Locating all the Zeros of an Analytic Function in one Complex Variable

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Abstract

Based on the argument principle we propose an adaptive multilevel subdivision algorithm for the computation of all the zeros of an analytic function $f : \mathbb{C} \to \mathbb{C}$ within a bounded domain. We illustrate the reliability of this method by several numerical examples.

Key words: Global zero finding, argument principle

MSC2000 - Classification: 30C15, 65E05
1 Introduction

Dynamical systems are frequently used as models for the temporal evolution of technical processes. In this case the stability analysis for an equilibrium state of the system naturally leads to the problem of finding all the zeros – or at least bounds on the set of zeros – of a certain analytic function $f : \mathbb{C} \rightarrow \mathbb{C}$. For instance, if there is no temporal delay to be taken into account in the underlying system then one has to consider the spectrum of the Jacobian of a vector field evaluated at the equilibrium. This can e.g. be done by using efficient eigenvalue solvers. However, if the technical process has to be modeled by a delay differential equation then the zero set of a non-polynomial but holomorphic function has to be approximated.

Motivated by this application we propose in this paper a robust numerical method for the computation of all the zeros of a holomorphic function $f : \mathbb{C} \rightarrow \mathbb{C}$ within a certain bounded domain. The underlying idea is to use numerically the argument principle and to combine this with an adaptive multilevel subdivision strategy. This way we construct tight box coverings of the set of zeros of $f$. The reliability of the method is due to the fact that by the argument principle one has to check whether or not a certain number is a nonvanishing integer, and this test is typically quite robust.

The underlying idea of this approach, namely to use the argument principle in combination with a subdivision procedure, already occurs in [4, 5]. However, we go one step further and propose an adaptive subdivision technique. Moreover, in contrast to [4, 5] we also describe in detail a specific numerical realization. This approach is similar in spirit to the topological methods developed in [3] where degree theory is the underlying concept for the approximation of the set of zeros of a given function. In fact, the argument principle as used here has to be viewed as the specific holomorphic situation for the computation of the degree of a mapping (cf. [1]).

A detailed outline of the article is as follows. In Section 2 we briefly restate the argument principle. Then, in Section 3, we develop our adaptive multilevel algorithm, prove its convergence and discuss a particular numerical realization. Finally we present three examples indicating the robustness and efficiency of this numerical approach (Section 4).

2 Theoretical Background

Our numerical approach is based on an elementary fact from complex analysis namely the so-called “argument principle”. For a given meromorphic function $f$ this result states that the number of zeros minus the number of singularities of $f$ (counting multiplicities) within a specified region in $\mathbb{C}$ can in principle be computed by a certain integration:
Theorem 2.1 (Argument Principle) Let $f : U \to \mathbb{C}$ be a meromorphic nonconstant function on the open subset $U \subset \mathbb{C}$ and let $\gamma$ be a closed curve on the boundary of a compact set $K$ inside $U$. Finally denote by $q_j$, $j = 1, \ldots, n$, and by $p_\ell$, $\ell = 1, \ldots, m$, the zeros resp. the singular points of $f$ inside $K$. Then

$$
\frac{1}{2\pi i} \int_{\gamma} \frac{f'(z)}{f(z)} \, dz = \sum_{j=1}^{n} n(\gamma, q_j)\mu(q_j) - \sum_{\ell=1}^{m} n(\gamma, p_\ell)\mu(p_\ell),
$$

where $n(\gamma, q_j)$, $n(\gamma, p_\ell)$ denote the winding numbers of the curve $\gamma$ with respect to $q_j$ resp. $p_\ell$ and $\mu(q_j)$, $\mu(p_\ell)$ are the multiplicities of $q_j$ resp. $p_\ell$.

In our applications we are particularly interested in the situation where $f$ is a holomorphic function and where the winding number of $\gamma$ is one. For this specific case we immediately obtain

Corollary 2.2 Let $f : U \to \mathbb{C}$ be a holomorphic nonconstant function on the open subset $U \subset \mathbb{C}$ and let $\gamma$ be a closed curve on the boundary of a compact set $K$ inside $U$ with winding number one for all the points surrounded by $\gamma$. Finally denote by $q_j$, $j = 1, \ldots, n$, the zeros of $f$ inside $K$. Then

$$
\int_{\gamma} \frac{f'(z)}{f(z)} \, dz = 2\pi i \sum_{k=1}^{n} \mu(q_j)
$$

(2.1)

where $\mu(q_j)$ are the multiplicities of the zeros $q_j$.

In the following we will denote by $\mu(f, \gamma)$ the right hand side in (2.1).

3 Algorithmic Description

Our aim is to find all the zeros of an analytic function $f$ in one complex variable inside a given compact domain. The underlying idea of the algorithm is as follows. We start with a (big) rectangle $B$ in $\mathbb{C}$ inside which we would like to find all the zeros of $f$. Then we compute the integral in the left hand side in (2.1) where $\gamma$ is a parametrization of the boundary of the rectangle $B$ with winding number one. If this integral is zero then there are no zeros inside $B$ and we are done. Otherwise we subdivide $B$ into smaller rectangles and compute the integrals in (2.1) over their boundaries. Proceeding this way and disregarding rectangles for which the integral is zero we obtain a close covering of all the zeros of $f$ inside $B$.

3.1 Description of a Basic Subdivision Scheme

We now formalize the idea stated above and present the abstract multilevel subdivision procedure in detail. The general structure of the following abstract algorithmic scheme is essentially known and can be found in the literature (see [4, 5]).
Basic Subdivision Scheme

Let $\mathcal{B}_0$ be an initial collection of finitely many rectangles in $\mathbb{C}$. Then $\mathcal{B}_k$ is inductively obtained from $\mathcal{B}_{k-1}$ in two steps:

(i) Subdivision step Construct from $\mathcal{B}_{k-1}$ a new system $\tilde{\mathcal{B}}_k$ of rectangles such that

$$
\bigcup_{B \in \tilde{\mathcal{B}}_k} B = \bigcup_{B \in \mathcal{B}_{k-1}} B
$$

and

$$
\text{diam}(\tilde{\mathcal{B}}_k) = \theta_k \text{diam}(\mathcal{B}_{k-1}),
$$

where $0 < \theta_{\text{min}} \leq \theta_k \leq \theta_{\text{max}} < 1$. (Here $\text{diam}(\mathcal{B}_k)$ denotes the diameter of the largest rectangle inside $\mathcal{B}_k$.)

(ii) Selection step Define the new collection $\mathcal{B}_k$ by

$$
\mathcal{B}_k = \left\{ B \in \tilde{\mathcal{B}}_k : \mu(f, \gamma_B) \neq 0 \right\}.
$$

Remarks 3.1  
(a) If at some stage in the subdivision process a zero of $f$ is lying on the boundary of one of the rectangles $B$ then $\mu(f, \gamma_B) = \infty$. We explicitly allow this possibility in the selection step and keep the corresponding rectangle in this case.

(b) Observe that we do not require that the rectangles inside the collection $\mathcal{B}_k$ are disjoint. However, in our modification and realization of the basic subdivision scheme we are always working with collections having this property in order to avoid unnecessary numerical computations.

Denote by $z(f, B)$ the set of zeros of the holomorphic function $f$ inside the rectangle $B$ and let

$$
Z_k = \bigcup_{B \in \mathcal{B}_k} B.
$$

Observe that $\lim_{k \to \infty} Z_k$ does exist since the $Z_k$ form a nested sequence of compact sets. Moreover, it is immediate from the construction of the general algorithm that the following result holds.

Proposition 3.2 An application of the basic subdivision scheme to the rectangle $B = \mathcal{B}_0$ yields a sequence of collections $\mathcal{B}_k$ such that

$$
\lim_{k \to \infty} h(Z_k, z(f, B)) = 0,
$$

where $h(\cdot, \cdot)$ denotes the standard Hausdorff distance.
3.2 Adaptive Version of the Basic Subdivision Scheme: the QZ-40 Algorithm

We now present a modification of the basic subdivision scheme which will lead to a robust and efficient numerical realization. The crucial difference consists essentially of two ingredients: first an adaptive subdivision strategy is used and second we introduce an additional search step. The structure of the following algorithm is significantly different to that of the basic subdivision scheme. Therefore – in order to avoid any potential confusion – we will from now on use the letter $R$ instead of $B$ in the notation for rectangles or their collections, respectively.

The QZ-40 Algorithm

Let $\mathcal{R}_0$ be an initial collection of finitely many rectangles in $\mathbb{C}$. Then $\mathcal{R}_k$ is inductively obtained from $\mathcal{R}_{k-1}$ in three steps:

(i) **Selection step** For every rectangle $R \in \mathcal{R}_{k-1}$ denote by $\gamma_R$ a parametrization of the boundary of the rectangle and compute the winding number $\mu(f, \gamma_R)$. Remove all rectangles $R$ from $\mathcal{R}_{k-1}$ for which $\mu(f, \gamma_R) = 0$.

(ii) **Search step** Search for a zero inside each rectangle $R \in \mathcal{R}_{k-1}$ with $\mu(f, \gamma_R) = 2\pi i$ using Newton's method with a starting point inside $R$. If a zero is found then store this point and remove the rectangle $R$ from the collection $\mathcal{R}_{k-1}$.

(iii) **Adaptive subdivision step** Construct from $\mathcal{R}_{k-1}$ a new system $\tilde{\mathcal{R}}_k$ of rectangles according to a certain specified subdivision strategy satisfying (3.1). Then additionally subdivide each rectangle inside $\tilde{\mathcal{R}}_k$ which is a subset of a rectangle $R \in \mathcal{R}_{k-1}$ with the property that $\mu(f, \gamma_R)/2\pi i > 2$. Let $\mathcal{R}_k$ be the resulting collection of boxes.

As in the case of the basic subdivision scheme the QZ-40 algorithm produces a nested sequence of compact sets $Z_k$ covering the (remaining) zeros of $f$. Since the diameter of the boxes is shrinking to zero we have the following result:

**Proposition 3.3** Suppose that all the zeros of $f$ inside the rectangle $R$ are simple. Then the QZ-40 algorithm applied to the rectangle $R = \mathcal{R}_0$ terminates after finitely many steps returning a complete list of all the zeros of $f$ inside $R$.

**Remarks 3.4**

(a) It is an easy task to modify the algorithm in such a way that also zeros of higher multiplicity can be found.

(b) One has to expect that in general in the first subdivision steps the integers $\mu(f, \gamma_R)/2\pi i$ will be greater than two for almost every rectangle within the
selected box collections. From this point of view it would seem natural to modify the subdivision step (iii) in such a way that additional subdivisions are just considered from a certain subdivision level $k > 1$ on. We have performed several numerical experiments along these lines, and these indicated that – somewhat counter-intuitively – the most efficient strategy is indeed to consider additional subdivisions right from the beginning.

### 3.3 Numerical Realization

A crucial part in the numerical realization of the QZ-40 algorithm is the computation of the integral (2.1) for the different rectangles. In our current implementation the computation of $\mu(f, \gamma_R)$ is done via an adaptive Romberg quadrature as described in [2] along the four different edges of the rectangle. More precisely we perform the three steps of the QZ-40 algorithm as follows:

- In a first step we parametrize each of the edges $R_j$ of a rectangle by $\gamma_j$ ($j = 1, 2, 3, 4$) and compute the value of

$$I_j \approx \Re \left( \frac{1}{2\pi i} \int_{\gamma_j} \frac{f'(z)}{f(z)} \, dz \right)$$

via an adaptive Romberg quadrature, see Figure 1. Then

$$\mu(f, \gamma_R) \approx 2\pi i \sum_{j=1}^{4} I_j.$$  

Observe that the value of the tolerance in the adaptive Romberg scheme can be chosen quite large since we only have to decide whether or not the approximation of $\sum_{j=1}^{4} I_j$ is zero or a nonvanishing integer.

- In the search step we perform a search for a zero of $f$ using the classical Newton method. This method either terminates with a zero inside the rectangle under consideration or the iteration is stopped if an iterate is more than a specified distance away from the center of the rectangle. In the examples which we considered it turned out to be quite efficient to choose at random a few (five, say) starting points for Newton’s method inside the rectangle.

- The subdivision rule used in the adaptive subdivision step is simply given by bisection alternating between the two different coordinate directions. That is, if a rectangle is created via bisection with respect to the $z_1$-direction then, if necessary, it will be bisected in the next step with respect to the $z_2$-direction and vice versa. Obviously by this rule the condition (3.1) is satisfied.
4 Numerical Examples

The following examples indicate both the efficiency and in particular the robustness of the QZ-40 algorithm.

4.1 Academic Example

We consider the function
\[ f_1 : \mathbb{C} \to \mathbb{C}, \quad f_1(z) = z^{50} + z^{12} - 5 \sin(20z) \cos(12z) - 1, \]
and compute its zeros inside the rectangle \([-20.3, 20.7] \times [-20.3, 20.7]\). A couple of coverings of the zeros of \(f_1\) produced by the QZ-40 algorithm are shown in Figure 2. The computations indicate that there are precisely 424 zeros of \(f\) inside the initial rectangle.

We have compared the numerical effort of the QZ-40 algorithm with the one obtained by two alternative approaches namely

- the classical Newton method performing at most 100 iterations with a certain number of initial points chosen at random. The numbers in Table 1 are averages over 20 different computations.

- the zero finding procedure c05pbc of the NAG library with a certain number of initial points chosen at random. In these computations we have specified a tolerance of 1e-15.

It can be observed, see Table 1, that the QZ-40 algorithm is much more efficient than these two approaches.

4.2 Stability of an Annular Combustion Chamber

Within a project at the Corporate Technology Department of Siemens (Munich), the stability of a flow inside an annular combustion chamber had to be analyzed. In
Figure 2: Box coverings of the set of zeros of $f_1$ obtained by the QZ-40 algorithm.
Table 1: Performance of the different zero finding procedures.

<table>
<thead>
<tr>
<th>Method</th>
<th># initial points</th>
<th># function calls</th>
<th># derivative calls</th>
<th># zeros</th>
</tr>
</thead>
<tbody>
<tr>
<td>Classical Newton</td>
<td>1500</td>
<td>140.130</td>
<td>140.130</td>
<td>153</td>
</tr>
<tr>
<td></td>
<td>5000</td>
<td>470.038</td>
<td>470.038</td>
<td>322</td>
</tr>
<tr>
<td></td>
<td>7000</td>
<td>655.879</td>
<td>655.879</td>
<td>361</td>
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<td></td>
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</tr>
<tr>
<td></td>
<td>15000</td>
<td>1405.903</td>
<td>1405.903</td>
<td>419</td>
</tr>
<tr>
<td>NAG c05pbc</td>
<td>1500</td>
<td>454.856</td>
<td>6.966</td>
<td>177</td>
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<td>23.672</td>
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<tr>
<td></td>
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</tr>
<tr>
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<td>406</td>
</tr>
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<td>QZ-40</td>
<td>-</td>
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<td>89.619</td>
<td>424</td>
</tr>
</tbody>
</table>

A simplified model this lead to the problem of finding all the zeros of the following holomorphic function:

\[ f_2 : \mathbb{C} \to \mathbb{C}, \quad f_2(z) = z^2 + Az + Be^{-Tz} + C, \]

where \( A, B, C \) and \( T \) are real parameters. Motivated by the actual underlying model for the combustion chamber we choose the values

\[ A = -0.19435, \quad B = 1000.41, \quad C = 522463 \quad \text{and} \quad T = 0.005. \]

In Figure 3 all the roots of \( f_2 \) found by the QZ-40 algorithm inside the rectangle \( R = [-15000, 5000] \times [-15000, 15000] \) are shown.

4.3 Stability of a Ring Oscillator

In [6] the detection of Hopf bifurcations in a ring consisting of coupled oscillators has been investigated. Taking the symmetry of the problem into account – i.e. by restricting to the bifurcation of so-called discrete rotating waves – one has to find all the zeros of the following function:

\[ f_3 : \mathbb{C} \to \mathbb{C}, \]

\[ f_3(\lambda) = \det \begin{pmatrix} -0.0166689 - 2.12 \cdot 10^{-14} \lambda & \frac{1}{60} + 6.0 \cdot 10^{-16} e^{-\tau \lambda} \\ 0.0166659 + e^{-\lambda}(-0.000037485 + 6.0 \cdot 10^{-16} \lambda) & -0.0166667 - 6.0 \cdot 10^{-16} \lambda \end{pmatrix}, \]

where we have chosen the delay to be \( \tau = 2.0 \). The result is shown in Figure 4. For more detailed information concerning this problem we refer to [6].
Figure 3: All the roots of $f_2$ inside $R = [-15000, 5000] \times [-15000, 15000]$.

Figure 4: All the roots of $f_3$ within the rectangle $R = [-12, 0] \times [-40, 40]$. 
References


