |
| 20 | $2.74 \cdot 10^{-1}$ | $1.59 \cdot 10^{-1}$ | 1 |

As can be seen the radius of the inclusion interval corresponds nicely to the sensitivity of the root. For a simple root almost maximum accuracy is achieved. In all examples only one interval iteration (27) is necessary. Note that the nearest other roots of $f_{k}$ are 0 and $\pi / 2$.

Next we test the influence of the nearness of another root to a multiple root. Consider $f(x):=(3 x-$ $2)^{3} \sin (x)\left(x-\frac{2}{3}+e\right)$ for different values of $e:=10^{-k}$. There is a triple root $\frac{2}{3}$ and a nearby root $\frac{2}{3}-e$.

An increase of the radius and thus decrease of accuracy can be observed in Table II when another root approaches the cluster. This effect becomes worse when two clusters are near each other.

Table II. Radius of inclusion for nearby root.

| $e$ | $\operatorname{rad}(Y), k=3$ | iter | $\operatorname{rad}(Y), k=4$ | iter |
| :---: | :---: | :---: | :---: | :---: |
| $10^{-2}$ | $4.74 \cdot 10^{-5}$ | 1 | $7.48 \cdot 10^{-3}$ | 1 |
| $10^{-3}$ | $1.11 \cdot 10^{-4}$ | 1 | $7.51 \cdot 10^{-4}$ | 1 |
| $10^{-4}$ | $2.08 \cdot 10^{-4}$ | 1 | $1.86 \cdot 10^{-4}$ | 1 |
| $10^{-5}$ | $4.71 \cdot 10^{-4}$ | 1 | $1.78 \cdot 10^{-4}$ | 1 |
| $10^{-6}$ | $9.64 \cdot 10^{-4}$ | 1 | $1.84 \cdot 10^{-4}$ | 1 |
| $10^{-7}$ | failed | 3 | $1.90 \cdot 10^{-4}$ | 1 |
| $10^{-8}$ | failed | 3 | $1.80 \cdot 10^{-4}$ | 1 |
| $10^{-9}$ | failed | 3 | $1.79 \cdot 10^{-4}$ | 1 |
| $10^{-10}$ | failed | 3 | $1.81 \cdot 10^{-4}$ | 1 |

However, when the cluster at $\frac{2}{3}$ and the extra root $\frac{2}{3}-e$ are too close, they may be regarded as one cluster. As can be seen in Table II, the inclusion of four roots as one cluster is achieved in a wide range.

If the distance is too large, however, the quality of the inclusion must deteriorate. Note that the radius of the enclosing disc is displayed, so for example the radius $7.48 \cdot 10^{-3}$ of the inclusion in the first line for $e=10^{-2}$ is not too far from the optimal radius $5 \cdot 10^{-3}$.

The final Table III shows the results for $f(x):=(3 x-2)^{3} \sin (x)\left(x-\frac{2}{3}+e\right)^{3}$ for different values of $e:=k \cdot 10^{-2}$, so that we have two triple roots $\frac{2}{3}$ and $\frac{2}{3}-e$.

Table III. Radius of inclusion for nearby cluster.

| $e$ | $\operatorname{rad}(Y), k=3$ | iter | $\operatorname{rad}(Y), k=6$ | iter |
| :---: | :---: | :---: | :---: | :---: |
| $5 \cdot 10^{-2}$ | $2.35 \cdot 10^{-4}$ | 1 | $4.93 \cdot 10^{-2}$ | 1 |
| $4 \cdot 10^{-2}$ | $3.28 \cdot 10^{-4}$ | 1 | $3.94 \cdot 10^{-2}$ | 1 |
| $3 \cdot 10^{-2}$ | $3.97 \cdot 10^{-4}$ | 1 | $2.95 \cdot 10^{-2}$ | 1 |
| $2 \cdot 10^{-2}$ | $6.16 \cdot 10^{-4}$ | 1 | $1.97 \cdot 10^{-2}$ | 1 |
| $10^{-2}$ | failed | 3 | $9.83 \cdot 10^{-3}$ | 1 |
| $9 \cdot 10^{-3}$ | failed | 3 | $8.85 \cdot 10^{-3}$ | 1 |
| $8 \cdot 10^{-3}$ | failed | 3 | $7.88 \cdot 10^{-3}$ | 1 |
| $7 \cdot 10^{-3}$ | failed | 3 | $6.92 \cdot 10^{-3}$ | 1 |

As can be seen the inclusion fails when the difference between the two clusters becomes 0.01 or smaller. As before, inclusions are always possible when regarding the roots as a cluster of 6 roots.

One may ask, why the algorithm fails for the distance 0.01 . In Figure 1 we display the function plot near both triple roots. As can be seen it seems not easy to separate the clusters numerically. In Figure 2 we show the behavior of the function near the individual triple roots. Here it becomes clear that we basically see roundoff errors because of the numerical instability. Concerning the lengthy expression

$$
\begin{aligned}
& 61162984 * \sin (x)+(-554658228 * \sin (x)+(2095781 \\
& 742 * \sin (x)+(-4223382471 * \sin (x)+(4787318700 * \\
& \sin (x)+(-2894130000 * \sin (x)+729000000 * \sin (x) * \\
& x) * x) * x) * x) * x) * x
\end{aligned}
$$

of the function we expect some overestimation due to interval arithmetic. In that sense the achieved results seem not bad.

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## References

[1] F. Bünger. private communication, 2008.
[2] Darboux,G. Sur les dèveloppements en série des fonctions d’une seule variable. Journal des Mathématiques pures et appl., 3:291-312, 1876.
[3] R.B. Kearfott, J. Dian, and A. Neumaier. Existence verification for singular zeros of complex nonlinear systems. SIAM J. Numer. Anal. (SINUM), 38(2):360-379, 2000.


Fig. 1. Plot near first and second triple root.


Fig. 2. Individual plots near first and second triple root.
[4] MATLAB User's Guide, Version 7. The MathWorks Inc., 2004.
[5] A. Neumaier. An Existence Test for Root Clusters and Multiple Roots. Zeitschrift für Angewandte Mathematik und Mechanik (ZAMM), 68(6):256-257, 1988.
[6] S.M. Rump. Kleine Fehlerschranken bei Matrixproblemen. PhD thesis, Universität Karlsruhe, 1980.
[7] S.M. Rump. Solving Algebraic Problems with High Accuracy. Habilitationsschrift. In U.W. Kulisch and W.L. Miranker, editors, A New Approach to Scientific Computation, pages 51-120. Academic Press, New York, 1983.
[8] S.M. Rump. INTLAB - INTerval LABoratory. In Tibor Csendes, editor, Developments in Reliable Computing, pages 77-104. Kluwer Academic Publishers, Dordrecht, 1999.
[9] S.M. Rump. Ten methods to bound multiple roots of polynomials. J. Comput. Appl. Math. (JCAM), 156:403-432, 2003.
[10] S.M. Rump and S. Graillat. Verified error bounds for multiple roots of systems of nonlinear equations. submitted for publication, 2009.


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