IMA Journal of Numerical Analysis (2002) **22**, 167–185

Finding zeros by multilevel subdivision techniques

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[Received on 21 July 2000; revised on 16 April 2001]

We present a new set oriented numerical method for the detection of all the zeros of a given (smooth) function $g : \mathbb{R}^n \to \mathbb{R}^n$ within a compact region. The underlying idea is to view classical iteration schemes as specific dynamical systems and to apply adaptive multilevel subdivision techniques for the computation of their fixed points. These techniques have previously been developed for the identification of arbitrary invariant sets of dynamical systems. Based on this idea we construct a subdivision algorithm which allows us to create close coverings of the set of zeros of g. We prove convergence of this algorithm in a general abstract context and propose three different realizations which are motivated by the theoretical results. Finally, we discuss the numerical efficiency of these algorithms by a comparison with a standard zero finding procedure using a routine from the NAG library.

Keywords: Newton's method, step size control, global zero finding

1. Introduction

In many applications in natural science or engineering the problem arises to detect all the zeros of a given smooth function $g : \mathbb{R}^n \to \mathbb{R}^n$ within a certain compact region $Q \subset \mathbb{R}^n$. One way to attack this problem is to choose randomly a large number of initial points inside Q and to apply a classical iteration scheme—e.g. a damped Newton method—to these points for a certain number of times. Using this approach there is a fair amount of uncertainty as to whether or not one has found all the zeros of g within Q. In principle, this problem can be avoided by applying zero finding procedures which are based on *interval analysis* (see e.g. Alefeld & Herzberger, 1983; Hansen, 1992 or Kearfott, 1996). However, due to the nature of these techniques there is a tradeoff between rigour and computing time so that these methods are typically just applicable in the case where the dimension n is not too large.

Another way for locating all the zeros of a given function is given by *homotopy methods* (see e.g. Chow *et al.*, 1978 and Allgower & Georg, 1990). Although these methods are in general non-rigorous they can in certain cases be used to find the entire zero set (see e.g. Morgan, 1987 and Verschelde & Haegemans, 1994) in the situation where the underlying function is polynomial. Finally, there are also global numerical techniques which are based on the adaptive refinement of Q into smaller subsets and by which all the zeros of g are approximated by outer coverings (see e.g. Ying & Katz, 1988, 1989 and Dellnitz *et al.*, 2002) in the case where $g : \mathbb{C} \to \mathbb{C}$ is a holomorphic function or Horst & Tuy (1996) in the context of problems in global optimization.

In this paper we propose a new approach which in principle fits into the last category: that is, we propose an adaptive multilevel scheme for the outer approximation of the set of zeros of g inside a specified compact set Q. The underlying idea is to view iteration schemes such as Newton's method as dynamical systems and then to apply adaptive set-oriented numerical methods which have recently been developed for the approximation of invariant sets of dynamical systems (Dellnitz & Hohmann, 1997; Dellnitz & Junge, 1998). Observe that the zeros of g are fixed points for the iteration schemes and therefore represent particular low-dimensional invariant sets.

In practice we would like to work with iteration schemes with variable step size such as the damped Newton method since this makes the computations both more reliable and more efficient. But this implies that the dynamical systems under consideration (i.e. the numerical iteration schemes) are depending on a parameter (i.e. the step size). This is the reason why we have to extend previous work on the approximation of invariant sets of single dynamical systems to the situation where one is interested in the computation of the common invariant sets of a finite number of different dynamical systems $f_1, \ldots, f_s$. In fact, in Section 2 we generalize the analytical results in Dellnitz & Hohmann (1997) to this situation and develop a subdivision algorithm for the outer approximation of the common global attractor of $f_1, \ldots, f_s$ inside a compact subset of state space. Moreover, we prove convergence of this abstract multilevel algorithm as long as every dynamical system is applied infinitely often in the course of the subdivision procedure (Proposition 2.7).

The theoretical results in Section 2 are not restricted to the situation where the underlying dynamical systems are produced by iteration schemes, and in Section 3 we show how these general results apply in the particular context of zero finding. Moreover, we discuss the effect of choosing different step sizes on the behaviour of the subdivision algorithm by a couple of motivating examples. This experience leads to the development of two algorithms based on different *a priori* step size strategies (Section 4) and of an adaptive algorithm based on the Armijo step size (Section 5). In principle, these algorithms allow us to determine arbitrarily close coverings of the set of zeros of the function g. However, in practice we would switch to a classical iteration scheme as soon as a particular level of refinement has been reached. Finally, we compare and discuss the numerical efficiency of these different approaches, and we also compare our method with a global zero finding procedure based on a routine taken from the NAG[†] library (Section 6).

2. The generalized subdivision algorithm

We consider a finite collection of discrete dynamical systems of the type

$$x_{j+1} = f_l(x_j), \qquad j = 0, 1, 2, \ldots,$$

where we assume for simplicity that each $f_l : \mathbb{R}^n \to \mathbb{R}^n$ $(l = 1, \ldots, s)$ is a diffeomorphism. The purpose is to develop a set-oriented numerical method for the approximation of those subsets of state space which are invariant for the *entire collection* of dynamical systems. More precisely, we want to approximate a subset $A \subset \mathbb{R}^n$ such that

$$f_l(A) = A \quad \text{for } l = 1, \ldots, s.$$

[†]http://www.nag.com

With this technique we generalize a known subdivision algorithm for the computation of invariant sets of single dynamical systems. See Dellnitz & Hohmann (1997); Dellnitz & Junge (1998) or Dellnitz *et al.* (2000) for generalizations of this approach. This new version of the subdivision algorithm will be the basis for the detection of zeros of a given function using Newton's method with different step sizes as the family of dynamical systems. In fact, in this case the set A consists of all the fixed points of the family of (damped) Newton iterations.

2.1 *Relative global attractors*

Given a compact subset $Q \subset \mathbb{R}^n$ the subdivision algorithm in Dellnitz & Hohmann (1997) allows us to compute the backward invariant set

$$A_{Q,f} = \bigcap_{j \geqslant 0} f^j(Q) \tag{2.1}$$

of a dynamical system $f : Q \to \mathbb{R}^n$. We now modify this definition to the present context in which we have to consider a finite set of different dynamical systems.

We begin by introducing some notations. Denote by

$$\Omega = \{1, 2, \ldots, s\}^{\mathbb{N}_0}$$

the set of all sequences of the symbols $\{1, 2, \ldots, s\}$. For $\omega = (\omega_i) \in \Omega$ set $\omega^j = (\omega_0, \omega_1, \ldots, \omega_{j-1})$ and define for $j \geqslant 1$

$$f_{\omega^j} = f_{\omega_{j-1}} \circ \cdots \circ f_{\omega_0}.$$

DEFINITION 2.1 Let $f_1, \ldots, f_s : \mathbb{R}^n \to \mathbb{R}^n$ be diffeomorphisms and let $Q \subset \mathbb{R}^n$ be compact. Then we define the *relative global attractor* of $f_1, \ldots, f_s$ with respect to Q as

$$A_{Q,f_1,\ldots,f_s} = \bigcap_{\omega \in \Omega} \bigcap_{j \geqslant 1} f_{\omega^j}(Q) \cap Q. \tag{2.2}$$

Observe that $A_{Q,f_1,\ldots,f_s}$ is contained in the intersection of all the standard relative global attractors A_{Q,f_i}, see (2.1). Moreover, it contains every set A which is invariant for each f_l, $l = 1, \ldots, s$.

EXAMPLE 2.2 Let $f_l : \mathbb{R}^n \to \mathbb{R}^n$, $l = 1, 2$, be defined as

$$f_1(x) = 3x \qquad \text{and} \qquad f_2(x) = \tfrac{1}{2}x,$$

and let $Q \subset \mathbb{R}^n$ be a compact convex subset containing the origin. Then the relative global attractors are given by

$$A_{Q,f_1} = Q \quad \text{and} \quad A_{Q,f_2} = \{0\}.$$

It follows that in this case $A_{Q,f_1,f_2} = \{0\}$.

The following basic facts on relative global attractors can immediately be obtained from the definitions.

LEMMA 2.3 Let $A_{Q,f_1,\ldots,f_s}$ be the relative global attractor for the dynamical systems $f_1, \ldots, f_s$ with respect to Q. Then

$$A_{Q,f_1,\ldots,f_s} = \{x \in Q : f_{\omega^j}^{-1}(x) \in Q \quad \text{for all } \omega \in \Omega \text{ and } j \geqslant 0\}.$$

In particular, $A_{Q,f_1,\ldots,f_s}$ is backward invariant for every f_l, that is

$$f_l^{-1}(A_{Q,f_1,\ldots,f_s}) \subset A_{Q,f_1,\ldots,f_s} \quad \text{for all } l \in \{1, \ldots, s\}. \tag{2.3}$$

2.2 *Computation of relative global attractors*

We now present an algorithm for the numerical computation of the relative global attractor $A_{Q,f_1,\ldots,f_s}$ where $f_1, \ldots, f_s$ are diffeomorphisms. Using a multilevel subdivision scheme this method produces a sequence of sets $\mathcal{B}_0, \mathcal{B}_1, \mathcal{B}_2, \ldots$ where each $\mathcal{B}_k$ consists of finitely many subsets of Q covering the relative global attractor $A_{Q,f_1,\ldots,f_s}$. In the following we will call the elements B of $\mathcal{B}_k$ *boxes*. By our construction, the diameter

$$\operatorname{diam}(\mathcal{B}_k) = \max_{B \in \mathcal{B}_k} \operatorname{diam}(B)$$

converges to zero for $k \to \infty$.

In order to guarantee convergence we have to assume that each dynamical system is applied infinitely often in the subdivision procedure. To make this precise we choose a sequence $\{u_k\}_{k=1}^{\infty}$ with $u_k \in \{1, \ldots, s\}$ which has the property

$$|\{k : u_k = l\}| = \infty \quad \text{for each } l = 1, \ldots, s. \tag{2.4}$$

We now describe the multilevel subdivision procedure in detail.

The subdivision algorithm. Let $\mathcal{B}_0$ be an initial collection of finitely many subsets of the compact set Q such that $\cup_{B \in \mathcal{B}_0} B = Q$. Then $\mathcal{B}_k$ is inductively obtained from $\mathcal{B}_{k-1}$ in two steps:

(i) Subdivision. Construct from $\mathcal{B}_{k-1}$ a new system $\hat{\mathcal{B}}_k$ of subsets such that

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

and

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

where $0 < \theta_{\min} \leqslant \theta_k \leqslant \theta_{\max} < 1$.

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

$$\mathcal{B}_k = \{B \in \hat{\mathcal{B}}_k : \text{there exists } \hat{B} \in \hat{\mathcal{B}}_k \text{ such that } f_{u_k}^{-1}(B) \cap \hat{B} \neq \emptyset\}.$$

(Here u_k is an element of the sequence defined above, see (2.4).)

Our aim is to show that this algorithm indeed converges to the relative global attractor as k tends to infinity.

Let Q_k be the union of subsets in $\mathcal{B}_k$,

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

In particular, we have $Q_0 = Q$. In analogy to the proof of the convergence result for the classical subdivision procedure we divide the proof into three parts. In a first step we show that the relative global attractor is always covered by the sets Q_k.

LEMMA 2.4 Let $A_{Q,f_1,\ldots,f_s}$ be the relative global attractor of $f_1, \ldots, f_s$ with respect to Q. Then

$$A_{Q,f_1,\ldots,f_s} \subset Q_k \quad \text{for all } k \in \mathbb{N}.$$

Proof. By definition, see (2.2), we have that $A_{Q,f_1,\ldots,f_s} \subset Q_0 = Q$. Now suppose that there is an $x \in A_{Q,f_1,\ldots,f_s} \subset Q_{k-1}$ such that $x \notin Q_k$. Then there is a box $B \in \hat{\mathcal{B}}_k$ with $x \in B$, and B is removed from the collection in step k. In particular, $f_{u_k}^{-1}(B) \cap Q_{k-1} = \emptyset$ and therefore $f_{u_k}^{-1}(x) \notin Q_{k-1}$. But this contradicts the fact that $f_{u_k}^{-1}(A_{Q,f_1,\ldots,f_s}) \subset A_{Q,f_1,\ldots,f_s} \subset Q_{k-1}$, see Lemma 2.3. □

In the next step we show that a subset $A \subset Q$ is contained in the relative global attractor $A_{Q,f_1,\ldots,f_s}$ if it is backward invariant for each f_l, $l = 1, \ldots, s$.

LEMMA 2.5 Let $A \subset Q$ be a subset which is backward invariant for each $f_1, \ldots, f_s$, that is

$$f_l^{-1}(A) \subset A \quad \text{for } l = 1, \ldots, s.$$

Then A is contained in the relative global attractor of $f_1, \ldots, f_s$, that is

$$A \subset A_{Q,f_1,\ldots,f_s}.$$

Proof. By assumption we have

$$A \subset f_l(A) \quad \text{for all } l \in \{1, \ldots, s\},$$

and this implies that

$$A \subset f_{\omega^j}(A) \quad \text{for all } \omega \in \Omega \text{ and } j \geqslant 0.$$

Moreover, $A \subset Q$ and therefore

$$A \subset \bigcap_{\omega \in \Omega} \bigcap_{j \geqslant 1} f_{\omega^j}(A) \cap Q \subset \bigcap_{\omega \in \Omega} \bigcap_{j \geqslant 1} f_{\omega^j}(Q) \cap Q = A_{Q,f_1,\ldots,f_s}.$$

□

Now the Q_k form a nested sequence of compact subsets of Q and therefore the limit

$$Q_\infty = \bigcap_{k=0}^{\infty} Q_k$$

does exist. We now show that Q_∞ is backward invariant for each dynamical system f_l ($l = 1, \ldots, s$).

LEMMA 2.6 The set Q_∞ is contained in Q and backward invariant for each f_l $(l = 1, \ldots, s)$, that is

$$f_l^{-1}(Q_\infty) \subset Q_\infty \quad \text{for } l = 1, \ldots, s.$$

Proof. Obviously $Q_\infty \subset Q$. For contradiction suppose that there is an $l \in \{1, \ldots, s\}$ and a $y \in Q_\infty$ such that $f_l^{-1}(y) \notin Q_\infty$. Since Q_∞ is compact it follows that there is a $\delta > 0$ with

$$d(f_l^{-1}(y), Q_\infty) > \delta.$$

Here d denotes the usual distance between a point and a set. Thus, there is an $N \in \mathbb{N}$ such that

$$d(f_l^{-1}(y), Q_k) > \delta/2 \quad \text{for all } k \geqslant N.$$

Now $y \in Q_\infty$ and therefore there exist boxes $B_k(y) \in \mathcal{B}_k$ with $y \in B_k(y)$ for all $k \in \mathbb{N}_0$. Since $\lim_{k\to\infty} \operatorname{diam}(\mathcal{B}_k) = 0$ and since f_l is continuous there exists an $m > N$ such that $u_m = l$ and $f_l^{-1}(B_m(y)) \cap Q_m = \emptyset$. (Here we have used the property (2.4) of the sequence $\{u_k\}$.) By the selection step of the subdivision algorithm this is a contradiction to the fact that $y \in Q_\infty \subset Q_{m+1}$. □

Combining the lemmas we now show that the subdivision algorithm indeed converges to the relative global attractor $A_{Q,f_1,\ldots,f_s}$.

PROPOSITION 2.7 Let $A_{Q,f_1,\ldots,f_s}$ be the relative global attractor of $f_1, \ldots, f_s$ with respect to $Q \subset \mathbb{R}^n$. Then the subdivision algorithm converges to $A_{Q,f_1,\ldots,f_s}$, that is

$$A_{Q,f_1,\ldots,f_s} = Q_\infty.$$

Proof. Lemma 2.4 states that $A_{Q,f_1,\ldots,f_s} \subset Q_k$ for all $k \in \mathbb{N}$ which implies that $A_{Q,f_1,\ldots,f_s} \subset Q_\infty$. By Lemma 2.6 Q_∞ is a backward invariant subset of Q for each $f_1, \ldots, f_s$. Therefore Lemma 2.5 implies that $Q_\infty \subset A_{Q,f_1,\ldots,f_s}$ and we obtain

$$A_{Q,f_1,\ldots,f_s} \subset Q_\infty \subset A_{Q,f_1,\ldots,f_s}$$

as desired. □

Observe that the limit Q_∞ does not depend on the particular sequence $\omega = \{u_k\}$ which is chosen in the subdivision algorithm. The only criterion which has to be satisfied is (2.4). Moreover, the following example shows that in general

$$A_{Q,f_1,\ldots,f_s} \neq \bigcap_{j\geqslant 1} f_{\omega^j}(Q) \cap Q,$$

where $\omega^j = (u_1, u_2, \ldots, u_j)$.

EXAMPLE 2.8 Let $Q = [-1, 1]$ and consider the dynamical systems $f_i : \mathbb{R} \to \mathbb{R}$ $(i = 1, 2)$ with $f_1(x) = 0{\cdot}5x$ and $f_2(x) = 2x$. Then we choose the sequence

$$\{u_k\}_{k=1}^\infty = \{2, 2, 1, 2, 2, 1, 2, 2, 1, \ldots\}.$$

Obviously this sequence satisfies (2.4), but it is easy to see that

$$\bigcap_{j\geqslant 1} f_{\omega^j}(Q) \cap Q = [-1, 1] \neq \{0\} = A_{Q,f_1,f_2}.$$

REMARKS 2.9

(a) Since Q_∞ is the limit of the Q_k, we can reformulate Proposition 2.7 as

$$\lim_{k\to\infty} h(A_{Q,f_1,\ldots,f_s}, Q_k) = 0,$$

where $h(B, C)$ denotes the standard Hausdorff distance between two compact sets $B, C \subset \mathbb{R}^n$.

(b) It is obvious that the speed of convergence to the relative global attractor will in general crucially depend on the choice of the sequence $\{u_k\}$. In fact, for an efficient numerical realization one would expect that the u_k should not be constant for a large number of successive indices k.

(c) Proposition 2.7 can be extended to the case where one has countably many different dynamical systems f_l with $l \in \mathbb{N}$. However, the sequence $\{u_k\}$ still has to be chosen in such a way that (2.4) holds for each $l \in \mathbb{N}$.

2.3 *Realization of the subdivision algorithm*

The numerical realization of the subdivision procedure is very similar to the one for the classical subdivision algorithm in Dellnitz & Hohmann (1997): rather than working explicitly with centres and radii of the boxes these are stored within a binary tree which leads to a significant reduction in the memory requirement.

The selection step is discretized via *test points* which are typically chosen within each box by one of the following strategies:

(i) The test points lie on an *a priori* specified fixed grid within each single box. This typically works quite well in low-dimensional problems.

(ii) The test points are chosen at random. This strategy is chosen in higher-dimensional problems.

(iii) More recently an adaptive choice for the set of test points has been suggested in Junge (1999) where Lipschitz estimates on the underlying dynamical system are taken into account. This method works particularly well for dynamical systems which do not arise via a discretization of an underlying ordinary differential equation.

For a detailed discussion of aspects concerning the implementation see Dellnitz & Hohmann (1997) and Junge (1999).

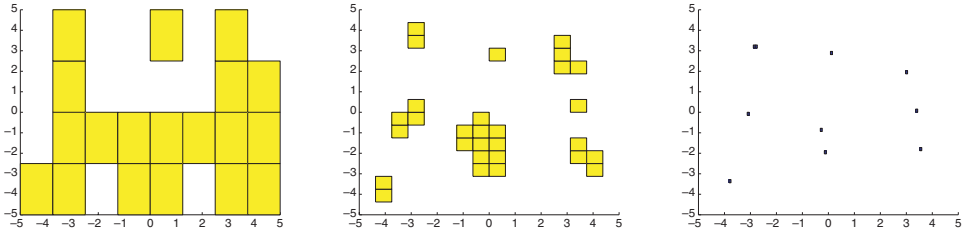
3. The location of zeros

Based on the theoretical results that we have developed so far we now consider the problem of finding all the zeros of a given function $g : \mathbb{R}^n \to \mathbb{R}^n$ inside a specified compact subset $Q \subset \mathbb{R}^n$. We motivate our techniques with the following two examples.

EXAMPLES 3.1

(a) First we consider the function $g : \mathbb{R}^2 \to \mathbb{R}^2$

$$g(x_1, x_2) = \begin{pmatrix} 4x_1(x_1^2 + x_2 - 11) + 2(x_1 + x_2^2 - 7) \\ 2(x_1^2 + x_2 - 11) + 4x_2(x_1 + x_2^2 - 7) \end{pmatrix}$$



(a) $k = 5$ (b) $k = 8$ (c) $k = 11$

FIG. 1. Application of the subdivision algorithm using Newton's method as the only dynamical system. The box collections $\mathcal{B}_5$, $\mathcal{B}_8$ and $\mathcal{B}_{11}$ are shown.

which is the gradient of an objective function proposed in Himmelblau (1972). We would like to find all the zeros of g within the compact set $Q = [-5, 5] \times [-5, 5]$.

In this example we set $s = 1$ and use the classical Newton function Ng as the only underlying dynamical system. The result of the computations is quite promising, see Fig. 1. All the nine zeros within the given domain Q can be located after only a few subdivision steps (Fig. 1(c)). In the computations we have chosen five test points in each box $B \in \mathcal{B}_k$ according to (ii) in Section 2.3 for an evaluation of $Ng(B)$.

(b) As a second example we consider the following function $g : \mathbb{R}^2 \to \mathbb{R}^2$:

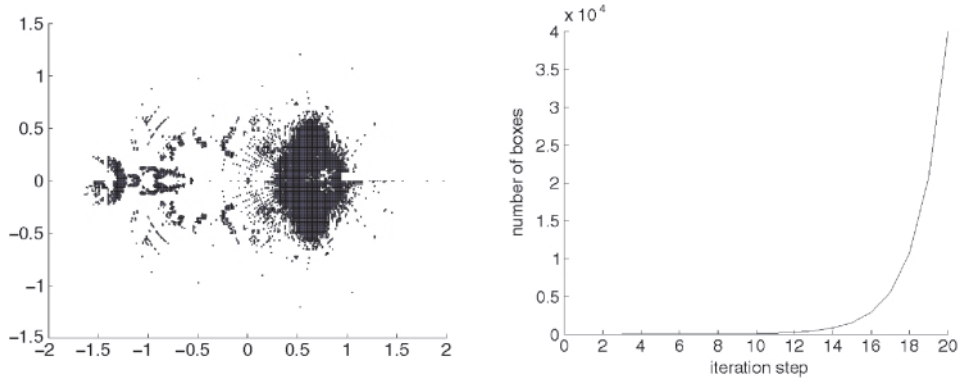
$$g(x_1, x_2) = \begin{pmatrix} x_1^3 - 3x_1x_2^2 - x_1 + \frac{1}{\sqrt{2}} \\ -x_2^3 + 3x_1^2x_2 - x_2 \end{pmatrix}.$$

The aim is to find all the zeros inside $Q = [-5, 5] \times [-5, 5]$. Again we set $s = 1$ and use just the classical Newton method in the subdivision process. In the computations we have used nine test points per box lying on a 3×3 grid inside the box (i.e. strategy (i) in Section 2.3). The result of this computation after 20 subdivision steps is shown in Fig. 2. It can be observed that the number of boxes is rapidly growing, and that no close covering of the set of zeros $\mathcal{Z} = \{(-1{\cdot}251, 0), (0{\cdot}625, 0{\cdot}417), (0{\cdot}625, -0{\cdot}417)\}$ is obtained. The reason is that we do not just obtain a covering of $\mathcal{Z}$ alone but of all the invariant sets of Newton's method. For instance, in this case it can be shown that the Newton iteration has an asymptotically stable periodic orbit $\{(0, 0), (\frac{1}{\sqrt{2}}, 0)\}$. Thus, we have to develop step size strategies which allow us to eliminate the computation of invariant sets of the iteration schemes besides their common fixed points.

Denote by

$$\mathcal{N}_{Q,g} = \{x \in Q : g(x) = 0\}$$

the set of all the zeros of g inside Q. If we are using the classical Newton method alone as the dynamical system for an approximation of $\mathcal{N}_{Q,g}$ then—as indicated by Example 3.1(b)—we may cover much more than just $\mathcal{N}_{Q,g}$ by the box collections obtained in the subdivision procedure. In order to avoid this problem we are going to use the damped



(a) Box covering (b) Number of boxes

FIG. 2. (a) The box collection $\mathcal{B}_{20}$ consisting of 40 648 boxes; (b) the number of boxes increases permanently with each subdivision step up to depth 20. Note that the box collection is not perfectly symmetric with respect to the x-axis. This is due to the occurrence of round-off errors in the numerical computation of Ng.

Newton method

$$x_{j+1} = x_j - hDg(x_j)^{-1}g(x_j), \quad j = 0, 1, \ldots, \tag{3.1}$$

where $h > 0$ denotes the step length. More precisely, denoting the right-hand side in (3.1) by

$$Ng_h(x) = x - hDg(x)^{-1}g(x),$$

we are going to work with finitely many different step lengths h_l, $l = 1, \ldots, s$, and define s dynamical systems $f_l : \mathbb{R}^n \to \mathbb{R}^n$ $(l = 1, \ldots, s)$ by

$$f_l(x) = Ng_{h_l}(x).$$

By this construction we have

$$\mathcal{N}_{Q,g} \subset A_{Q,f_1,\ldots,f_s}, \tag{3.2}$$

where $A_{Q,f_1,\ldots,f_s}$ denotes the relative global attractor of $f_1, \ldots, f_s$ with respect to Q, see (2.2), and therefore we can compute an outer covering of the set of zeros of g by an application of the subdivision algorithm to $f_1, \ldots, f_s$.

REMARK 3.2 Observe that formally the convergence result in Proposition 2.7 does not apply in this context since the mappings $f_1, \ldots, f_s$ will in general not be diffeomorphisms on the set Q. However, in practice we expect to rapidly lose neighbourhoods of the singular points of $f_1, \ldots, f_s$ within the subdivision process. Moreover, Proposition 2.7 certainly applies to the damped Newton method in the case when we choose Q to be a compact neighbourhood of the set $\mathcal{N}_{Q,g}$ of regular zeros of g within Q.

The following result shows that for different step sizes h_1 and h_2 the dynamical systems f_1 and f_2 cannot have common periodic points of period greater or equal to two.

PROPOSITION 3.3 Let f_1 and f_2 be dynamical systems belonging to the step sizes h_1 and h_2. For $\bar{x} \in \mathbb{R}^n$ suppose that $g(\bar{x}) \neq 0$ and that the Jacobian $Dg(\bar{x})$ is invertible. Then

$$f_1(\bar{x}) = f_2(\bar{x}) \Longrightarrow h_1 = h_2.$$

Proof. We compute

$$\begin{aligned} & f_1(\bar{x}) = f_2(\bar{x}) \\ \Longleftrightarrow\ & \bar{x} - h_1 \underbrace{Dg(\bar{x})^{-1} g(\bar{x})}_{=:y \neq 0} = \bar{x} - h_2 Dg(\bar{x})^{-1} g(\bar{x}) \\ \Longleftrightarrow\ & (h_1 - h_2) y = 0 \\ \Longrightarrow\ & h_1 = h_2. \end{aligned}$$

□

REMARK 3.4 Suppose that Q is chosen in such a way that $f_1, \ldots, f_s$ are diffeomorphisms on a neighbourhood of Q. Then we expect that generically equality will hold in (3.2) if $s \geqslant 2$ and the different step sizes h_l ($l = 1, \ldots, s$) are chosen randomly in (0, 1]. In fact, Proposition 3.3 indicates that common invariant sets of $f_1, \ldots, f_s$ do not contain periodic points which on the other hand would at least be generic for C^1 diffeomorphisms. (This is Pugh's celebrated Closing Lemma, see e.g. Shub (1987).) Also observe that the smaller we choose the step size h the closer is the map Nf_h to the identity.

4. Basic algorithms

A crucial aspect for an application of the subdivision algorithm lies in the selection procedure for the different step sizes h_l. If the step size is not varied at all then we expect to obtain in the limit not just the zeros of g but also additional invariant sets of the (damped) Newton method (see Devaney, 1989; Peitgen *et al.*, 1988 and also Example 3.1b). On the other hand we expect to lose this additional dynamical behaviour when we use quite small step sizes (see Hirsch & Smale, 1979; Kellogg *et al.*, 1976 and Remark 3.4). But in this case the number of boxes in the covering of $A_{Q,f_1,\ldots,f_s}$ will grow significantly and therefore one has to choose a step length control mechanism which balances these two different goals.

We now describe our first basic algorithm. In the following $g : \mathbb{R}^n \to \mathbb{R}^n$ is the function for which we would like to find all the zeros inside the compact set $Q \subset \mathbb{R}^n$.

Algorithm A

In this algorithm we prescribe *a priori* two step lengths $h_1, h_2 \in (0, 1]$ together with four integers $q_1, q_2, n_1, n_2 \in \mathbb{N}$. Then we work with two dynamical systems

$$\begin{aligned} f_1 &: \mathbb{R}^n \to \mathbb{R}^n, \quad f_1(x) = (Ng_{h_1})^{q_1}(x), \\ f_2 &: \mathbb{R}^n \to \mathbb{R}^n, \quad f_2(x) = (Ng_{h_2})^{q_2}(x). \end{aligned}$$

Using the integers n_1 and n_2 we define the sequence

$$\{u_k\}_{k=1}^{\infty} = \{\underbrace{1, \ldots, 1}_{n_1}, \underbrace{2, \ldots, 2}_{n_2}, \underbrace{1, \ldots, 1}_{n_1}, 2, \ldots\}.$$

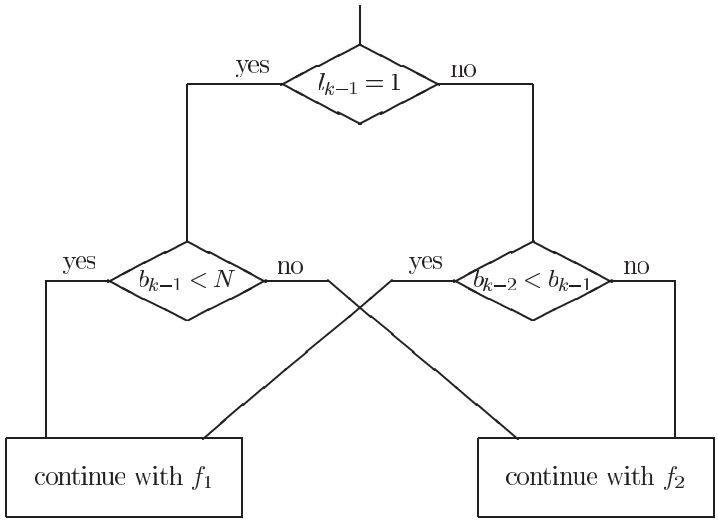


FIG. 3. Schematic description of step k of Algorithm B. b_k denotes the number of boxes in the box collection $\mathcal{B}_k$ and l_k the chosen step length.

By this definition it is clear that the condition (2.4) is satisfied and therefore, in principle, the convergence of the subdivision algorithm to A_{Q,f_1,f_2} is guaranteed.

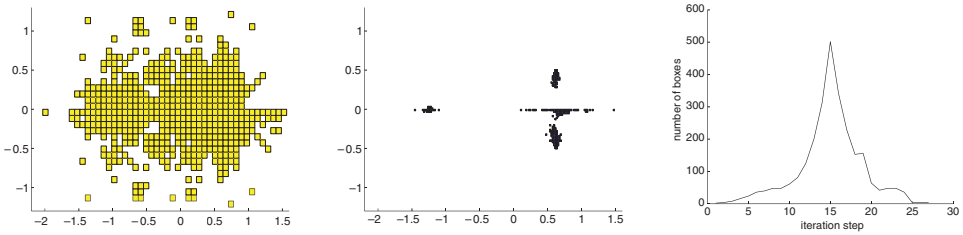
In the realization of Algorithm A we typically choose $(h_1, q_1) = (1, 1)$ and $(h_2, q_2) = (0{\cdot}1, 10)$. That is, we choose the classical Newton method and a strongly damped version.

Algorithm A has the disadvantage that the numbers n_1 and n_2 have to be defined in advance and that no adjustment is made in the course of the subdivision procedure. However, in the case that the number of boxes is growing too fast then it would be desirable to adjust the step size in Newton's method according to this observation. This leads to

Algorithm B

Set $(h_1, q_1) = (1, 1)$ and specify an integer $N \in \mathbb{N}$. Moreover, choose a (small) step size $h_2 \in (0, 1)$ and $q_2 \in \mathbb{N}$. Then proceed in the kth step of the algorithm according to the diagram in Fig. 3.

During the subdivision procedure the number of boxes is monitored and h_2 is chosen as a damping parameter when the number of boxes b_{k-1} is increasing beyond the prescribed number N. Otherwise, one proceeds with the classical Newton method: that is, with step length $h_1 = 1$. The reason for this strategy is that the occurrence of a large number of boxes indicates that the subdivision procedure has found more than just the fixed points of Newton's method. A significant change in the damping parameter should lead to an elimination of these additional boxes. On the other hand, if the number of boxes is increasing again when the step length h_2 is repeatedly chosen then this is an indication for the fact that the contraction around the fixed points is not fast enough. In this case we switch back to the classical Newton method.



(a) $k = 15$ (b) $k = 18$ (c) Number of boxes

FIG. 4. Application of Algorithm B: the box collections $\mathcal{B}_{15}, \mathcal{B}_{18}$ and the number of boxes during the subdivision process are shown.

EXAMPLE 4.1 We now apply Algorithm B to Example 3.1(b) by choosing $N = 500$, $(h_1, q_1) = (1, 1)$ and $(h_2, q_2) = (0{\cdot}1, 10)$. The results are shown in Fig. 4. After 15 steps 502 boxes are computed by the subdivision algorithm. The algorithm then switches to the function $f_2 = (Ng_{0{\cdot}1})^{10}$. In step 19 the number of boxes is again increasing so that the algorithm switches back to the classical Newton method. A close covering of the roots can be obtained after 23 subdivision steps.

5. An adaptive algorithm

We now present a refined version of Algorithm B as described in Section 4. In this algorithm the step length h is chosen to be the Armijo step length (see Dennis & Schnabel, 1983) and therefore the step size h becomes a function of x, i.e. $h = h(x)$. Moreover, we specify in each subdivision step a power $q = q(x) \geqslant 1$ and apply the dynamical system $(Ng_{h(x)})^{q(x)}$ at the point x. Observe that this algorithm still fits into the underlying theoretical framework since in practice we only perform finitely many subdivision steps and since we are evaluating $(Ng_h)^q$ only at finitely many points.

We now state the underlying theoretical result which will allow us to find an appropriate choice for the power $q = q(x)$. Its proof can be found in Dellnitz & Hohmann (1997).

PROPOSITION 5.1 For $q \geqslant 1$ let A_{Q,f^q} be the global attractor of f^q relative to the compact set $Q \subset \mathbb{R}^n$ (cf. (2.1)). Moreover, suppose that A_{Q,f^q} is an attracting compact hyperbolic set. Let $\rho \geqslant 1$ be a constant such that for each compact neighbourhood $\tilde{Q}$ of A_{Q,f^q} we have

$$h(A_{Q,f^q}, \tilde{Q}) \leqslant \delta \Longrightarrow \tilde{Q} \subset U_{\rho\delta}(A_{Q,f^q}).$$

Then the coverings Q_k obtained by the subdivision algorithm for f^q satisfy

$$h(A_{Q,f^q}, Q_k) \leqslant \operatorname{diam}(\mathcal{B}_k)(1 + \alpha + \alpha^2 + \cdots + \alpha^k). \tag{5.1}$$

Here $\alpha = C\rho\lambda^q/\theta_{\min}$, where C is a constant, $\lambda \in (0, 1)$ is the number quantifying the contractivity of the hyperbolic set A_{Q,f^q} and $\theta_{\min}$ is defined in the subdivision step of the subdivision algorithm.

REMARK 5.2 In Proposition 5.1 $h(E, F)$ denotes the Hausdorff distance between two compact sets E, F. Moreover, $U_{\rho\delta}(A_{Q,f^q})$ is defined as

$$U_{\rho\delta}(A_{Q,f^q}) = \{y \in \mathbb{R}^n : \text{there is an } x \in A_{Q,f^q} \text{ such that } y \in W^s(x) \text{ and } \operatorname{dist}(x, y) < \rho\delta\}.$$

($W^s(x)$ is the *stable manifold* of the point x.)

Let us consider Proposition 5.1 in the specific context where A_{Q,f^q} is a fixed point of the damped Newton method Ng_h. In that case we have close to the fixed point

$$C \approx 1, \quad \rho \approx 1 \quad \text{and} \quad \lambda = 1 - h.$$

For a verification of this fact recall that fixed points of Ng_h are asymptotically stable with contraction rate $1 - h$.

Taking the estimate (5.1) into account we would like to choose q such that $\alpha < \epsilon$ for a specified (small) $\epsilon > 0$ which implies fast convergence of the algorithm. This leads to the following choice for the power q:

$$\epsilon > \alpha = \frac{\lambda^q}{\theta_{\min}} \Longleftrightarrow \lambda^q < \epsilon\theta_{\min} \Longleftrightarrow (1-h)^q < \epsilon\theta_{\min} \Longleftrightarrow q > \frac{\ln(\epsilon\theta_{\min})}{\ln(1-h)}.$$

This computation suggests that, as expected, one should choose a large q if the step length is small. Since in practice we do not want to exclude the case where $h = 1$, that is the case where we are working with the classical Newton method, we choose the power q as follows:

$$q = \left\lceil \frac{\ln(\epsilon\theta_{\min})}{\ln(\max(1-h, \delta))} \right\rceil, \tag{5.2}$$

where $\delta \in (0, 1)$ is a prescribed constant.

Thus, we suggest the following adaptive subdivision algorithm.

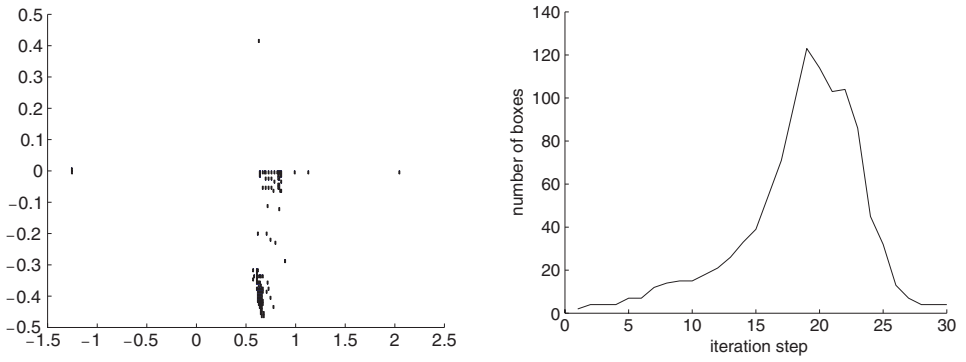
> In each subdivision step choose the Armijo step length $h = h(x)$ at the test point x. Then choose the power $q = q(x)$ according to (5.2) and apply $(Ng_{h(x)})^{q(x)}$ at the point x.

EXAMPLE 5.3 We reconsider Example 3.1(b) and show the result obtained by the adaptive algorithm in Fig. 5. The maximum number of boxes calculated by this strategy is 123.

Finally, we compare the three algorithms that we have described so far in Fig. 6.

6. Comparison with another approach

We now investigate the computational efficiency of the adaptive algorithm by a comparison with another global root finding method based on the NAG routine `c05pbc()`. Our approach is expected to be particularly advantageous in the situation where the zeros of the given function g are not uniformly distributed inside the compact set Q but rather occur



(a) (b)

FIG. 5. (a) The box collection $\mathcal{B}_{20}$ containing 114 boxes obtained by the adaptive algorithm. (b) Number of boxes in the box collections using the adaptive strategy.

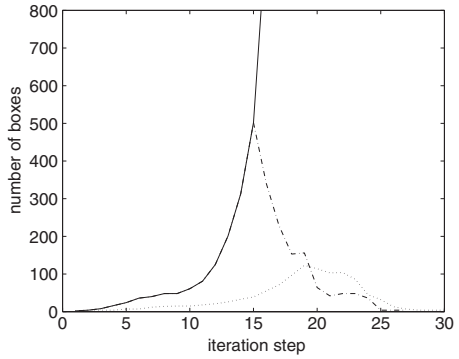


FIG. 6. A comparison of the proposed algorithms: the respective number of boxes in the subdivision procedure is shown (classical Newton (solid), Algorithm B (dash-dotted) and the adaptive algorithm (dotted)).

in clusters. In fact, by the construction of the subdivision process these clusters should always be covered by the box collections. On the other hand, it seems very unlikely to find all the zeros inside the clusters by an application of Newton's method to a certain number of randomly chosen initial conditions since the basins of attraction of the zeros are very different in size. We illustrate this fact by the following Examples (a) and (b). Examples (c) and (d) are taken from the literature and indicate the efficiency of our approach even in the case where the zeros do not occur in clusters.

In all the computations we have used the following set of parameter values for the adaptive algorithm:

$$\epsilon = 0{\cdot}2 \quad \text{and} \quad \delta = 0{\cdot}1,$$

see (5.2). Moreover, the test points have been chosen randomly (i.e. strategy (ii) in Section 2.3).

(a) Consider the following test function:

$$g_1 : \mathbb{R}^2 \to \mathbb{R}^2$$
$$g_1(x, y) = \left(\psi(y) \prod_{i=1}^{40} (x - x_i), \quad \phi(x) \prod_{i=1}^{40} (y - y_i) \right),$$

where

$$x_i = y_i = \begin{cases} 0{\cdot}1 + \frac{-10+i}{1000} : & \text{for } i = 1, \ldots, 20 \\ 0{\cdot}9 + \frac{-30+i}{1000} : & \text{for } i = 21, \ldots, 40 \end{cases}$$

and

$$\psi(y) = \sin(4y), \quad \phi(x) = \sin(4x).$$

By construction g_1 possesses 1649 roots in the domain $Q = [-3, 3] \times [-3, 3]$ and most of them are concentrated in four clusters, Fig. 7(c). In addition to an application of our adaptive algorithm we have tried to find all the roots by using the NAG-solver `c05pbc()` with 10 000 randomly distributed initial points. By this strategy only 300 roots were found (including some spurious zeros, see Fig. 7(a)). In the right-hand side of this figure the roots located by this method in one of the four clusters are shown. Observe that, as expected, almost all the zeros on the 'boundary' of the cluster have been found but very few inside.

In Fig. 7(b) we show the box collection obtained after 24 subdivision steps of the adaptive algorithm. All the roots are covered by the boxes. Moreover, by switching to the classical Newton method with a few initial conditions per box all the roots could be computed (see Fig. 7(c)).

(b) In order to illustrate that our method also works in higher dimensions we now embed the previous example into an n-dimensional context: consider the function

$$g_2 : \mathbb{R}^n \to \mathbb{R}^n,$$
$$g_2(x_1, \ldots, x_n) = (g_1(x_1, x_2), (x_3 - 3)^2, \ldots, (x_n - n)^2),$$

where g_1 denotes the function from the previous example. Using this function we have performed numerical tests up to dimension $n = 10$. Some of the results are presented in Table 1 and illustrate the efficiency of our approach.

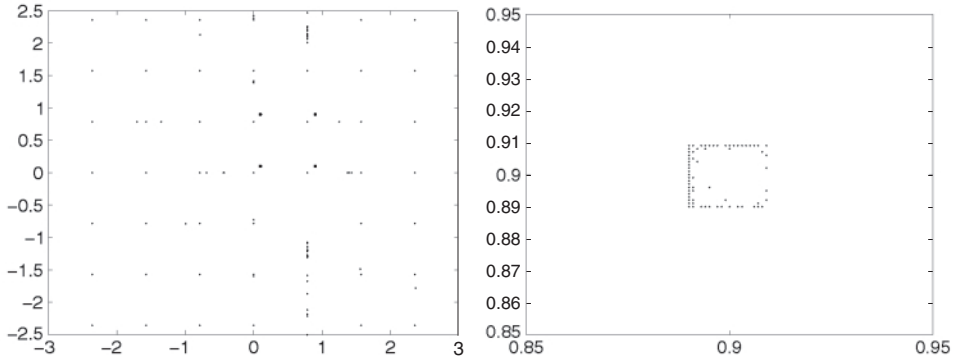
(c) In this example we consider a polynomial function taken from Stewart *et al.* (2000):

$$g_3 : \mathbb{R}^n \to \mathbb{R}^n,$$
$$g_3(x) = (f_1(x), \ldots, f_n(x))$$

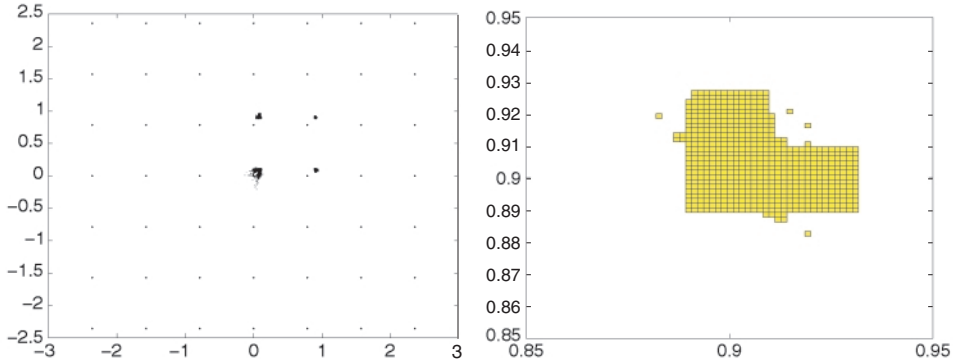
where

$$f_j(x) = -\sum_{i=1}^{n} x_i + \lambda x_i + x_i^2 - x_i^3.$$

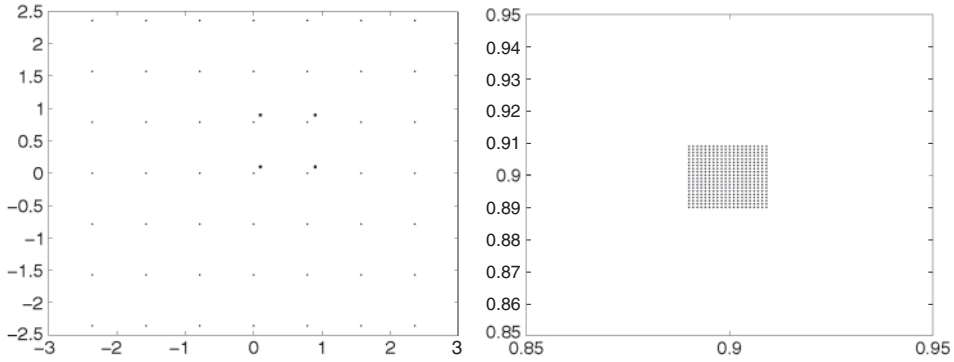
Here $\lambda \in [-50, 1000]$ is a bifurcation parameter and the equations can be viewed as a model describing speciation phenomena occurring in the evolution process. For $n = 8$ and $\lambda = 100$ the function has 6561 roots in $Q = [-40, 40]^n$ see Fig. 8. In



(a) Zeros found by the NAG-solver c05pbc ()



(b) The box collection B_{24} computed by the adaptive subdivision algorithm



(c) All the roots of g inside $Q = [-3, 3] \times [-3, 3]$

FIG. 7. Numerical results for Example (a).

TABLE 1 *Performance of the different zero finding procedures. In the table #IP denotes the number of test points per box (subdivision procedure) or the total number of initial points (NAG solver). #FC denotes the number of function calls and #DC the number of derivative calls. The computations have been done on a SUN Ultra* 10 *workstation*

Dim	Method	#IP	#FC	#DC	CPU time (min)	#zeros found
5	Subdivision	5	$0{\cdot}4 \cdot 10^7$	$2{\cdot}6 \cdot 10^6$	5	1624
		12	$4{\cdot}0 \cdot 10^7$	$27 \cdot 10^6$	47	1649
	NAG `c05pbc()`	50 000	$0{\cdot}7 \cdot 10^7$	$0{\cdot}8 \cdot 10^6$	5	570
		300 000	$4{\cdot}0 \cdot 10^7$	$4{\cdot}6 \cdot 10^6$	33	991
		400 000	$5{\cdot}4 \cdot 10^7$	$6{\cdot}2 \cdot 10^6$	44	1062
10	Subdivision	4	$0{\cdot}6 \cdot 10^7$	$4{\cdot}3 \cdot 10^6$	10	1609
		10	$9{\cdot}6 \cdot 10^7$	$65 \cdot 10^6$	150	1649
	NAG `c05pbc()`	50 000	$0{\cdot}7 \cdot 10^7$	$0{\cdot}8 \cdot 10^6$	10	578
		600 000	$8{\cdot}1 \cdot 10^7$	$9{\cdot}2 \cdot 10^6$	124	1176
		800 000	$11 \cdot 10^7$	$12 \cdot 10^6$	164	1256

Table 2 we have summarized our results in comparison with the NAG-solver. Since g_3 is polynomial, all the roots could in principle also be found by a global homotopy algorithm as implemented in the package PHC[†].

Finally, we remark that we have also tried to find all the zeros for this example using the software GLOBSOL[‡] taking the standard parameter values. However, this computation has not been successful since the maximal number of iteration steps has been exceeded in the course of the computation.

(d) Our final example is a test example taken from Moré *et al.* (1981):

$$g_4 : \mathbb{R}^n \to \mathbb{R}^n,$$
$$g_4(x) = (f_1(x), \ldots, f_n(x)),$$

with

$$f_i(x) = n - \sum_{j=1}^{n} \cos(x_j) + i(1 - \cos(x_i)) - \sin(x_i).$$

For $n = 10$ there exist 10 roots inside the box $Q = [-0{\cdot}3, 0{\cdot}8]^n$. Since in this case the basin of attraction for Newton's method is quite large for every root we do not have a computational advantage in comparison with the NAG-solver. However, it can be seen that also in this case the computational effort is comparable, see Table 3.

Acknowledgements

We thank Gary Froyland for helpful discussions on the contents of this paper. Research is partly supported by the Deutsche Forschungsgemeinschaft under Grant De 448/5-4.

[†]http://www.math.uic.edu/∼jan/download.html

[‡]http://interval.usl.edu/GLOBSOL

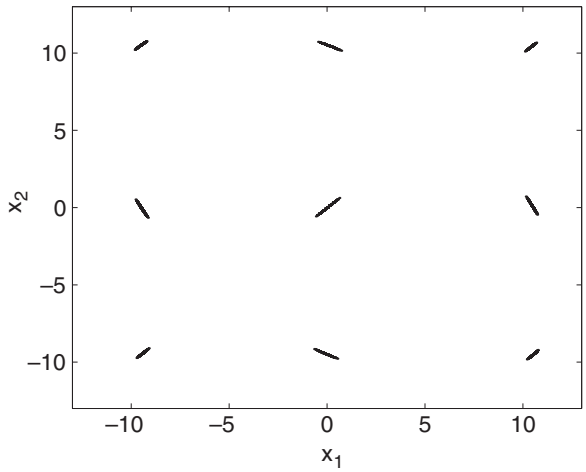


FIG. 8. All the roots of g_3. A projection onto the first two coordinates is shown.

TABLE 2 *Comparison for the test function g_3. The notation is the same as in Table* 1

Dim	Method	#IP	#FC	#DC	#zeros found
8	Subdivision	5	$2{\cdot}2 \cdot 10^7$	$1{\cdot}6 \cdot 10^7$	6463
		12	$5{\cdot}9 \cdot 10^7$	$4{\cdot}2 \cdot 10^7$	6561
	NAG `c05pbc()`	100 000	$2{\cdot}8 \cdot 10^6$	$1{\cdot}5 \cdot 10^5$	5716
		200 000	$5{\cdot}5 \cdot 10^6$	$3{\cdot}6 \cdot 10^5$	6128
		400 000	$1{\cdot}1 \cdot 10^7$	$7{\cdot}3 \cdot 10^5$	6392
		1000 000	$2{\cdot}7 \cdot 10^7$	$1{\cdot}8 \cdot 10^6$	6522
		2000 000	$5{\cdot}6 \cdot 10^7$	$3{\cdot}6 \cdot 10^6$	6556
		4000 000	$8{\cdot}3 \cdot 10^7$	$5{\cdot}5 \cdot 10^6$	6560

TABLE 3 *Comparison for the test function g_4. The notation is the same as in Table* 1

Dim	Method	#IP	#FC	#DC	#zeros found
10	Subdivision	3	9 200	6 800	8
		5	26 747	19 741	10
		8	137 900	102 700	10
		12	$1{\cdot}0 \cdot 10^7$	$0{\cdot}77 \cdot 10^7$	10
	NAG `c05pbc()`	250	13 300	2 300	6
		500	26 400	4 800	9
		750	39 800	7 400	10
		1000	52 800	9 800	10

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