

# Effective Subdivision Algorithm for Isolating Zeros of Real Systems of Equations, with Complexity Analysis

Juan Xu  
Beihang University  
Beijing, China  
xujuan@buaa.edu.cn

Chee Yap\*  
Courant Institute, NYU  
New York, NY  
yap@cs.nyu.edu

## ABSTRACT

We describe a new algorithm *Miranda* for isolating the simple zeros of a function  $f : \mathbb{R}^n \rightarrow \mathbb{R}^n$  within a box  $B_0 \subseteq \mathbb{R}^n$ . The function  $f$  and its partial derivatives must have interval forms, but need not be polynomial. Our subdivision-based algorithm is “effective” in the sense that our algorithmic description also specifies the numerical precision that is sufficient to certify an implementation with any standard BigFloat number type. The main predicate is the Moore-Kioustelides (MK) test, based on Miranda’s Theorem (1940). Although the MK test is well-known, this appears to be the first synthesis of this test into a complete root isolation algorithm.

We provide a complexity analysis of our algorithm based on intrinsic geometric parameters of the system. Our algorithm and complexity analysis are developed using 3 levels of description (Abstract, Interval, Effective). This methodology provides a systematic pathway for achieving effective subdivision algorithms in general.

## KEYWORDS

Root Isolation; System of Real Equations; Certified Computation; Subdivision Algorithms; Miranda Theorem; Moore-Kioustelides Test; Effective Certified Algorithm; Complexity Analysis;

## ACM Reference Format:

Juan Xu and Chee Yap. 2019. Effective Subdivision Algorithm for Isolating Zeros of Real Systems of Equations, with Complexity Analysis. In *Proceedings of ACM Conference (Conference’17)*. ACM, New York, NY, USA, 10 pages. <https://doi.org/10.1145/nnnnnnn.nnnnnnn>

## 1 INTRODUCTION

Solving multivariate zero-dimensional systems of equations is a fundamental task with many applications. We focus on the problem of isolating simple real zeros of a real function

$$f = (f_1, \dots, f_n) : \mathbb{R}^n \rightarrow \mathbb{R}^n$$

within a given bounded box  $B_0 \subseteq \mathbb{R}^n$ . We do not require  $f$  to be polynomial, only each  $f_i$  and its partial derivatives have interval

\*Partially supported NSF Grants Nos. CCF-1423228 and CCF-1564132. Further support under Chinese Academy of Science (Beijing) President’s International Fellowship Initiative (2018), and Beihang International Visiting Professor Program No. Z2018060.

Permission to make digital or hard copies of all or part of this work for personal or classroom use is granted without fee provided that copies are not made or distributed for profit or commercial advantage and that copies bear this notice and the full citation on the first page. Copyrights for components of this work owned by others than ACM must be honored. Abstracting with credit is permitted. To copy otherwise, or republish, to post on servers or to redistribute to lists, requires prior specific permission and/or a fee. Request permissions from [permissions@acm.org](https://permissions.acm.org).  
*Conference’17, July 2017, Washington, DC, USA*

© 2019 Association for Computing Machinery.  
ACM ISBN 978-x-xxxx-xxxx-x/YY/MM...\$15.00  
<https://doi.org/10.1145/nnnnnnn.nnnnnnn>

forms. We require that  $f$  has only isolated simple zeros in  $2B_0$ . We call  $B_0$  the region-of-interest (ROI) of the input instance. This formulation of root isolation is called<sup>1</sup> a **local problem** in [14], in contrast to the **global problem** of isolating all roots of  $f$ . The local problem is very important in higher dimensions because the global problem has complexity that is exponential in  $n$ . In geometric applications we typically can identify ROI’s and can solve the corresponding local problem much faster than the global problem. Moreover, if  $f$  is not polynomial, the global problem might not be solvable: E.g.,  $f = \sin x$ ,  $n = 1$ . But it is solvable as a local problem as in [28].

In their survey of root finding in polynomial systems, Sherbrooke and Patrikalakis [26] noted 3 main approaches: (1) algebraic techniques, (2) homotopy, (3) subdivision. They objected to the first two approaches on “philosophical grounds”, meaning that it is not easy in these methods to restrict its computation to some ROI  $B_0$ . Of course, one could solve the global problem and discard solutions that do not lie in  $B_0$ . But its complexity would not be a function of the roots in  $2B_0$ . Such local complexity behavior are provable in the univariate case (e.g., [4]), and we will also show similar local complexity in the algorithm of this paper.

Focusing on the subdivision approach, we distinguish two types of subdivision: algebraic and analytic. In algebraic subdivision,  $f$  is polynomial and one exploits representations of polynomials such as Bernstein form or B-splines [7, 11, 12, 22, 26]. Analytic subdivision [15, 23, 27] supports a broader class of functions; this is formalized in [28] and includes all the functions obtained from composition of standard elementary functions or hypergeometric functions. Many algebraic algorithms comes with complexity analysis, while the analytic algorithms typically lack such analysis, unless one views convergence analysis as a weak form of complexity analysis. This lack is natural because many analytic algorithms are what theoretical computer science call “heuristics” with no output guarantees. Any guarantees would be highly<sup>2</sup> conditional (cf. [27]). To our knowledge, there has been no subdivision algorithm that solves the root isolation problem until the present paper. The subdivision algorithms [7, 11, 12, 22, 26] suffer from two gaps. (1) Non-termination: they require an input  $\varepsilon > 0$  to serve as termination criterion. (2) Non-isolation: the output box is not guaranteed to be **isolating**, i.e., to contain a unique root. So an output box could err in one of two ways: it may contain no roots or may have more than one

<sup>1</sup> Sometimes, an algorithm is called “local” if it works in small enough neighborhoods (like Newton iteration), and “global” if no such restriction is needed. Clearly, this is a different local/global distinction.

<sup>2</sup> The issue of “unconditional algorithms” is a difficult one in analytic settings. Even the algorithm in this paper is conditional: we require the zeros of  $f$  to be simple within  $2B_0$ . But one should certainly specify any conditions upfront and try to avoid conditions which are “algorithm-induced” (see [29]).

root. To avoid the first error, some root existence test is needed: so Garloff and Smith [11, 12] considered the use of Miranda test. To avoid the second error, Elber and Kim [7] introduced a cone test to ensure that there is at most one solution. The cone test generalizes the hodograph test of Sederberg and Meyers (1988); unfortunately this is a nontrivial test and details on how to compute the cones are missing.

## 1.1 Generic Root Isolation Algorithms

It is useful to formulate a “generic algorithm” for local root isolation (cf. [19]). We postulate 5 abstract modules: three box tests (**exclusion**  $C_0$ , **existence**  $EC$ , **Jacobian**  $JC$ ) and two box operators (**subdivision** and **contraction**). Our tests (or predicates, which we use interchangeably) is best described using a notation: for any set  $B \subseteq \mathbb{R}^n$ ,  $\#(B) = \#_f(B)$  denotes the number of roots, counted with multiplicity, of  $f$  in  $B$ . These tests are abstractly defined by these implications:

$$\left. \begin{aligned} C_0(B) &\implies \#(B) = 0, \\ EC(B) &\implies \#(B) \geq 1, \\ JC(B) &\implies \#(B) \leq 1. \end{aligned} \right\} \quad (1)$$

Unlike exact predicates, these tests are “one-sided” (cf. [28]) since their failure may have no implications for the negation of the predicate. For root isolation, we need both  $EC(B)$  and  $JC(B)$  to prove uniqueness. These 3 tests can be instantiated in a variety of ways. The exclusion test  $C_0(B)$  is instantiated differently depending on the type of subdivision: exploiting the convex hull property of Bernstein coefficients (in algebraic case) or using interval forms of  $f$  (in analytic case). For  $EC$ , we can use various tests coming from degree theory or fixed point theory (e.g., [3]). This paper is focused on a test based on Miranda’s Theorem. The Jacobian test  $JC$  is related to the determinant of the Jacobian matrix but more geometric forms (e.g., cone test [7]) can be formulated. Next consider the box operators: An  $n$ -dimensional box  $B$  may be **subdivided** into  $2^k$  subboxes in  $\binom{n}{k}$  ways ( $k = 1, \dots, n$ ), giving a total of  $2^n - 1$  ways. In practice,  $k = 1$  and some heuristic will choose one of the  $n$  binary splits (see [12] for 3 heuristics). If Bernstein form is used, then de Casteljau’s algorithm is used to construct the Bernstein forms for the children. We **contract**  $B$  to  $B \cap N(B)$  where  $N(B)$  is a box returned by a Newton-like operator. Let us say the contraction “succeeds” if the width  $w(B \cap N(B))$  is less than  $w(B)$ . But success is not guaranteed, and so this operator always needs to be paired with some subdivision operator that never fails. It is well-known that  $N(B)$  can also provide exclusion and uniqueness tests:

$$\left. \begin{aligned} \text{exclusion: } & B \cap N(B) = \emptyset \\ \text{unique root: } & N(B) \subseteq B \end{aligned} \right\} \quad (2)$$

Given the above 5 modules, we are ready to synthesize them into a root isolation algorithm: In broad outline, our algorithm maintains a queue  $Q$  of candidate boxes. Initially,  $Q$  contains only the ROI  $B_0$ , the algorithm loops until  $Q$  is empty:

```

SIMPLE ISOLATE( $f, B_0$ )
  Output: sequence of isolating boxes for roots in  $B_0$ 
   $Q \leftarrow \{B_0\}$ 
  While  $Q \neq \emptyset$ 
     $B \leftarrow Q.pop()$ 
    If  $C_0(B)$  continue;      ◀ discard B and repeat loop
    If  $EC(B) \wedge JC(B)$       ◀ B has a unique root
      output  $B$  and continue;
    If  $w(N(B) \cap B) < w(B)$  ◀ if contraction succeeds
       $Q.push(B)$ 
    else
       $Q.push(subdivide(B))$ 

```

The **partial correctness** of SIMPLE ISOLATE is clear, i.e., if it terminates, the output is correct. But termination is a serious issue: clearly it depends on instantiations of the three tests. But independent of the tests, non-termination can arise in two other ways: (1) Success of contraction ensures a reduction in the width  $w(B)$ , but this alone may not suffice for termination. (2) Presence of roots on the boundary of a box (e.g.,  $B_0$ ). We next discuss the research issues around this framework.

## 1.2 How to derive effective algorithms

In this paper, we describe Miranda, a subdivision algorithm for root isolation, roughly along the above outline. We forgo the use of the contraction operator as it will not figure in our analysis. For simplicity, assume that all our boxes are hypercubes (equidimensional boxes); this means our subdivision splits each box into  $2^n$  children. With a little more effort, our analysis can handle boxes with bounded aspect ratios and thus support the bisection-based algorithms. As noted, termination depends on instantiations of our 3 tests: our exclusion and Jacobian tests are standard in the interval literature. Our existence test, called MK test, is from Moore-Kioustelides (MK) [20]. Our algorithm is similar<sup>3</sup> to one in the Appendix of [18, Appendix]. In the normal manner of theoretical algorithms, one would proceed to “prove that Miranda is correct and analyze its complexity”. This will be done, but the way we proceed is aimed at some broader issues discussed next.

**Effectivity:** how could we convert a mathematically precise algorithm (like Miranda) into an “effective algorithm”, i.e., certified and implementable. One might be surprised that there is an issue. The non-triviality of this question can be illustrated from the history of isolating univariate roots: for about 30 years, it is known that the “benchmark problem” of isolating all the roots of an integer polynomial with  $L$ -bit coefficients and degree  $n$  has bit-complexity  $\tilde{O}(n^2L)$ , a bound informally described as “near-optimal”. This is achieved by the algorithm of Schönhage and Pan (1981-1992). But this algorithm has never been implemented. What is the barrier? Basically, it is the formidable problem of mapping algorithms in the Real RAM model [2] or BSS model [6] into a bit-based Turing-computable model – see [30].

In contrast, recent progress in subdivision algorithms for univariate roots finally succeeded in achieving comparable complexity bounds of  $\tilde{O}(n^2(L + n))$ , and such algorithms were implemented

<sup>3</sup> In [18, Appendix], only termination was proved (up to the interval level). There was no complexity analysis and we will correct an error in a lemma.

shortly after! Thus, these subdivision algorithms were “effective”. For two parallel accounts of this development, see [17, 25] for the case of real roots, and to [4, 5, 14] for complex roots. What is the power conferred by subdivision? We suggest this: *the subdivision framework provides a natural way to control the numerical precision necessary to ensure correct operations of the algorithm. Moreover, the typical one-sided tests of subdivision avoid the “Zero Problem” and can be effectively implemented using approximations with suitable rounding modes.*

In this paper, we capture this pathway to effectivity by introducing 3 Levels of (algorithmic) Abstractions: (A) **Abstract Level**, (I) **Interval Level**, and (E) **Effective Level**. We normally identify Level (A) with the mathematical description of an algorithm or Real RAM algorithms. *We assume our effective algorithms approximate real numbers by BigFloat or dyadic numbers, i.e.,  $\mathbb{Z}[\frac{1}{2}]$ .* As illustration, consider the exclusion test  $C_0(B)$  (viewed as abstract) has correspondences in the next two levels:

$$\begin{aligned} \text{(A): } C_0(B) &\equiv 0 \notin f(B) \\ \text{(I): } \square C_0(B) &\equiv 0 \notin \square f(B) \\ \text{(E): } \tilde{\square} C_0(B) &\equiv 0 \notin \tilde{\square} f(B) \end{aligned}$$

where  $f(B)$  is the exact range of  $f$  on  $B$ ,  $\square f(B)$  is the interval form of  $f$ , and  $\tilde{\square} f(B)$  the effective form. The 3 range functions here are related as follows:

$$f(B) \subseteq \square f(B) \subseteq \tilde{\square} f(B). \quad (3)$$

In general, for any abstract test  $C(B)$ , we derive its interval and effective forms to ensure the implications

$$\tilde{\square} C(B) \Rightarrow \square C(B) \Rightarrow C(B). \quad (4)$$

This means, the success of  $\tilde{\square} C(B)$  implies the success of  $\square C(B)$ , and hence  $C(B)$ . An abstract algorithm  $A$  is first mapped into an interval algorithm  $\square A$ . But algorithms still involve real numbers. So we must map  $\square A$  to an effective algorithm  $\tilde{\square} A$ . Correctness must ultimately be shown at the Effective Level; the standard missing link in numerical (even “certified”) algorithms is that one often stops at Abstract or Interval Levels.

**Complexity:** The complexity of analytic algorithms is often restricted to convergence analysis. But in this paper, we will provide explicit bounds on complexity as a function of the geometry of the roots in  $2B_0$ . This complexity can be captured at each of our 3 levels, but we always begin by proving our theorems at the Abstract Level, subsequently transferred to the other levels. Although it is the Effective Level that really matters, it would be a mistake to directly attempt such an analysis at the Effective level: that would obscure the underlying mathematical ideas, incomprehensible and error prone. The 3-level description enforces an orderly introduction of new concerns appropriate to each level. Like structured programming, the design of effective algorithms needs some structure. Currently, outside of the subdivision framework, it is hard to see a similar path way to effectivity.

### 1.3 Literature Survey

There is considerable literature associated with each of our three tests: the exclusion test comes down to bounding range of functions, a central topic in Interval Analysis [24]. The Jacobian test is connected to the question of local injectivity of functions, the

Bieberbach conjecture (or de Branges Theorem), Jacobian Conjecture, and theory of univalent functions. In our limited space, we focus on the “star” of our 3 tests, i.e., the existence test. It is the most sophisticated of the 3 tests in the sense that some nontrivial global/topological principle is always involved in existence proofs. In our case, the underlying principle is the fixed point theorem of Brouwer, in the form of Miranda’s Theorem (1940), and intimately related to degree theory.

We compare two box tests  $C$  and  $C'$  in terms of their relative **efficacy**: say  $C$  is **as efficacious as**  $C'$ , written  $C \geq C'$ , if for all  $B$ ,  $C'(B)$  succeeds implies that  $C(B)$  succeeds. The relative efficacy of several existence tests have been studied [3, 9, 10, 13]. Goldsztejn considers four common existence tests, and argues that “in practice” there is an efficacy hierarchy

$$(IN) \geq (HS) \geq (FLS) \geq (K) \quad (5)$$

where (K) refers to Krawczyk, (HS) to Hansen-Sengupta, (FLS) to Frommer-Lang-Schnurr, and (IN) to Interval-Newton. Note that (K), (HS) and (IN) are all based on Newton-type operators (see (2)). Our Moore-Kioustelidis (MK) test is essentially (FLS). We say “essentially” because the details of defining the tests may vary to render the comparisons invalid. In our MK tests, we evaluate  $f$  on each box face using the Mean Value Form expansion at the center of the face. But the above analysis assumes an expansion is at the center of the box, which is less accurate. But we may also compare these tests in terms of their complexity (measured by the worst case number of arithmetic operations, or number of function evaluations); a complexity-efficacy tradeoff may be expected. Such complexity comparisons do not account for adaptive costs: Newton-type existence tests have non-adaptive costs while the Miranda-type tests are adaptive (we are testing  $n$  pairs of faces, and can break off as soon as one pair fails the test. Finally, evaluating these tests in isolation does not tell us how they might perform in the context of an algorithm. It is therefore premature to decide on the best existence test.

### 1.4 Overview

In section 2, we introduce some basic concepts of interval arithmetic and establish notations. Section 3 introduces the key existence test based on Miranda’s theorem. Section 4 proves conditions that ensure the success of these existence test. Section 5 introduces two Jacobian tests. Section 6 describes our main algorithm. Section 7 is the complexity analysis of our algorithm. We conclude in Section 8. All proofs are relegated to the Appendix.

## 2 INTERVAL FORMS

We first establish notations for standard concepts of interval arithmetic. Bold fonts indicate vector variables: e.g.,  $\mathbf{f} = (f_1, \dots, f_n)$  or  $\mathbf{x} = (x_1, \dots, x_n)$ .

Let  $\square \mathbb{R}$  denote the set of compact intervals in  $\mathbb{R}$ . Extend this to  $\square \mathbb{R}^n$  for the set of compact  $n$ -boxes. In the remaining paper, we assume that all  $n$ -boxes are hypercubes (i.e., the width in each dimension is the same). For any box  $B \in \square \mathbb{R}^n$ , let  $\mathbf{m}_B = \mathbf{m}(B)$  denote its center and  $w_B = w(B)$  be the width of any dimension. Besides boxes, we will also use ball geometry: let  $\Delta = \Delta(\mathbf{a}, r) \subseteq \mathbb{R}^n$  denote the closed ball centered at  $\mathbf{a} \in \mathbb{R}^n$  of radius  $r > 0$ . If  $r \leq 0$ ,  $\Delta(\mathbf{a}, r)$  is



just the point  $\mathbf{a}$ . For any positive  $k > 0$ , let  $k\Delta$  and  $kB$  denote the dilation of the ball  $\Delta$  and box  $B$  relative to their centers. Let  $A, B \subseteq \mathbb{R}^n$  be two sets. We will quantify their “distance apart” in two ways: their usual Hausdorff distance is denoted  $q(A, B)$  and their **separation**,  $\inf \{\|\mathbf{a} - \mathbf{b}\| : \mathbf{a} \in A, \mathbf{b} \in B\}$  is denoted as  $sep(A, B)$ . Note that  $q$  is a metric on closed subsets of  $\mathbb{R}^n$  but  $sep(A, B)$  is no metric.

Consider two kinds of extensions of a function  $f : \mathbb{R}^n \rightarrow \mathbb{R}$ . First, the **set extension** of  $f$  refers to the function (still denoted by  $f$ ) that maps  $S \subseteq \mathbb{R}^n$  to  $f(S) := \{f(\mathbf{x}) : \mathbf{x} \in S\}$ . The second kind of extension is not unique: an **interval form** of  $f$  is any function  $\square f : \square \mathbb{R}^n \rightarrow \square \mathbb{R}$ , satisfying two properties: (i) (inclusion)  $f(B) \subseteq \square f(B)$ ; (ii) (convergence) if  $\mathbf{p} = \lim_{i=0}^{\infty} B_i$  then  $f(\mathbf{p}) = \lim_{i=0}^{\infty} \square f(B_i)$ . For short, we call  $\square f$  a **box form** of  $f$ .

If  $\mathbf{f} = (f_1, \dots, f_n) : \mathbb{R}^n \rightarrow \mathbb{R}^n$ , we have corresponding set extension  $\mathbf{f}(S)$  and interval forms  $\square \mathbf{f} : \square \mathbb{R}^n \rightarrow \square \mathbb{R}^n$ ,

For any set  $S \subseteq \mathbb{R}^n$ , let  $\text{Zero}_{\mathbf{f}}(S)$  denote the multiset of zeros of  $\mathbf{f}$  in  $S$ . We assume that  $\mathbf{f}$  is analytic and its zeros are counted with the proper multiplicity. Then  $\#\mathbf{f}(S)$  is the size of the multiset  $\text{Zero}_{\mathbf{f}}(S)$ . We may write  $\text{Zero}(S)$  and  $\#(S)$  when  $\mathbf{f}$  is understood.

The notation “ $\square f$ ” is a generic box form; we use subscripts to indicate specific box forms. Thus, the **mean value form** of  $f$  is

$$\square_M f(B) = f(\mathbf{m}(B)) + \square \nabla f(B)^T \cdot (B - \mathbf{m}(B))$$

where  $\nabla f$  is the gradient of  $f$  (viewed as a column vector) and  $\nabla f(B)^T$  is the transpose. The box  $B - \mathbf{m}(B)$  is now at the origin, i.e.,  $\mathbf{m}(B - \mathbf{m}(B)) = \mathbf{0}$ . The appearance of the generic “ $\square \nabla f(B)$ ” in the definition of  $\square_M f$  means that  $\square_M f$  is still not fully specified. In our complexity analysis, we assume that for any box form, if not fully specified, will have at least linear convergence. *In this paper, all the box forms used in our predicates will be mean value forms.* Next, we intend to convert the interval form  $\square_M$  to some effective version  $\tilde{\square}_M$ . One reason that this is necessary may be seen in the fact that  $\square_M$  assumes an exact value  $f(\mathbf{m}(B))$ . Even if  $\mathbf{m}(B)$  is a dyadic number, we may need to approximate  $f(\mathbf{m}(B))$  (e.g.,  $f(x) = \sin(x)$ ).

### 3 MIRANDA AND MK TESTS

In the rest of this paper, we fix

$$\mathbf{f} := (f_1, \dots, f_n) : \mathbb{R}^n \rightarrow \mathbb{R}^n \quad (6)$$

to be a  $C^2$ -function (twice continuously differentiable), and  $\mathbf{f}$  and its partial derivatives have interval forms. We further postulate that  $\mathbf{f}$  has only finitely many simple zeros in any bounded region of interest (this means  $2B_0$  in our algorithms). A zero  $\boldsymbol{\alpha}$  of  $\mathbf{f}$  is simple if the Jacobian matrix  $J_{\mathbf{f}}(\boldsymbol{\alpha})$  is non-singular. For any set  $S \subseteq \mathbb{R}^n$ , its **magnitude** is defined as  $|S| := \max \{ |x| : x \in S \}$ .

We consider a classical test from Miranda (1940) to confirm that a box  $B \in \square \mathbb{R}^n$  contains a zero of  $\mathbf{f}$ . If the box  $B$  is written as  $B = \prod_{i=1}^n I_i$  with  $I_i = [a_i^-, a_i^+]$ , then it has two  $i$ -th **faces**, namely

$$B_i^- := I_1 \times \dots \times I_{i-1} \times \{a_i^-\} \times I_{i+1} \times \dots \times I_n.$$

and  $B_i^+$ , defined similarly. Write  $B_i^{\pm}$  to mean either  $B_i^-$  or  $B_i^+$ . Consider the following box predicate called<sup>4</sup> the **simple Miranda Test**:

$$\text{MT}_{\mathbf{f}}(B) \equiv \bigwedge_{i=1}^n (f_i(B_i^+) > 0) \wedge (f_i(B_i^-) < 0) \quad (7)$$

where  $\mathbf{f}$  is given in (6). The following result is classic:

PROPOSITION 1. [Miranda (1940)]

If  $\text{MT}_{\mathbf{f}}(B)$  holds then  $\#\mathbf{f}(B) \geq 1$ .

For a box  $B$  and  $k > 0$ , let  $kB$  denote the box centered at  $\mathbf{m}(B)$  of width  $k \cdot w(B)$ , called the  $k$ -**dilation** of  $B$ . Next, we introduce the **MK Test** test  $\text{MK}(B) = \text{MK}_{\mathbf{f}}(B)$  that amounts an application of the simple Miranda test to the box  $2B$  (instead of  $B$ ), using a preconditioned form of  $\mathbf{f}$ :

ABSTRACT MK TEST

Input:  $\mathbf{f}$  and box  $B$

Output: true iff  $\text{MK}_{\mathbf{f}}(B)$  succeeds

1.  $C \leftarrow J_{\mathbf{f}}(\mathbf{m}(B))$ , Jacobian matrix at  $\mathbf{m}(B)$   
If  $C^{-1}$  does not exist, return false.

2. Construct a “preconditioned version”  $\mathbf{g}$ :  
 $\mathbf{g} \leftarrow C^{-1} \mathbf{f} = (g_1(\mathbf{x}), \dots, g_n(\mathbf{x}))$

3. Apply the Simple Miranda Test to  $2B$  for  $\mathbf{g}$ :

For  $i \leftarrow 1, \dots, n$ :

If  $g_i(2B_i^+) \leq 0$  or  $g_i(2B_i^-) \geq 0$ , (\*)  
return false

4. Return true.

The notation “ $2B_i^{\pm}$ ” in (\*) refers to faces of the box  $2B$ , not the 2-dilation of the faces of  $B$ . Here “MK” refers to Moore and Kiousteliades [20]; the preconditioning idea first appearing in [16]. The MK Test was first introduced in [18].

Note that  $\text{MK}(B)$  is mathematically exact and generally not implementable (even if it were possible, we may still prefer approximations). We first define its interval form, denoted  $\square \text{MK}(B)$ : simply by replacing  $g_i(B_i^{\pm})$  in line (\*) by interval forms  $\square g_i(B_i^{\pm})$ . Finally, we must define the effective form  $\tilde{\square} \text{MK}(B)$  (Section 8). The key property is the relation (cf. (4)):

$$\tilde{\square} \text{MK}(B) \Rightarrow \square \text{MK}(B) \Rightarrow \text{MK}(B).$$

### 4 ON SURE SUCCESS OF MK TEST

The success of the MK test implies the existence of roots. In this section, we prove some (quantitative) converses.

We need preliminary facts about mean value forms. Given  $x, y \in \mathbb{R}$ , the notation  $x \pm y$  denotes a number of the form  $x + \theta y$ , where  $0 \leq |\theta| \leq 1$ ; thus “ $\pm$ ” hides the implicit  $\theta$  in the definition. This notation is not symmetric:  $x \pm y$  and  $y \pm x$  are generally different. This notation extends to matrices: let  $A = (a_{ij})_{i,j=1}^n$  and  $B = (b_{ij})_{i,j=1}^n$  be two matrices. Then  $A \pm B := (a_{ij} \pm b_{ij})_{i,j=1}^n$ . Similarly, for a scalar  $\lambda$ , we have  $A \pm \lambda := (a_{ij} \pm \lambda)_{i,j=1}^n$ . Also, let  $\|\mathbf{x}\|$  denote the vector  $(|x_1|, \dots, |x_n|)$  where  $\mathbf{x} = (x_1, \dots, x_n)$ . For  $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$ , we write  $[\mathbf{x}, \mathbf{y}]$  to denote the line segment connecting  $\mathbf{x}$  and  $\mathbf{y}$ . We write  $\|\mathbf{x}\|$

<sup>4</sup> We call it “simple” as we ignore some common generalizations that allow an interchange of “ $< 0$ ” with “ $> 0$ ”, or replace  $\mathbf{f}$  by  $\sigma(F) = (f_{\sigma(1)}, \dots, f_{\sigma(n)})$  for any arbitrary permutation  $\sigma$  of the indices.

and  $\|A\|$  for the infinity norms of vector  $\mathbf{x}$  and matrix  $A$ . For convex set  $C \subseteq \mathbb{R}^n$ , define the matrix  $K(C)$  with entries  $(K(C)_{ij})_{i,j=1}^n$  where

$$K(C)_{ij} := \sum_{k=1}^n \left| \frac{\partial^2 f_i}{\partial x_j \partial x_k}(C) \right|. \quad (8)$$

Below,  $C$  may be a disc  $\Delta$  or a line  $[\mathbf{x}, \mathbf{y}]$ . Denote by  $J_f(\mathbf{x})$  the Jacobian matrix of  $f$  at  $\mathbf{x}$ . We write  $J_f(\mathbf{x})$  as  $J(\mathbf{x})$  when  $f$  is understood. The following is a simple application of the Mean Value Theorem (MVT):

LEMMA 2 (MVT). *Given two points  $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$ , we have:*

- (a)  $J(\mathbf{x}) = J(\mathbf{y}) \pm K([\mathbf{x}, \mathbf{y}])\|\mathbf{x} - \mathbf{y}\|,$   
 (b)  $f(\mathbf{x}) - f(\mathbf{y}) = (J(\mathbf{y}) \pm K([\mathbf{x}, \mathbf{y}])\|\mathbf{x} - \mathbf{y}\|) \cdot (\mathbf{x} - \mathbf{y}).$

#### 4.1 Sure Success of abstract MK Test

In this and the next subsection, we consider boxes that contain a root  $\alpha$  of  $f$ . We prove conditions that ensures the success of the MK Test. We first prove this for the abstract test  $\text{MK}(B)$ . The next section extends this result to the interval test  $\square\text{MK}(B)$ .

The key definition here is a bound  $\lambda_1(\alpha)$  which depends on  $\alpha$  and  $f$ . We prove that if  $w(B) \leq \lambda_1(\alpha)$ , then the abstract MK test will succeed on  $B$ . By a **critical point** we mean  $\alpha \in \mathbb{R}^n$  where the determinant of  $J(\alpha)$  is zero. By definition, a root  $\alpha$  of  $f$  is simple if  $\alpha$  is not a critical point.

Suppose  $S_1$  and  $S_2$  are two sets in  $\mathbb{R}^n$ . Define

$$\|J^{-1}(S_1)\| := \max_{\mathbf{x} \in S_1} \|J^{-1}(\mathbf{x})\| \quad \text{and}$$

$$\|J^{-1}(S_1) \cdot K(S_2)\| := \max_{\mathbf{x} \in S_1, \mathbf{y} \in S_2} \|J^{-1}(\mathbf{x}) \cdot K(\mathbf{y})\|.$$

We see that both  $\|J^{-1}(S_1)\|$  and  $\|J^{-1}(S_1) \cdot K(S_2)\|$  are finite if  $S_1$  does not contain a critical point of  $f$ . Consider the following function

$$s(r) := r - \frac{1}{18n \|J^{-1}(\Delta(\alpha, 2\sqrt{nr})) \cdot K(\Delta(\alpha, 2\sqrt{nr}))\|}. \quad (9)$$

We then define  $\lambda_1(\alpha)$  to be the smallest  $r$  such that  $s(r) = 0$ , i.e.,  $\lambda_1(\alpha) := \text{argmin}_r \{s(r) = 0\}$ .

LEMMA 3. *For any simple root  $\alpha$  of  $f$ ,  $\lambda_1(\alpha)$  is well-defined.*

From now on, let  $\Delta_\alpha$  denote the disc

$$\Delta_\alpha := \Delta(\alpha, 2\sqrt{n}\lambda_1(\alpha)). \quad (10)$$

The following lemma corrects an gap in the appendix of [18].

LEMMA 4. *Let box  $B$  contain a simple root  $\alpha$  of  $f$ .*

*If  $w_B \leq \lambda_1(\alpha)$ , the preconditioned system  $\mathbf{g}_B := J^{-1}(\mathbf{m}(B))f = (g_1, \dots, g_n)$  is well-defined, and for all  $i = 1, \dots, n$ ,*

$$g_i(2B_i^+) \geq \frac{w_B}{4}, \quad g_i(2B_i^-) \leq -\frac{w_B}{4}.$$

#### 4.2 Sure Success of Interval MK Test

We now extend the previous subsection on the abstract MK Test  $\text{MK}(B)$  to the interval version  $\square\text{MK}(B)$ . Again, assume  $B$  is a box containing exactly one root  $\alpha$  of  $f$ . We will give  $\lambda_2(\alpha)$  which is analogous to  $\lambda_1(\alpha)$  and prove that if  $w_B \leq \lambda_2(\alpha)$ , then  $\square\text{MK}(B)$  will succeed.

To prove the existence of such a  $\lambda_2(\alpha)$  as mentioned above, we need to make some assumptions on the property of the box

functions. As in [21], a box function  $\square f$  is called **Lipschitz** in a region  $S \subseteq \mathbb{R}^n$  if there exists a constant  $L$  such that

$$w(\square f(B)) \leq L \cdot w(B), \quad \forall B \subseteq S. \quad (11)$$

We call any such  $L$  a **Lipschitz constant** of  $\square f$  on  $S$ . For our theorem, we need to know the specific box function in order to derive a Lipschitz constant. Consider the mean value form  $\square_{\text{M}}f$  on a region  $S \subseteq \mathbb{R}^n$ .

LEMMA 5. *Let  $f$  be a continuously differentiable function defined on a convex region  $S \subseteq \mathbb{R}^n$ . Then a Lipschitz constant for  $\square_{\text{M}}f$  on  $S$  is  $\sum_{k=1}^n \left| \square \frac{\partial f}{\partial x_k}(S) \right|$ .*

Consider the sign tests of  $\square\text{MK}(B)$ :

$$\square_{\text{M}}g_i(2B_i^+) > 0 \quad \text{and} \quad \square_{\text{M}}g_i(2B_i^-) < 0$$

where  $g_i$  is the  $i$ -th component of the system  $J(\mathbf{m}(B))^{-1}f$ . We consider the mean value form  $\square_{\text{M}}g_i(2B_i^+) = g_i(\mathbf{m}(2B_i^+)) + \square \nabla g_i(2B_i^+) \cdot (\mathbf{m}(2B_i^+) - 2B_i^+)$  and assume that the components of  $\square \nabla g_i(2B_i^+)$  are evaluated via the linear combination of  $\square \frac{\partial f_j(2B_i^+)}{\partial x_k}$  for  $j, k = 1, \dots, n$ .

We now prove that if  $B$  is small enough,  $\square\text{MK}(B)$  will succeed. Recalling the Hausdorff distance  $q(I, J)$  on intervals, we have this bound from [23].

PROPOSITION 6. *Let  $f : D \subset \mathbb{R}^n \rightarrow \mathbb{R}$  be a continuously differentiable function. Then*

$$q(\square_{\text{M}}f(B), f(B)) \leq 2w_B \sum_{i=1}^n w(\square \frac{\partial f(B)}{\partial x_i}). \quad (12)$$

For the next theorem, define

$$\widehat{\lambda}_1(\alpha) := \frac{1}{64n^2L \cdot \|J^{-1}(\Delta_\alpha)\|}. \quad (13)$$

where  $L = L_\alpha$  is a Lipschitz constant for  $\square \frac{\partial f_j}{\partial x_k}$  on  $\Delta_\alpha$  (for all  $j, k = 1, \dots, n$ ).

THEOREM 7. *Let  $B$  be a box containing a simple root  $\alpha$  of width  $w_B \leq \lambda_1(\alpha)$ .*

(a) *If  $w(\square \frac{\partial g_i(2B_i^+)}{\partial x_j}) \leq \frac{1}{32n}$  for each  $j = 1, \dots, n$ , then  $\mathbf{g}_B := J^{-1}(\mathbf{m}(B))f$  is well-defined and  $\square\text{MK}(B)$  will succeed.*

(b) *If  $w_B \leq \lambda_2(\alpha)$  with  $\lambda_2(\alpha) := \min \{ \lambda_1(\alpha), \widehat{\lambda}_1(\alpha) \}$ , then  $\square\text{MK}(B)$  will succeed.*

## 5 TWO JACOBIAN CONDITIONS

We define the **Jacobian test** as follows:

$$\text{JC}(B) \equiv 0 \notin \det(J_f(3B)). \quad (14)$$

The order of operations in  $\det(J_f(3B))$  should be clearly understood: first we compute the **interval Jacobian matrix**  $J_f(3B)$ , i.e., entries in this matrix are the intervals  $\partial_{x_j} f_i(3B)$ . Then we compute the determinant of the interval matrix. Also note that we use  $3B$  instead of  $B$ . The following is well-known in interval computation (see [1, Corollary to Theorem 12.1]):

PROPOSITION 8. [*Jacobian test*]

*If  $\text{JC}(B)$  holds then  $\#_f(3B) \leq 1$ .*

```

581 ABSTRACT  $\text{Miranda}(f, B_0)$ 
582 OUTPUT: Queue  $P$  of non-overlapping isolating boxes of  $f$  s.t.
583  $\mathcal{Z}_f(B_0) \subseteq \bigcup_{B \in P} \mathcal{Z}_f(B) \subseteq \mathcal{Z}_f(2B_0)$ 
584
585 1. Initialize output queue  $P \leftarrow \emptyset$  and priority queue  $Q \leftarrow \{B_0\}$ .
586 2. While  $Q \neq \emptyset$  do:
587 3. Remove a biggest box  $B$  from  $Q$ .
588 4. If  $C_0(B)$  succeeds, continue;
589 5. If  $JC(B)$  succeeds then
590 6. Initialize new queue  $Q' \leftarrow \{B\}$ .
591 7. While  $Q' \neq \emptyset$  do:
592 8.  $B' \leftarrow Q'.\text{pop}()$ .
593 9. If  $(B' = B) \vee C_0(B')$  fails then
594 10. If  $MK(B')$  succeeds then
595 11.  $P.\text{add}(2B')$ .
596 12. Discard from  $Q$  the boxes contained in  $3B$ .
597 13. Break.
598 14.  $Q.\text{push}(\text{subdivide}(B))$ .
599 15. Else
600 16.  $Q.\text{push}(\text{subdivide}(B))$ .
601

```

Figure 1: Root Isolation Algorithm

We next introduce the following **strict Jacobian test**:

$$JC_s(B) \equiv 0 \notin (\det J_f)(3B) \quad (15)$$

where  $(\det J_f)(\mathbf{x})$  denotes expression obtained by evaluating the determinant of the Jacobian matrix  $J_f(\mathbf{x})$  with functional entries  $\partial_{x_j} f_i(\mathbf{x})$ . Finally, we evaluate  $(\det J_f)(\mathbf{x})$  on  $3B$ . Note that  $JC(B) \Rightarrow JC_s(B)$  and so the strict test is more efficacious. Unfortunately  $JC_s(B)$  cannot be used by our algorithm since it is known that  $JC_s(B)$  does not imply  $\#_f(3B) \leq 1$ . Nevertheless, we now show that it can serve as a uniqueness test in conjunction with the MK test:

**THEOREM 9.**

*If both  $JC_s(B)$  and  $MK(\frac{3}{2}B)$  succeed then  $\#_f(3B) = 1$ .*

It follows that we could use  $JC_s(B) \wedge MK(B)$  in our SIMPLE ISOLATE algorithm in the introduction.

## 6 THE MIRANDA ALGORITHM

Our main algorithm for root isolation is given in Figure 1. We use  $MK(B)$  and  $JC(B)$  (respectively) for its existence and Jacobian tests. It remains to specify the exclusion test  $C_0(B)$ :

$$C_0(B) \equiv (\exists i = 1, \dots, n)[0 \notin f_i(B)] \quad (16)$$

The algorithm in Figure 1 is abstract. To introduce the interval version  $\square\text{Miranda}$ , just replace the abstract tests by their interval analogues:  $\square MK(B)$ ,  $\square C_0(B)$  and  $\square JC(B)$ . In amounts to replacing the set theoretic function in the abstract definition by their interval analogues:

- $\square C_0(B)$ :  $\exists i = 1, \dots, n$  such that  $0 \notin \square f_i(B)$ ;
- $\square JC(B)$ :  $0 \notin \square \det(J(3B))$ ;
- In the definition of  $MK(B)$  (Section 3), replace each  $g_i(2B_i^\pm)$  by  $\square g_i(2B_i^\pm)$ .

Note that all these box forms are really mean value forms  $\square_M$ . For the effective version, we use the tests  $\square MK(B)$ ,  $\square C_0(B)$  and  $\square JC(B)$ , which is discussed in Section 8.

Termination of each version of *Miranda* follows from the complexity analysis below. Even if there are roots on the boundary of  $B_0$ , we will terminate, although the isolated root might lie in  $2B_0 \setminus B_0$ . But we first show that the output is correct when *Miranda* halts:

**THEOREM 10 (PARTIAL CORRECTNESS).**

1. If *Miranda* halts, the output queue  $P$  is correct.
2. The same holds for  $\square\text{Miranda}$  and  $\square_M\text{Miranda}$ .

## 7 COMPLEXITY UPPER BOUNDS

In this section, we derive a lower bound  $\lambda > 0$  on the size of boxes produced by *Miranda*. That is, any box  $B$  with width  $w(B) \leq \lambda$  would either be output or rejected. This implies that the subdivision tree is no deeper than  $\log_2(w(B_0)/\lambda)$ , yielding an upper bound on computational complexity. This bound  $\lambda$  will be expressed in terms of quantities determined by the zeros in  $2B_0$ . We first prove this for the abstract *Miranda*, then extend the results to  $\square\text{Miranda}$  and  $\square_M\text{Miranda}$ . From the algorithm, we see that a box  $B$  is output if  $\neg C_0(B) \wedge JC(B) \wedge MK(B)$  holds in line 10; it is rejected if one of the 2 following cases is true: (1)  $C_0(B)$  holds or (2) it is contained in  $3B'$  where  $JC(B')$  holds and a box in  $B'$  is output, as indicated in line 12. The boxes that contain a root of  $f$  will be finally verified by the former predicate and the boxes that contain no root of  $f$  will eventually be rejected in one of the 2 cases.

To prove the existence of such a  $\lambda$ , we need to look into the tests  $C_0(B)$ ,  $JC(B)$  and  $MK(B)$ . We will give bounds  $\lambda_{JC}$ ,  $\lambda_{MK}$  and  $\lambda_{C_0}$  for the 3 tests respectively and show that for any box  $B$  produced in the algorithm

- (1) if  $\#(B) > 0$ , it will pass  $MK(B)$  when  $w_B \leq \lambda_{MK}$ ,
- (2) if  $\#(B) > 0$ , it will pass  $JC(B)$  when  $w_B \leq \lambda_{JC}$ ;
- (3) if  $\#(B) = 0$  and  $B$  keeps a certain distance from the roots, it will pass  $C_0(B)$  when  $w_B \leq \lambda_{C_0}$ .

We have essentially proved item (1) in the Section 4. More precisely, for each root  $\alpha$ , we had defined a constant  $\lambda_2(\alpha)$ . We now set

$$\lambda_{MK} := \min_{\alpha \in \text{Zero}(2B_0)} \lambda_2(\alpha). \quad (17)$$

### 7.1 Sure Success for $C_0(B)$ and $JC(B)$

We study conditions to ensure the success of the tests  $JC$  and  $C_0$ . We will introduce constants  $\lambda_{JC}$ ,  $\lambda_{C_0}$  in analogy to (17).

First consider  $JC(B)$ . Let box  $B$  contain a simple root  $\alpha$ . By Mean Value Theorem,  $w(\frac{\partial f_i}{\partial x_j}(3B)) \leq 3w_B \cdot K(3B)_{ij}$  (see (8) for definition). Since  $\frac{\partial f_i}{\partial x_j}(\alpha) \in \frac{\partial f_i}{\partial x_j}(3B)$ , it holds  $\frac{\partial f_i}{\partial x_j}(3B) \subseteq [\frac{\partial f_i}{\partial x_j}(\alpha) - 3w_B \cdot K(3B)_{ij}, \frac{\partial f_i}{\partial x_j}(\alpha) + 3w_B \cdot K(3B)_{ij}]$  ( $\forall i, j = 1, \dots, n$ ). Denoting  $U(\alpha) := \max_{1 \leq i, j \leq n} |\frac{\partial f_i}{\partial x_j}(\alpha)|$  and  $V := \max_{1 \leq i, j \leq n} K(3B)_{ij}$ , we get  $|\frac{\partial f_i}{\partial x_j}(3B)| \leq U(\alpha) + 3Vw_B$  and  $w(\frac{\partial f_i}{\partial x_j}(3B)) \leq 3Vw_B$ . By applying the rules  $w(I_1 + I_2) = w(I_1) + w(I_2)$  and  $w(I_1 \cdot I_2) \leq w(I_1) \cdot |I_2| + w(I_2) \cdot |I_1|$  where  $I_1, I_2$  are intervals, we may verify by induction that  $w(\prod_{i=1}^n (\frac{\partial f_i}{\partial x_{\sigma_i}}(3B)) \leq 3nV(U(\alpha) + 3w_BV)^{n-1}w_B$

for any permutation  $\sigma$ . Hence, it follows  $w(\det(J_f(3B))) \leq 3n \cdot n! \cdot V(U(\alpha) + 3Vw_B)^{n-1}w_B$ .

Set  $\lambda_3(\alpha)$  to be the smallest positive root of the equation

$$|\det(J(\alpha))| - 3n \cdot n! \cdot V(U(\alpha) + 3Vx)^{n-1} \cdot x = 0. \quad (18)$$

The following lemma implies the existence of  $\lambda_{JC}$ :

**LEMMA 11.** *If box  $B$  contains a simple root  $\alpha$  and  $w_B < \lambda_3(\alpha)$  then  $JC(B)$  succeeds.*

Thus we may choose  $\lambda_{JC} := \min_{\alpha \in \text{Zero}(2B_0)} \lambda_3(\alpha)$  and set

$$\ell_1 := \min \{\lambda_{JC}, \lambda_{MK}\}$$

**LEMMA 12 (Lemma A).** *If  $\#(B) > 0$  and  $w_B \leq \ell_1$  then  $MK(B)$  and  $JC(B)$  holds.*

**COROLLARY 13.** *Each root in  $B_0$  will be output in a box of width  $> 3\ell_1/2$ .*

Let  $R_0 \subseteq 2B_0$  be a region that excludes discs around roots:

$$R_0 := 2B_0 \setminus \bigcup_{\alpha \in \text{Zero}(2B_0)} \mathring{\Delta}(\alpha, \ell_1)$$

where  $\mathring{\Delta}$  is the interior of  $\Delta$ . Denote the zero set of  $f_i$  as  $S_i$  for  $i = 1, \dots, n$  and define  $d_0 := \inf_{p \in R_0} \max_{i=1}^n \text{sep}(p, S_i)$ . Since all the roots in  $2B_0$  are removed from the set  $R_0$ , we can verify that  $\max_{i=1}^n \text{sep}(p, S_i) > 0$  for all  $p \in R_0$ . Combining with the compactness of  $R_0$ , we obtain  $d_0 > 0$ . Finally we set

$$\lambda_{C_0} := \frac{d_0}{2\sqrt{n}}.$$

**LEMMA 14 (Lemma B).** *Suppose  $\#(B) = 0$  with  $\text{sep}(\mathbf{m}_B, \text{Zero}(2B_0)) \geq \ell_1$ , if  $w_B \leq \lambda_{C_0}$  then  $C_0(B)$  holds.*

**LEMMA 15 (Lemma C).** *Every box produced by the Miranda has width  $\geq \frac{1}{4} \min \{\lambda_{C_0}, \lambda_{JC}, \lambda_{MK}\}$ .*

## 7.2 Sure Success for $C_0(B)$ and $JC(B)$

We now consider the interval tests  $JC$  and  $C_0$  under the assumption that the underlying interval forms involved are Lipschitz. Let  $\widehat{L}$  be a global Lipschitz constant for  $f_i$  and  $\frac{\partial f_i}{\partial x_j}$  for all  $i, j = 1, \dots, n$  in  $3B_0$ . We will develop corresponding bounds  $\lambda_{JC}$ ,  $\lambda_{C_0}$ . Observe that if we replace the bounds  $\lambda_{MK}, \lambda_{JC}, \lambda_{C_0}$  in the abstract version by the bounds  $\lambda_{MK}, \lambda_{JC}, \lambda_{C_0}$ , all the statements and proofs in the previous section remain valid. So in this section, we do not repeat the statements, except to give the bounds  $\lambda_{JC}$  and  $\lambda_{C_0}$ .

First look at the test  $JC(B)$ . With the same arguments as in abstract level, we obtain

$$\lambda_{JC} := \min_{\alpha \in \text{Zero}(2B_0)} \lambda_4(\alpha)$$

where  $\lambda_4(\alpha)$  is the smallest positive root of the

$$|\det(J(\alpha))| - 3n \cdot n! \cdot \widehat{L}(U(\alpha) + 3\widehat{L}x)^{n-1} \cdot x = 0. \quad (19)$$

With  $\lambda_{JC}$  and  $\lambda_{MK}$ , we have an interval analogue of Lemma A:

**LEMMA 16 (Lemma A).** *If  $\#(B) > 0$  and  $w_B \leq \ell'_1$  with*

$$\ell'_1 := \min \{\lambda_{JC}, \lambda_{MK}\},$$

*then  $MK(B)$  and  $JC(B)$  succeeds.*

Next look at the test  $C_0(B)$ . Arguing as in the abstract level, we only consider the boxes in the region  $R'_0 := 2B_0 \setminus \bigcup_{\alpha \in \text{Zero}(2B_0)} \mathring{\Delta}(\alpha, \ell'_1)$  with  $\ell'_1 := \min \{\lambda_{JC}, \lambda_{MK}\}$ . Define  $u := \inf_{p \in R'_0} \max_{i=1}^n \frac{|f_i(p)|}{\widehat{L}}$ .

It is easy to see that  $\max_{i=1}^n \frac{|f_i(p)|}{\widehat{L}} > 0$  for any  $p \in R'_0$ . Since the function  $|f_i(x)|$  is continuous and the set  $R'_0$  is compact, we obtain that  $u > 0$ . Setting  $\lambda_{C_0} := \frac{u}{2}$ , we have the following lemma:

**LEMMA 17 (Lemma B).** *Let  $\text{sep}(\mathbf{m}_B, \text{Zero}(2B_0)) > \ell'_1$  with  $\ell'_1 := \min \{\lambda_{JC}, \lambda_{MK}\}$ . If  $\#(B) = 0$  and  $w_B \leq \lambda_{C_0}$ , then  $C_0(B)$  succeeds.*

Combining Lemma A and Lemma B, we obtain:

**LEMMA 18 (Lemma C).** *Every box produced by the Miranda has width  $\geq \frac{1}{4} \min \{\lambda_{C_0}, \lambda_{JC}, \lambda_{MK}\}$ .*

## 8 EFFECTIVE MIRANDA

We now extend our results from  $\square$ Miranda to  $\widetilde{\square}$ Miranda by introducing the effective tests  $\widetilde{\square}MK(B)$ ,  $\widetilde{\square}JC(B)$  and  $\widetilde{\square}C_0(B)$ . Inside these tests are various box forms, say  $\square h(B)$ . Recall that they are actually mean value forms  $\square_M h(B)$  (we write " $\square h(B)$ " for simplicity). We convert each  $\square h(B)$  to its effective version  $\widetilde{\square} h(B)$ , whose output interval has dyadic endpoints and which satisfies  $\square h(B) \subseteq \widetilde{\square} h(B)$ . The main issue is the accuracy of the effective forms, which we express by upper bounds on the Hausdorff distance  $q(\square h(B), \widetilde{\square} h(B))$ . It is always bounded as a linear function of the width  $w_B$ , i.e.,  $q(\square h(B), \widetilde{\square} h(B)) = O(w_B)$ . However, we cannot stop here – the implicit constant in the asymptotic notation must be made explicit for implementation purposes.

Specifically, in  $\widetilde{\square}C_0(B)$ , we require  $q(\square f_i(B), \widetilde{\square} f_i(B)) \leq \frac{1}{16} w_B$  for each  $i = 1, \dots, n$ . In  $\widetilde{\square}MK(B)$ , we require  $q(\square_M g_i(2B_i^\pm), \square_M g_i(2B_i^\pm)) \leq \frac{1}{16} w_B$ . In  $\widetilde{\square}JC(B)$  we require that  $q(\square J_{ij}(3B), \widetilde{\square} J_{ij}(3B)) \leq \frac{1}{16} \cdot 3w_B$  for each entry  $\square J_{ij}(3B)$  of  $\square J(3B)$ . We get effective versions of all our lemmas and theorems, with modified constants such as  $\lambda_{JC}$  and  $\lambda_{C_0}$ .

## 9 CONCLUSION

We have provided the first effective subdivision algorithm Miranda for isolating simple real roots of a system of equations  $\mathbf{f} = \mathbf{0}$ , provided  $\mathbf{f}$  and its derivatives have interval forms. Our result are novel for its completeness (previous algorithms need  $\varepsilon$ -termination and has no isolation guarantees), its generality (going beyond the polynomial case), and its complexity analysis (going beyond termination proofs). We also contributed to the theory of subdivision algorithms by formalizing a 3-level description to provide a pathway from abstract algorithms to effective ones. Given that many existing numerical algorithms still lack effective versions, this is a promising line of work. In the future, we plan to implement and develop our algorithm into a practical tool.

## REFERENCES

- [1] Oliver Aberth. *Introduction to Precise Numerical Methods*. Elsevier Inc, Oxford, UK, second edition, 2007.
- [2] A. V. Aho, J. E. Hopcroft, and J. D. Ullman. *The Design and Analysis of Computer Algorithms*. Addison-Wesley, Reading, Massachusetts, 1974.



- [3] Götz Alefeld, Andreas Frommer, Gerhard Heindl, and Jan Mayer. On the existence theorems of Kantorovich, Miranda and Borsuk. *Electronic Transactions on Numerical Analysis*, 17:102–111, 2004.
- [4] Ruben Becker, Michael Sagraloff, Vikram Sharma, Juan Xu, and Chee Yap. Complexity analysis of root clustering for a complex polynomial. In *41st Int'l Symp. Symbolic and Alge. Comp.*, pages 71–78, 2016. ISSAC 2016. July 20–22, Wilfrid Laurier University, Waterloo, Canada.
- [5] Ruben Becker, Michael Sagraloff, Vikram Sharma, and Chee Yap. A near-optimal subdivision algorithm for complex root isolation based on Pellet test and Newton iteration. *J. Symbolic Computation*, 86:51–96, May–June 2018.
- [6] Lenore Blum, Felipe Cucker, Michael Shub, and Steve Smale. *Complexity and Real Computation*. Springer-Verlag, New York, 1998.
- [7] Gershon Elber and Myung-Soo Kim. Geometric constraint solver using multivariate rational spline functions. In *Proc. 6th ACM Symp. on Solid Modeling and Applications*, pages 1–10. ACM Press, 2001.
- [8] Peter Franek and Stefan Ratschan. Effective topological degree computation based on interval arithmetic. *CoRR*, abs/1207.6331, 2012.
- [9] Andreas Frommer and Bruno Lang. Existence Tests for Solutions of Nonlinear Equations Using Borsuk's Theorem. *SIAM J. Numer. Anal.*, 43(3):1348–1361, 2005.
- [10] Andreas Frommer, Bruno Lang, and Marco Schnurr. A comparison of the Moore and Miranda existence tests. *Computing*, 72(3–4):349–354, 2004.
- [11] Jürgen Garloff and Andrew P. Smith. Investigation of a subdivision based algorithm for solving systems of polynomial equations. *J. Nonlinear Analysis: Series A Theory and Methods*, 47(1):167–178, 2001.
- [12] Jürgen Garloff and Andrew P. Smith. Solution of systems of polynomial equations by using Bernstein expansion. In G. Alefeld, S. Rump, J. Rohn, and T. Yamamoto, editors, *Symbolic Algebraic Methods and Verification Methods (Dagstuhl 1999)*, pages 87–97. Springer, Vienna, 2001.
- [13] Alexandru Goldsztejn. Comparison of the Hansen-Sengupta and the Frommer-Lang-Schnurr existence tests. *Computing*, 79(1):53–60, 2007.
- [14] Rémi Imbach, Victor Pan, and Chee Yap. Implementation of a near-optimal complex root clustering algorithm. In *Proc. Int'l Congress on Mathematical Software*, 2018. 6th ICMS, Notre Dame University. July 24–27, 2018.
- [15] R Baker Kearfott. *Rigorous global search: continuous problems*, volume 13. Springer Science & Business Media, 2013.
- [16] John B Kioustelidis. Algorithmic error estimation for approximate solutions of nonlinear systems of equations. *Computing*, 19(4):313–320, 1978.
- [17] Alexander Kobel, Fabrice Rouillier, and Michael Sagraloff. Computing real roots of real polynomials ... and now for real! In *41st Int'l Symp. Symbolic and Alge. Comp.*, pages 303–310, 2016. July 19–22, Waterloo, Canada.
- [18] Jyh-Ming Lien, Vikram Sharma, Gert Vegter, and Chee Yap. Isotopic arrangement of simple curves: An exact numerical approach based on subdivision. In *ICMS 2014*, pages 277–282. Springer, 2014. LNCS No. 8592. Download from <http://cs.nyu.edu/exact/papers/> for version with Appendices and details on MK Test.
- [19] Long Lin and Chee Yap. Adaptive isotopic approximation of nonsingular curves: the parameterizability and nonlocal isotopy approach. *Discrete and Comp. Geom.*, 45(4):760–795, 2011.
- [20] R. E. Moore and J. B. Kioustelidis. A simple test for accuracy of approximate solutions to nonlinear (or linear) systems. *SIAM J. Numer. Anal.*, 17(4):521–529, 1980.
- [21] Ramon E. Moore. *Methods and Applications of Interval Analysis*. SIAM, Philadelphia, PA, 1995. Second Reprint.
- [22] B. Mourrain and J.-P. Pavone. Subdivision methods for solving polynomial equations. *J. Symbolic Computation*, 44(3):292–306, 2009.
- [23] Arnold Neumaier. *Interval Methods for Systems of Equations*. Cambridge University Press, Cambridge, 1990.
- [24] Helmut Ratschek and Jon Rokne. *Computer Methods for the Range of Functions*. Horwood Publishing Limited, Chichester, West Sussex, UK, 1984.
- [25] Michael Sagraloff and Kurt Mehlhorn. Computing real roots of real polynomials. *J. Symbolic Computation*, 73:46–86, 2016.
- [26] Evan C. Sherbrooke and Nicholas M. Patrikalakis. Computation of the solutions of nonlinear polynomial systems. *Computer Aided Geometric Design*, 10:379–405, 1993.
- [27] Pascal van Hentenryck, David McAllester, and Deepak Kapur. Solving polynomial systems using a branch and prune approach. *Siam J. Num. Analysis*, 34(2):797–827, 1997.
- [28] C. Yap, M. Sagraloff, and V. Sharma. Analytic root clustering: A complete algorithm using soft zero tests. In *The Nature of Computation. Logic, Algorithms, Applications*, volume 7921 of LNCS, pages 434–444. Springer, 2013.
- [29] Chee K. Yap. Symbolic treatment of geometric degeneracies. *J. Symbolic Computation*, 10:349–370, 1990.
- [30] Chee K. Yap. In praise of numerical computation. In S. Albers, H. Alt, and S. Näher, editors, *Efficient Algorithms*, volume 5760 of LNCS, pages 308–407. Springer-Verlag, 2009.

## A APPENDIX: ALL PROOFS

LEMMA 2 (MVT). *Given two points  $x, y \in \mathbb{R}^n$ , we have:*

(a)

$$J(x) = J(y) \pm K([\mathbf{x}, \mathbf{y}])\|\mathbf{x} - \mathbf{y}\| \quad (20)$$

(b)

$$f(\mathbf{x}) - f(\mathbf{y}) = (J(\mathbf{y}) \pm K([\mathbf{x}, \mathbf{y}])\|\mathbf{x} - \mathbf{y}\|) \cdot (\mathbf{x} - \mathbf{y}) \quad (21)$$

*Proof.* (a) We apply the Mean Value Theorem to each entry  $J_{ij} = \frac{\partial f_i}{\partial x_j}$ :

$$\begin{aligned} J_{ij}(\mathbf{x}) &= J_{ij}(\mathbf{y}) + \nabla J_{ij}(\tilde{\mathbf{y}}) \cdot (\mathbf{x} - \mathbf{y}) \quad \text{with } \tilde{\mathbf{y}} \in [\mathbf{x}, \mathbf{y}] \\ &= J_{ij}(\mathbf{y}) \pm K([\mathbf{x}, \mathbf{y}])_{ij}\|\mathbf{x} - \mathbf{y}\| \end{aligned}$$

(b) We apply the Mean Value Theorem twice. The first application gives:

$$\begin{aligned} f_i(\mathbf{x}) - f_i(\mathbf{y}) &= \nabla f_i(\tilde{\mathbf{y}}) \cdot (\mathbf{x} - \mathbf{y}) \\ &= (J_{i1}(\tilde{\mathbf{y}}), \dots, J_{in}(\tilde{\mathbf{y}})) \cdot (\mathbf{x} - \mathbf{y}) \end{aligned}$$

where  $\tilde{\mathbf{y}} \in [\mathbf{x}, \mathbf{y}]$  and  $J_{ij} := \frac{\partial f_i}{\partial x_j}$ . Applying the Mean Value Theorem again to each  $J_{ij}(\tilde{\mathbf{y}})$ :

$$\begin{aligned} J_{ij}(\tilde{\mathbf{y}}) &= J_{ij}(\mathbf{y}) + \nabla J_{ij}(\hat{\mathbf{y}}) \cdot (\mathbf{y} - \tilde{\mathbf{y}}) \quad \text{with } \hat{\mathbf{y}} \in [\mathbf{y}, \tilde{\mathbf{y}}] \\ &= J_{ij}(\mathbf{y}) \pm K([\mathbf{x}, \mathbf{y}])_{ij}\|\mathbf{x} - \mathbf{y}\| \end{aligned}$$

Hence

$$\begin{aligned} f_i(\mathbf{x}) - f_i(\mathbf{y}) &= (J_{i1}(\mathbf{y}) \pm K([\mathbf{x}, \mathbf{y}])_{i1}\|\mathbf{x} - \mathbf{y}\|, \dots, \\ &\quad J_{in}(\mathbf{y}) \pm K([\mathbf{x}, \mathbf{y}])_{in}\|\mathbf{x} - \mathbf{y}\|) \cdot (\mathbf{x} - \mathbf{y}) \end{aligned}$$

for  $i = 1, \dots, n$ . This proves (21). **Q.E.D.**

LEMMA 3. *For any simple root  $\alpha$  of  $f$ ,  $\lambda_1(\alpha)$  is well-defined.*

*Proof.* Note that  $s(0)$  is well-defined since  $\alpha$  is a simple root. We also deduce that  $s(0) < 0$  and that  $s(r) = s(0)$  for all  $r < 0$ . Thus  $\lambda_1(\alpha) > 0$  if it is well-defined. Let  $r^*$  be the smallest radius such that  $\Delta(\alpha, r^*)$  contains a critical point; if  $f$  has no critical point, then  $r^*$  is defined to be  $\infty$ . It follows that  $s(r^*) = r^* - \frac{1}{\infty} = r^*$ . Thus  $s(0) < 0 < s(r^*)$ . From the fact that  $\|J^{-1}(\Delta(\alpha, 2\sqrt{nr})) \cdot K(\Delta(\alpha, 2r))\|$  is a continuous non-decreasing function of  $r$  in the range  $[0, r^*)$ , we conclude that there exists some  $r \in (0, r^*)$  such that  $s(r) = 0$ . **Q.E.D.**

LEMMA 4. *Let box  $B$  contain a simple root  $\alpha$  of  $f$ .*

*If  $w_B \leq \lambda_1(\alpha)$ , the preconditioned system  $\mathbf{g}_B := J^{-1}(\mathbf{m}(B))\mathbf{f} = (g_1, \dots, g_n)$  is well-defined, and for all  $i = 1, \dots, n$ ,*

$$g_i(2B_i^+) \geq \frac{w_B}{4}, \quad g_i(2B_i^-) \leq -\frac{w_B}{4}.$$

*Proof.* For simplicity, we write  $\mathbf{m}(B)$  as  $\mathbf{m}$ . From the definition of  $\lambda_1(\alpha)$  and the fact that  $B$  contains  $\alpha$  we know that  $J^{-1}(\alpha)$  is well-defined.



Let  $\mathbf{x}$  be a point on the boundary of the box  $2B$ . Then

$$\begin{aligned} \mathbf{g}_B(\mathbf{x}) &= J^{-1}(\mathbf{m})\mathbf{f}(\mathbf{x}) && \text{(by definition of } \mathbf{g}_B) \\ &= J^{-1}(\mathbf{m})(\mathbf{f}(\boldsymbol{\alpha}) + (J(\boldsymbol{\alpha}) \pm K([\mathbf{x}, \boldsymbol{\alpha}])\|\mathbf{x} - \boldsymbol{\alpha}\|) \cdot (\mathbf{x} - \boldsymbol{\alpha})) && \text{(by MVT (21))} \\ &= J^{-1}(\mathbf{m})(J(\boldsymbol{\alpha}) \pm K([\mathbf{x}, \boldsymbol{\alpha}])\|\mathbf{x} - \boldsymbol{\alpha}\|) \cdot (\mathbf{x} - \boldsymbol{\alpha}) && \text{(since } \boldsymbol{\alpha} \text{ is a root)} \\ &= J^{-1}(\mathbf{m})(J(\mathbf{m}) \pm K([\boldsymbol{\alpha}, \mathbf{m}])\|\boldsymbol{\alpha} - \mathbf{m}\| \pm K([\mathbf{x}, \boldsymbol{\alpha}])\|\mathbf{x} - \boldsymbol{\alpha}\|) \cdot (\mathbf{x} - \boldsymbol{\alpha}) && \text{(by MVT (20))} \\ &= J^{-1}(\mathbf{m})(J(\mathbf{m}) \pm 2K(2B)\|\mathbf{x} - \boldsymbol{\alpha}\|) \cdot (\mathbf{x} - \boldsymbol{\alpha}) && \text{(since } \|\mathbf{m} - \boldsymbol{\alpha}\| \leq \|\boldsymbol{\alpha} - \mathbf{x}\|) \\ &= (\mathbf{1} \pm 2J^{-1}(\mathbf{m})K(2B)\|\mathbf{x} - \boldsymbol{\alpha}\|) \cdot (\mathbf{x} - \boldsymbol{\alpha}) && \text{(1 is the identity matrix).} \end{aligned}$$

The  $i$ -th component in  $\mathbf{g}_B(\mathbf{x})$  is the  $g_i$ ; thus

$$g_i(\mathbf{x}) = (x_i - \alpha_i) \pm 2(J^{-1}(\mathbf{m})K(2B)\|\mathbf{x} - \boldsymbol{\alpha}\|) \cdot (\mathbf{x} - \boldsymbol{\alpha}).$$

In the following, we write  $\lambda_1$  for  $\lambda_1(\boldsymbol{\alpha})$  and note that  $\boldsymbol{\alpha} \in B$  and  $w_B \leq \lambda_1$  implies

$$\left. \begin{aligned} m &\in \Delta_{\boldsymbol{\alpha}} \\ 2B &\subseteq \Delta_{\boldsymbol{\alpha}} \end{aligned} \right\}. \quad (22)$$

Thus:

$$\begin{aligned} &|g_i(\mathbf{x}) - (x_i - \alpha_i)| \\ &\leq 2\|J^{-1}(\mathbf{m})K(2B)\| \cdot \|\mathbf{x} - \boldsymbol{\alpha}\| \sum_{j=1}^n |x_j - \alpha_j| \\ &\leq 3nw_B \|J^{-1}(\mathbf{m})K(2B)\| \cdot \|\mathbf{x} - \boldsymbol{\alpha}\| && \text{(as } \sum_{j=1}^n |x_j - \alpha_j| \leq \frac{3}{2}nw_B) \\ &\leq \frac{9}{2}nw_B^2 \|J^{-1}(\mathbf{m})K(2B)\| && \text{(as } \|\mathbf{x} - \boldsymbol{\alpha}\| \leq \frac{3}{2}w_B) \\ &\leq \frac{w_B^2}{4} (18n\|J^{-1}(\mathbf{m})K(2B)\|) \\ &\leq \frac{w_B^2}{4} (18n\|J^{-1}(\Delta_{\boldsymbol{\alpha}})K(\Delta_{\boldsymbol{\alpha}})\|) && \text{from (22)} \\ &= \frac{w_B^2}{4} \cdot \frac{1}{\lambda_1} && \text{(definition of } \lambda_1) \\ &\leq \frac{w_B}{4} && \text{(since } w_B \leq \lambda_1). \end{aligned}$$

This last inequality gives

$$|g_i(\mathbf{x}) - (x_i - \alpha_i)| \leq w_B/4. \quad (23)$$

It remains to show that  $g_i(2B_i^+) \geq \frac{w_B}{4}$  (the proof that  $g_i(2B_i^-) \leq -\frac{w_B}{4}$  is similar). This amounts to proving  $g_i(\mathbf{x}) \geq \frac{w_B}{4}$  holds for all  $\mathbf{x} \in 2B_i^+$ . First we note that

$$x_i - \alpha_i \geq w_B/2 \quad (24)$$

since  $\mathbf{x} \in 2B_i^+$  and  $\boldsymbol{\alpha} \in B$ . The inequalities (23) and (24) together implies  $g_i(\mathbf{x})$  and  $x_i - \alpha_i$  must have the same sign. Since  $x_i - \alpha_i$  is positive, we conclude that  $g_i(\mathbf{x})$  must be positive. Combined with (23) and (24), we conclude that  $g_i(\mathbf{x}) \geq w_B/4$ , as claimed. **Q.E.D.**

**LEMMA 5.** Let  $f$  be a continuously differentiable function defined on a convex region  $S \subseteq \mathbb{R}^n$ . Then a Lipschitz constant for  $\square_{\mathbf{M}}f$  on  $S$  is

$$\sum_{k=1}^n \left| \square \frac{\partial f}{\partial x_j}(S) \right|.$$

*Proof.* Recall that  $\square_{\mathbf{M}}f(B) = f(\mathbf{m}(B)) + \square \nabla f(B)^T \cdot (B - \mathbf{m}(B)) = f(\mathbf{m}(B)) + \frac{1}{2}w_B \cdot \sum_{k=1}^n \square \frac{\partial f}{\partial x_j}(B)$  for any  $B \subseteq S$ . Thus  $w(\square_{\mathbf{M}}f(B)) = \frac{1}{2}w_B \cdot w(\sum_{k=1}^n \square \frac{\partial f}{\partial x_j}(B)) = \frac{1}{2}w_B \cdot \sum_{k=1}^n w(\square \frac{\partial f}{\partial x_j}(B)) \leq w_B \cdot$

$$\sum_{k=1}^n \left| \square \frac{\partial f}{\partial x_j}(B) \right| \leq w_B \cdot$$

$$\sum_{k=1}^n \left| \square \frac{\partial f}{\partial x_j}(S) \right|. \text{ The lemma follows. } \quad \mathbf{Q.E.D.}$$

**THEOREM 7.** Let  $B$  be a box containing a simple root  $\boldsymbol{\alpha}$  of width  $w_B \leq \lambda_1(\boldsymbol{\alpha})$ .

- (a) If  $w(\square \frac{\partial g_i(2B_i^+)}{\partial x_j}) \leq \frac{1}{32n}$  for each  $j = 1, \dots, n$ , then  $\mathbf{g}_B := J^{-1}(\mathbf{m}(B))\mathbf{f}$  is well-defined and  $\square \text{MK}(B)$  will succeed.
- (b) If  $w_B \leq \lambda_2(\boldsymbol{\alpha})$  with  $\lambda_2(\boldsymbol{\alpha}) := \min \{ \lambda_1(\boldsymbol{\alpha}), \widehat{\lambda}_1(\boldsymbol{\alpha}) \}$ , then  $\square \text{MK}(B)$  will succeed.

*Proof.* (a) We show the first part of the theorem. In Lemma 4, it is proven that when  $w_B \leq \lambda_1(\boldsymbol{\alpha})$ , the system  $\mathbf{g}_B$  is well-defined and it holds that  $g_i(B_i^+) \geq \frac{w_B}{4}$  and  $g_i(B_i^-) \leq -\frac{w_B}{4}$ . From Proposition 6, we have

$$\begin{aligned} q(\square_{\mathbf{M}}g_i(2B_i^+), g_i(2B_i^+)) &\leq 2w(2B) \sum_{j=1, j \neq i}^n w(\square \frac{\partial g_i(2B_i^+)}{\partial x_j}) \\ &\leq 4nw_B \cdot \max_{1 \leq j \leq n, j \neq i} w(\square \frac{\partial g_i(2B_i^+)}{\partial x_j}). \end{aligned}$$

By the convergence property of box functions,  $w(\square \frac{\partial g_i(2B_i^+)}{\partial x_j})$  approaches 0 when  $w_B$  approaches 0 for  $j = 1, \dots, n$ . Thus when  $w_B$  is small enough, we have  $w(\square \frac{\partial g_i(2B_i^+)}{\partial x_j}) \leq \frac{1}{32n}, \forall j = 1, \dots, n$ . Then

$$\begin{aligned} \square_{\mathbf{M}}g_i(2B_i^+) &\geq g_i(2B_i^+) - q(\square_{\mathbf{M}}g_i(2B_i^+), g_i(2B_i^+)) \\ &\geq \frac{w_B}{4} - 4nw_B \cdot \frac{1}{32n} = \frac{w_B}{8} > 0. \end{aligned}$$

Similar argument applies to  $\square_{\mathbf{M}}g_i(2B_i^-)$ . This gives the first part of the theorem.

(b) Now we prove the second part of the theorem. From the proof of the first part, it suffices to prove that when  $w_B \leq \lambda_2(\boldsymbol{\alpha})$ , the inequality  $w(\square \frac{\partial g_i(2B_i^+)}{\partial x_j}) \leq \frac{1}{32n}$  holds for all  $i, j = 1, \dots, n$ . To show this, we observe that

$$\begin{aligned} &w(\square \frac{\partial g_i(2B_i^+)}{\partial x_j}) \\ &= \sum_k [J^{-1}(\mathbf{m}(B))]_{ik} \cdot \square \frac{\partial f_j}{\partial x_k}(2B_i^+) \\ &\quad ([J^{-1}(\mathbf{m}(B))]_{ik} \text{ are the entries of } J^{-1}(\mathbf{m}(B))) \\ &< \sum_k \|J^{-1}(\Delta_{\boldsymbol{\alpha}})\| \cdot \square \frac{\partial f_j}{\partial x_k}(2B_i^+) \quad (2B \subset \Delta_{\boldsymbol{\alpha}}) \\ &< \|J^{-1}(\Delta_{\boldsymbol{\alpha}})\| \cdot 2nLw_B \quad (\square \frac{\partial f_j}{\partial x_k} \text{ are Lipschitz on } \Delta_{\boldsymbol{\alpha}}) \\ &\leq \frac{1}{32n} \quad (w_B \leq \frac{1}{64n^2L \cdot \|J^{-1}(\Delta_{\boldsymbol{\alpha}})\|}). \end{aligned}$$

**Q.E.D.**

**LEMMA 9.** If both  $\text{JC}_s(B)$  and  $\text{MK}(\frac{3}{2}B)$  succeed then  $\#_{\mathbf{f}}(3B) = 1$ .

*Proof.* From [8], the success of  $\text{MK}(\frac{3}{2}B)$  implies

$$\sum_{\mathbf{y} \in \text{Zero}(3B)} \text{sign}(\det J_{\mathbf{f}}(\mathbf{y})) = \pm 1$$

where  $\text{sign}(\det J_{\mathbf{f}}(\mathbf{y}))$  is the sign of  $\det J_{\mathbf{f}}(\mathbf{y})$ . By the success of  $\text{JC}(B)$ , we further know that  $\text{sign}(\det J_{\mathbf{f}}(\mathbf{y}))$  is the same for all  $\mathbf{y} \in 3B$ . Thus there is only one root in  $3B$ . **Q.E.D.**

## THEOREM 10 (PARTIAL CORRECTNESS).

1. If `Miranda` halts, the output queue  $P$  is correct.
2. The same holds for  $\square$ `Miranda` and  $\widetilde{\square}$ `Miranda`.

*Proof.*

We first argue that the partial correctness of  $\square$ `Miranda` and  $\widetilde{\square}$ `Miranda` follows from the partial correctness of `Miranda` by the general observation<sup>5</sup> that the predicates in `Miranda` are one-sided, and (as can be verified below) none of our arguments are predicated upon the *failure* of the tests. We need to further note that for the effective version, we must assume that the ROI  $B_0$  is a dyadic box, so that all subdivisions are done without approximation.

Hence it remains to prove the partial correctness of `Miranda`:

(1) We note that each output box in  $P$  is isolating. A box  $2B$  is output in line 11 upon passing  $\text{MK}(B)$ . This is inside the inner while loop for subboxes of some  $B'$  which passes  $\text{JC}(B')$ . But  $\text{MK}(B)$  implies  $\#(2B) \geq 1$  and  $\text{JC}(B')$  implies  $\#(3B) \leq 1$ . Thus  $\#(2B) = 1$ .

(2) Next we claim no root is output twice in  $P$ . This follows by showing that if  $2B$  and  $2B'$  are output, then their interiors are disjoint. It does not matter if the boundaries of  $2B$  and  $2B'$  intersect because there are no roots on their boundary – this is ensured by the success of the Simple `Miranda` test on these output boxes. The reason for our concern comes from the fact that, although the boxes in  $Q$  have pairwise disjoint interiors, each  $B$  in  $Q$  can cause a larger box ( $2B$ ) to be output.

*CLAIM:* Suppose  $2B$  is output in line 11. Then immediately after line 12, every box  $B'$  in  $Q$ , the interior of  $2B'$  is disjoint from  $2B$ . Pf: Suppose the interior of  $2B'$  intersects  $2B$ . By the priority queue property, we have  $w(B') \leq w(B)$ . It follows that  $B'$  actually is contained in the annulus  $3B \setminus B$ . This follows from two facts<sup>6</sup> about aligned boxes: (a) any two aligned boxes have disjoint interiors or have a containment relationship, and (b)  $3B \setminus B$  is a union of 8 aligned boxes. If  $B'$  is contained in this annulus, then line 12 would have removed it. This proves our claim.

(3) We must show that

$$\mathcal{Z}_f(B_0) \stackrel{(*)}{\subseteq} \bigcup_{B \in P} \mathcal{Z}_f(B) \stackrel{(**)}{\subseteq} \mathcal{Z}_f(2B_0).$$

The second containment (\*\*) is immediate because all our output boxes have the form  $2B$  where  $B$  is an aligned box. Such boxes are contained in  $2B_0$ . To show (\*), it suffices to prove that if  $B'$  is a discarded box, then either  $B'$  has no roots, or any root in  $B'$  is already output. From the algorithm, a box  $B'$  is discarded in two lines: The first is Line 4, when  $\text{C}_0(B')$  succeeds. But this implies  $B$  has no roots. The second is Line 12 of the algorithm. Since  $B'$  is contained in  $3B$  (where  $2B$  is the output). We know that  $\text{JC}(B)$  holds, and thus there is at most one root in  $3B$ . So if  $B'$  contains any root, it must be the root already identified by  $2B$ . Thus, all discarded boxes are justified.

**Q.E.D.**

<sup>5</sup> If we were proving termination, the reverse implication hold: if  $\widetilde{\square}$ `Miranda` terminates then `Miranda` terminates.

<sup>6</sup> Here **aligned boxes** means those that can arise by repeated subdivision of  $B_0$ . Clearly  $B$  and  $B'$  are aligned, but  $kB$  and  $kB'$  are not aligned for any  $k > 1$ .

LEMMA 11. If box  $B$  contains a simple root  $\alpha$  and  $w_B < \lambda_3(\alpha)$  then  $\text{JC}(B)$  succeeds.

*Proof.* The fact  $\alpha \in B$  implies  $J(\alpha) \in J(3B)$ . Since  $\alpha$  is a simple root, we have  $\det(J(\alpha)) \neq 0$ , and thus  $\lambda_3(\alpha) \neq 0$ . From the definition of  $\lambda_3(\alpha)$ , we know that if  $w_B < \lambda_3(\alpha)$ , then  $3n \cdot n! \cdot V(U(\alpha) + 3Vw_B)^{n-1} \cdot w_B < |\det(J(\alpha))|$ , and thus  $w(\det(J(3B))) < |\det(J(\alpha))|$ . It follows  $0 \notin \det(J(3B))$ . The test  $\text{JC}(B)$  succeeds.

**Q.E.D.**

LEMMA 14 (**Lemma B**). Suppose  $\#(B) = 0$  with  $\text{sep}(\mathbf{m}_B, \text{Zero}(2B_0)) \geq \ell_1$ , if  $w_B \leq \lambda_{\text{C}_0}$  then  $\text{C}_0(B)$  holds.

*Proof.* Since  $\text{sep}(\mathbf{m}_B, \text{Zero}(2B_0)) > \ell_1$ , we have  $\mathbf{m}_B \in R_0$ . Thus  $\max_{i=1}^n \text{sep}(\mathbf{m}_B, \mathcal{S}_i) \geq d_0$ . Combining  $w_B \leq \lambda_{\text{C}_0}$ , it follows that  $\max_{i=1}^n \text{sep}(B, \mathcal{S}_i) \geq d_0 - \sqrt{n}w_B \geq d_0/2$ . Hence there exists  $i \in [1, n]$  such that  $B \cap \mathcal{S}_i = \emptyset$ . Thus  $\text{C}_0(B)$  holds.

**Q.E.D.**

LEMMA 15 (**Lemma C**). Every box produced by the `Miranda` has width  $\geq \frac{1}{4} \min \{\lambda_{\text{C}_0}, \lambda_{\text{JC}}, \lambda_{\text{MK}}\}$ .

*Proof.* We first give an equivalent statement of the lemma: for any box  $B$  produced in the algorithm, if  $w_B \leq \frac{1}{2} \min \{\lambda_{\text{C}_0}, \ell_1\}$ , then  $B$  has been output or rejected. In what follows, we will prove this equivalent statement.

Case 1,  $\#(B) > 0$ : Thus some ancestor of  $B$  should have output according to Lemma 12, a contradiction.

Case 2,  $\#(B) = 0$ ,  $\text{sep}(\mathbf{m}_B, \text{Zero}(2B_0)) \geq \ell_1$ . We contradict Lemma 14 directly.

Case 3,  $\#(B) = 0$ ,  $\text{sep}(\mathbf{m}_B, \text{Zero}(2B_0)) < \ell_1$ . Without loss of generality, assume that  $\text{sep}(\mathbf{m}_B, \alpha) < \ell_1$ . Since  $w_B \leq \frac{1}{2} \min \{\lambda_{\text{C}_0}, \ell_1\}$ , by the Corollary to Lemma 12, we know that some box  $B'$  containing  $\alpha$  of width  $> \ell_1/2$  has been output (this uses the fact that we process the boxes in a breadth-first-manner). This output also removes all the boxes in the process queue that intersect the interior of  $3B'$ . We can see that  $B$  intersects  $3B'$  because  $w_{B'} > \ell_1/2$ ,  $\alpha \in B'$  and  $\text{sep}(\mathbf{m}_B, \alpha) < \ell_1$ . Thus  $B$  should have been removed. Contradiction.

**Q.E.D.**

LEMMA 17 (**Lemma  $\square$ B**). Let  $\text{sep}(\mathbf{m}_B, \text{Zero}(2B_0)) > \ell'_1$  with  $\ell'_1 := \min \{\lambda_{\square \text{JC}}, \lambda_{\square \text{MK}}\}$ . If  $\#(B) = 0$  and  $w_B \leq \lambda_{\square \text{C}_0}$ , then  $\square \text{C}_0(B)$  succeeds.

*Proof.* The Proof is similar to that of Lemma 14. Since  $\text{sep}(\mathbf{m}_B, \text{Zero}(2B_0)) > \ell'_1$ , we have  $\mathbf{m}_B \in R'_0$ .

By the definition of  $u$ , we see  $\max_{i=1}^n \frac{|f_i(\mathbf{m}_B)|}{\widehat{L}} \geq u$ , which means that  $\exists j \in [1, n]$  such that  $\frac{|f_j(\mathbf{m}_B)|}{\widehat{L}} \geq u$ . By the inclusion property of box functions,  $f_j(\mathbf{m}_B) \in \square f_j(B)$ . Since  $w_B \leq \lambda_{\square \text{C}_0} = \frac{u}{2}$ , we have  $w(\square f_j(B)) \leq \widehat{L} \cdot w_B \leq \frac{u}{2}$ . It follows that  $\square f_j(B) \geq f_j(\mathbf{m}_B) - w(\square f_j(B)) \geq u - \frac{u}{2} > 0$ . Thus  $0 \notin \square f_j(B)$  and  $\square \text{C}_0$  holds.

**Q.E.D.**