HOMOTOPY METHODS FOR SOLVING SMOOTH NONLINEAR SYSTEMS OF EQUATIONS

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NONLINEAR SYSTEMS OF EQUATIONS

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PREFACE

The last twenty years have witnessed a constant stream of research in the general area of finding global algorithms for solving nonlinear systems of equations. A primary objective of this study is to explore some of the existing algorithms and the theories behind them, which are scattered in the literature, and put this in an integrated form. It is hoped that this will make these materials more accessible to those who are interested in this area of mathematics.

To do so, Chapter I contains the precise statement of the problem of this study, and some examples. Also, in this chapter a brief account of the historical development of this area as well as the necessary background materials for this study are given.

In Chapter II, a detailed construction of Hirsch and Smale's definition of a unit vector field is obtained by means of which an initial value problem is defined. Also, an alternative definition of this vector field by an explicit formula is given, and a detailed proof of Hirsch and Smale's convergence theorem for their algorithm to compute zeros of certain nonlinear maps presented.

In Chapter III, a constructive proof of Brouwer's fixed point theorem is given. Chapter IV deals with the global

Newton and global homotopy methods. and compares the solution curves of these two methods.

Chapter V describes several algorithms based on the continuous Newton and homotopy methods. Chapter VI concludes this thesis, highlighting its salient points.

A study of this type could not have been completed without the good will of my advisor, Professor Hermann Burchard, whose wise and critical comments helped to clarify my thinking on many points throughout this study, especially when things seemed to come to a dead end. My gratitude goes to him for his patient guidance and assistance throughout the preparation of this thesis.

I acknowledge my obligation to professors Gardiner, Haack, and Wolfe as my teachers and as members of my committee, for their time and effort on my behalf. I would like also to thank Professor Paul Duvall, an ex-member of my advisory committee, for his interest in this project and encouragement.

Special gratitude is expressed to my wife, children, and family for their understanding, patience, and numerous sacrifices. Last but not least, I would like to dedicate this study to the memories of my mother and father, without whom this project could not have been realized.

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CHAPTER I

INTRODUCTION

The objectives of this chapter are to state the problem under consideration and to give some examples in 1.1; to mention the historical development of finding global methods for solving nonlinear systems of equations in 1.2; to briefly discuss the continuation methods and the nature of this study in 1.3; and finally, to give the necessary background materials for this study in 1.4.

1.1 Statement of the Problem and Some Examples

Suppose a smooth nonlinear map $f : R^n \rightarrow R^n$ is given. It is of interest to find global algorithms that solve the system of equations:

$$f(x) = 0. \tag{1.1}$$

A global algorithm is considered as an algorithm for which the starting point of the solution may by chosen anywhere in R^n, or at least in a large portion of R^n.

The global methods, which are the subject of this study, will be introduced in the following chapters. Here,

it is emphasized that these global methods must be contrasted with the more familiar local methods such as the classical (discrete, local) Newton method. This can be very simply described by the iteration formula

$$x_{n+1} = x_n - [Df(x_n)]^{-1} f(x_n). \tag{1.2}$$

Beginning at some point x_0, which the user of this method must supply, successive iterates x_n are computed by means of formula (1.2), provided the current point x_n belongs to the domain of $f(x)$ and the Jacobian matrix $Df(x)$ is defined and invertible at x_n. The sequence $(x_n)_{n=1,2\ldots}$ thus generated may be assumed to converge to a solution x_* of equation (1.1), under fairly simple hypotheses on the map f such as $Df(x)$ being continuous in a neighborhood U of x_* for which $f(x_*) = 0$, and $Df(x_*)$ is nonsingular, if only the initial point x_0 was chosen sufficiently near the solution x_*.

This can be expressed by saying that the local Newton method (1.2) works in a neighborhood of the zeros of the map f, as sought in (1.1).

However, cases are known where the convergence works from an arbitrary starting point. For example, let f satisfy the following rather strong conditions:

1. f is continuously differentiable, convex;
2. the Jacobian matrix $Df(x)$ is nonsingular;
3. $[Df(x)]^{-1} \geq 0$ for all $x \in R^n$;
4. equation (1.1) has a solution x_*; and
5. $Df(x)$ is continuous on R^n. (1.3)

Then it follows that x_* is unique, and starting at any point $x_0 \in R^n$, the local Newton method converges to x_*.

Further discussion about this result and others can be found in Ortega and Rheinboldt [42].

Some problems from various fields, such as numerical analysis and optimization theory, may be formulated in the form (1.1).

An illustrative example: An illustration of how a system of nonlinear equations arises in a typical applied problem is given below. In numerical analysis, a simple form of the two point boundary value problem (BVP) is given by:

$$u'' = g(t,u),\ 0 \le t \le 1,\ u(0) = a,\ u(1) = b.$$

Assume $g(t,u)$ is C^2 function on the set

$$A = \{(t,u):\ 0 \le t \le 1,\ -\infty < u < +\infty\},$$

and $g(t,u)$ satisfies the following:

(1) $g(t,u)$ is Lipschitz, that is,

$$\|g(t,u) - g(t,u')\| \le K\|u-u'\| \text{ for all } (t,u),\ (t,u') \in A$$

and K is a constant.

$$(2)\quad \frac{\partial}{\partial u}\, g(t,u) \ge 0 \quad \text{for } (t,u) \in A. \tag{1.4}$$

Then the above BVP possesses a unique solution. Solutions to (1.4), as it is customary in nonlinear or linear

problems, are approximated by means of finite difference methods.

To this end, the interval [0,1] is partitioned by equally spaced grid points:

$$0 = t_0 < t_1 < t_2 <\ldots< t_n = 1,\ t_i = ih,\ h = \frac{1}{n},$$

$$i = 0,1,2,\ldots n.$$

At each t_i, $u''(t_i)$ is approximated by a second central difference; in fact, if $u \in C^3[0,1]$, then

$$u''(t_i) = \frac{1}{h^2}\,[u(t_{i+1}) - 2\,u(t_i) + u(t_{i-1})] + 0(h^2). \quad (1.5)$$

Suppose x_i is the approximation to $u(t_i)$, then (1.5) gives rise to the system of nonlinear equations

$$x_{i+1} - 2x_i + x_{i-1} = h^2\, g(t_i,x_i)\ ,$$

$$i = 1,2,3,\ldots,n,\ x_0 = a,\ x_n = b. \quad (1.6)$$

Equation (1.6) can be put in the compact form

$$AX + H(X) = 0,\ X = (x_1,\ldots,x_n) \in R^n$$

Here A is an n×n tridiagonal matrix, and H is a nonlinear map depending on g and the grid points. Under the conditions in (1.4), the above system of finite difference equations possesses a unique solution as well as the BVP, and this unique solution can be found by the Newton method for h

sufficiently small. Further discussion about this BVP problem can be found in Henrici [24].

If the strong conditions in (1.3) do not hold, the Newton method converges only locally. In this way arises the need of finding global methods for solving (1.1). Additional examples in numerical analysis can be found in Ortega and Rheinboldt [42].

In optimization theory, there are many problems which lead to problem (1.1). For example, in unconstrained optimization, one seeks to minimize the real valued function $h : R^n \rightarrow R$. Assuming that h is differentiable, then the gradient of h, denoted by ∇h, is given by

$$\nabla h = (\partial h/\partial x_1, \partial h/\partial x_2, \ldots, \partial h/\partial x_n).$$

Then the minima of h(x) are among the zeros of

$$f(x) = \nabla h(x).$$

Having introduced the problem and some typical examples, it is appropriate to mention the methods that will be considered in solving it. Existence theorems and algorithms for solving (1.1) that will be considered in this study originate from two global approaches: the Hirsch and Smale's approach, which is also called the *continuous Newton method*, (Li and Yorke [37]), and the *homotopy method*.

To find a zero of the system (1.1), both approaches follow a solution curve of an initial value problem (IVP)

until the zero is reached. To be more specific, in Hirsch and Smale's approach the following IVP is obtained

$$\frac{d\xi}{dt} = \phi(x),\ \xi(t_0) = x_0, \tag{1.7}$$

where $\phi(x)$ is a unit vector, which may be obtained by normalizing the vector $-[Df(x)]^{-1}f(x)$ provided that $Df(x)$ is nonsingular (when the rank $(Df(x)) = n-1$, and $f(x) \notin$ range$(Df(x)$ then ϕ may be extended by a continuity agrument).

In the homotopy approach, too, one gets the IVP

$$DH(Y)\dot{Y} = 0\ ,\ Y(0) = (t(0),x(0)) = (t_0,x_0),$$

where H: $R^{n+1} \rightarrow R^n$ and $\dot{Y} = (dt/ds,dx/ds)$ is a unit vector, too.

1.2 Historical Background

Finding zeros of nonlinear maps is a classical problem in numerical analysis. Until quite recently, methods and algorithms available to solve such problems were local in character in the sense that the starting point of the iterative process must be a good approximation for the zero that need to be found. The literature of the local theory is too vast to be reported here, but for details, the reader should consult the authoritative works by Householder [26],

Ostrowski [40], Traub [46], and the extensive bibliographies therein.

Global methods of solving nonlinear systems of equations seem to have been used for the first time by Lahaye [36] in 1934. He applied what is called the *discrete continuation* (imbedding, homotopy) approach to obtain global algorithms for solving such a problem. In fact, Lahaye first implemented this approach to find the zeros of a single equation where the Newton method was used to move along the continuation curve. Lahaye further applied this approach in 1948 to obtain zeros of nonalgebraic systems of equations.

In 1951, this continuation approach was considered in an abstract setting by Ficken [16]. In 1971, Avila [6] used this approach to globalize the Newton method. For the first time, Avila studied the feasibility of this approach. For example, when the Newton method is used in the continuation process, the process is called *feasible* if there exists a partition $\{t_k\}_{k=1}^{n}$ of the interval $I = [0,1]$ and finite integers $\{j_k\}$, $k = 1,\ldots,n$ such that the Newton method takes the form

$$x_k^{i+1} = x_k^i - [D_x H(t_k, x_k^i)]^{-1} H(t_k, x_k^i),$$

for $k = 1,\ldots,n$, $i = 0,\ldots,j_k$, and $x^0 = x(0)$, where $H: I \times R^n \to R^n$ in a homotopy map, and $D_x H$ is the Jacobian matrix of H with respect to x. If $D_x H$ and its inverse

$[D_X H]^{-1}$ exist and the latter is bounded in the neighborhood of the curve $x : I \to R^n$ with $H(t, x(x)) = 0$, then the above form of the Newton method converges to a zero of f.

In 1977, Wacker, Zarzer, and Zulehner [52] considered this continuation approach to globalize both the Newton and the modified Newton methods, that is, the iterative process of the form

$$x_{n+1} = x_n - [Df(x_0)]^{-1} f(x_n), \text{ for some fixed } x_0 \text{ and } n = 0,1,2,....$$

Another technique of continuation, called *analytic* (continuous) *continuation*, was initiated in 1953 by Davidenko [10] (for more details see 1.3). In a series of papers, Davidenko used this approach to deal with several problems in numerical analysis such as the eigenvalue problem, the evaluation of determinants, and the inversion of matrices. An English translation of Davidenko's complete work can be found in Rall [45]. The Davidenko's approach attracted many researchers such as Yokavlev [57], Davis [11], Meyer [40], and Wasserstrom [53], to mention a few.

The last twenty years have witnessed a constant stream of research in the general area of obtaining a global algorithm for solving nonlinear systems of equations. To be more specific, in 1967 a new line of development was opened by Scarf's algorithm [47], which computes fixed points of continuous maps. This approach uses a simplicial decomposition of the domain of the given map and a systematic search

technique based on *Sperner's Lemma* to find a simplex of the decomposition which contains or is near to a fixed point or a zero of a map. For example, a path which leads to a fixed point or a zero of the given nonlinear map is linearly approximated over those simplices of the decomposition which it crosses.

Since the introduction of Scarf's algorithm, a host of other algorithms have been published by many researchers: Allgower, Keller, and Reeves [2], Kuhn [32, 33], Eaves [13], Eaves and Saigal [14], Merrill [39], and Lann [35], to list a few.

The simplicial approach does not assume the smoothness of the map f and therefore does not depend on evaluating the Jacobian matrices, except possibly in the final stages, in order to take advantage of the smoothness if it is present.

In the mid-1970's, another approach, which uses differential topology techniques to obtain global algorithms, was introduced independently by Kellogg, Li, and Yorke [31], and Smale [49]. This new development and Davidenko's approach share one common feature; that is, both approaches translate the problem of solving nonlinear systems of equations into a problem of solving an initial value problem (IVP).

This approach also attracted many researchers: Alexander [1], Allgower and Georg [3], Chow, Mallet-Paret, and

Yorke [8], Garcia and Gould [17, 18], Garcia and Zangwill [19], Keller [34], Rheinboldt [46], and Watson [54], to mention a few. A survey of the development of this approach is given by Allgower [4].

Additional details and an extensive bibliography concerning the development of both the simplicial and continuation methods can be found in the two review articles by Allgower and Georg [3,5].

1.3 The Scope of the Study

As an introduction to this study, it will be advantageous to introduce the basic ideas behind the continuation methods and how they evolved. To begin, the following definition is stated:

Definition 1.1

Let I be the closed interval [0,1]. A map $H : R^n \times I \rightarrow R^n$ is a *homotopy* between the functions $f, g : R^n \rightarrow R^n$, if H is continuous with $H(x,0) = g(x)$, $H(x,1) = f(x)$ for all $x \in R^n$.

For the purpose of solving the nonlinear system (1.1), the system $g(x) = 0$ will be assumed to have either a solution that is known explicitly or can be found by a standard method.

Let f be a C^1 map and assume $Df(x)$ is nonsingular for all $x \in R^n$. Assume, also, that $\|[Df(x)]^{-1}\| \leq \beta$, $\beta > 0$, then there exists a continuous map $x : I \rightarrow R^n$ such that

$$H(x(t),t) = 0, \quad \text{for all } t \in I. \tag{1.8}$$

Thus, $x(t)$ is a curve in R^n with one end point at $x(0) = x_0$ and the other end point $x(1) = x_*$, the solution of (1.1) (Ortega and Rheinboldt [42]).

To find x_*, the interval I is divided into, say, $n + 1$ points

$$0 = t_0 < t_1 < t_2 < \ldots < t_n = 1$$

Then consider the family of problems

$$H(x,t_i) = 0 \quad , \quad i = 0,1,2,3,\ldots,n. \tag{1.9}$$

Using a local iterative method, such as Newton's, each problem in (1.9) may be solved with starting point at x^{i-1} and iterating until the solution x^i of the ith problem is obtained. If $h_i = t_{i+1} - t_i$ is small enough, then x^{i-1} will be a good starting approximation to x^i and the local Newton method is expected to succeed in finding x^i.

This approach runs into difficulties if the Jacobian matrix $D_x H(x,t)$ becomes singular at any point on the curve $x(t)$. Also, the precise spacing of the t_i for efficiency and stability is a major difficulty. Much of the work in this direction seems to have been towards obtaining an optimal step size $h_i = t_i - t_{i-1}$, so that computational effort in solving (1.9) is minimal. Additional details about this approach can be found in Ortega and Rheinboldt [42]. Also, Wacker [51] reviewed this approach and its development.

In the continuous homotopy, too, one works under conditions such as "x(t) is continuously differentiable on [0,1]" and "the homotopy H has continuous partial derivatives" [42].

Differentiating (1.8) with respect to t, one gets the Davidenko's differential equation

$$D_x H(x(t),t)\ dx/dt + D_t H(x(t),t) = 0$$

Thus the following IVP is obtained

$$dx/dt = - [D_x H]^{-1} D_t H,$$

$$H(x(0),0) = 0,\ x(0) = x^0. \qquad (1.10)$$

By means of numerical integration of the IVP in (1.10) an approximation to the homotopy path x(t) is obtained, and hence for $x(1) = x_*$.

A great deal of research has been done in this direction, especially in the case when the matrix $D_x H$ becomes singular during the integration process. After all, this contingency must be dealt with successfully if, as assumed, the initial point x_0 is far from x_*. Additional details about this approach can be found in Rall [45], Ortega and Rheinboldt [42], Wacker [51], and the more recent work by Georg [20].

As pointed out earlier, the 1970's witnessed the emergence of a powerful theory which uses differential topology techniques to obtain global algorithms for solving (1.1).

To be more specific, in 1976, Kellogg et al. [31] gave a constructive proof of Brouwer's fixed point theorem using the nonretraction principle; that is, there is no continuous map from the closure of a bounded open set into its boundary which acts as the identity function on the boundary of this set. As a consequence of this constructive proof, they also gave an algorithm based on following a solution curve of an IVP to a fixed point of the map f.

Smale [49], in the same year, introduced the so-called global Newton method along with existence theorems to zeros of certain maps. Although Smale's theorems asserts the existence of a solution curve of the global Newton equation, no algorithm was given on how to follow this curve. Smale's sketched proofs rested on Sard's Theorem and the utilization of a projection map of a compact set onto S^{n-1}.

Further development took place toward the end of the 1970's. For example, Chow et al. [8], in 1978, used the Parametrized Sard's Theorem to establish homotopy methods that find fixed points of maps with "Probability 1"; that is to say, if for almost every $u \in U \subseteq R^n$ in the n-dimensional Lebesque measure sense, there exists a point "P_u" and a solution curve, $C(P_u)$, of an IVP that starts at P_u and terminates at a fixed point of the map f.

Moreover, Watson [54,55,56], in a series of articles between 1978 and 1980, used the Chow et al. [8] algorithm to find fixed points of nonlinear maps, to solve the nonlinear complementarity problem, that is, finding a vector $u \in R^n$

such that $u > 0$, $f(u) > 0$, and $uf(u) = 0$, where the inequality sign to be understood as componentwise of both u and $f(u)$; to solve the two-point boundary value problem; and to deal with many engineering problems. Also, in 1978, Keller [34] extended the work of Smale.

Since the publication of Hirsch and Smale's [29] long paper in 1979, very little response has appeared in the literature. In that paper Hirsch and Smale [29] gave several existence and convergence theorems and algorithms.

One main objective of this study, on the one hand, is to fill out the missing details in Hirsch and Smale's proof of an existence and convergence theorem of zeros of certain nonlinear maps. In 2.1, the definition of Hirsch and Smale's vector field that defines the IVP (1.7) is reconstructed. In 2.2, an alternative definition to this vector field by an explicit formula is given. To obtain this formula, it is necessary to characterize the regular points in the domain of the *projection map* $g(x)$, which is related to the map f by the equation:

$$g(x) = \frac{f(x)}{\|f(x)\|}.$$

Another main objective of this study, on the one hand, is to report in Chapter III on existence theory of fixed points or zeros of maps which based on the new homotopy (Chow et al. [8]) approach. On the other hand, Chapter V describes algorithms that are based on this approach. In

Chapter IV, an extension to Smale's existence theorem [49] is given, and the relation between the global Newton and global homotopy methods is studied.

The final aim of this study is to report in Chapter V on some existing algorithms, and modify or formulate others.

1.4 Background Materials

During discussion of the historical development of the various global methods, the differential topology approach was mentioned as one of the most successful techniques used to establish and to justify existence theorems and algorithms.

Differential topology terminologies and results will be used throughout this study. Therefore, for ease of reference, some definitions are recalled and several theorems are listed.

This process begins with the basic definitions relating to smooth manifolds and maps between them.

Definition 1.2

Let U be an open subset of R^n. The map $f : U \to R^n$ is said to be a *C^r map* (or of class C^r) if f is r-times continuously differentiable. In general, let X, Y be arbitrary subsets of R^n, R^m respectively; a map $f : X \to Y$ is said to be a C^r map if for each $x \in X$ there exists a neighborhood of x, say $U \in R^n$, and a C^r map $F : U \to R^m$ such that $F(u) = f(u)$ for all $u \in U \cap X$.

Definition 1.3

A map $f : X \to Y$ between two subsets of Euclidian spaces is called a *homeomorphism* if f is bijective and both f and its inverse, f^{-1}, are continuous.

Next, a topological manifold is defined:

Definition 1.4

Let M be a Hausdorff space, then M is called an *n-dimensional topological manifold* if M is locally homeomorphic to R^n. More precisely, there exists an open cover, $U = \{U_i\}_{i \in \Lambda}$ of M such that for each $i \in \Lambda$ there is a homeomorphism Ψ_i of U_i onto an open subset of R^n. The pair (Ψ_i, u_i) is called a *chart* (or a coordinate system) and the collection $\Psi = \{(\Psi_i, u_i)\}_{i \in \Lambda}$ is called an *atlas*. Two charts (Ψ_i, u_i) and (Ψ_j, u_j) are said to have a C^r *overlap* if $\Psi_j \Psi_i^{-1} : \Psi_i(u_i \cap u_j) \to \Psi_j(u_i \cap u_j)$ is of class C^r.

An atlas Ψ on M is called C^r if every pair of its charts has C^r overlap. A maximal C^r atlas Φ on a topological manifold M is a C^r differentiable structure. The pair (M, Φ) is called a *manifold of class C^r* (or *M is a smooth manifold*).

Note that in this study it is not necessary to deal with the full generality of abstract manifolds, but rather with ones that are embedded in Euclidian spaces.

Definition 1.5

M is an (embedded) C^r submanifold of R^K if and only if $M \subseteq R^K$, and for all $x \in M$ and for all charts Φ of M defined at x there exists an open subset $U \subseteq R^K$, such that $x \in U$, $U \subseteq \text{domain}(\Phi)$ and such that Φ extends to a C^r map from U to R^m; i.e., Φ is a C^r in the sense of Definition 1.2.

Below, smooth maps and manifolds are frequently refered to. This is meant to be a short-hand expression for the standard condition of r-fold differentiability, or, membership in class C^r.

From this point on the reader should note that all manifolds under discussion may be assumed to be embedded in Euclidian space. This is important in the next definition, as it now may be assumed that all charts automatically extend to smooth maps on all of R^K.

Definition 1.6

If A, M are C^r manifolds and $A \subseteq M$, then A is called a *submanifold of M*.

Next, the notion of derivative of a C^r map is defined over a smooth manifold. For this purpose, a few more definitions are recalled.

Definition 1.7

A map $f : M \to N$ between two C^r manifolds is called a C^r *diffeomorphism* if f is bijective and both f and its

inverse, f^{-1}, are of class C^r. When such a map exists it is said that M and N are diffeomorphic and this is denoted by $M \approx N$.

Remark: As the concern here is not with general abstract manifolds, there appears to be no need for developing the full machinery of abstract tangent spaces and of derivatives of maps between manifolds. Therefore, in the following, when reference is made to tangent vectors and derivatives, it is assumed that these are defined by methods of advanced calculus. Thus, only the more pertinent definitions and results are formally stated below.

Definition 1.8

Let $U \subseteq R^n$, $V \subseteq R^K$ be open subsets, and $M \subseteq R^K$ be a smooth m-manifold. Let $f : U \to V \cap M$ be a smooth map,

$$f(x) = (f_1(x),\ldots,f_K(x)).$$

The derivative of f and x, denoted by $Df(x)$ or $D_x f$, is the linear operator $Df(x) : R^n \to R^K$, defined by the usual condition that

$$\|f(x+h)-f(x)-Df(x)h\| = o(\|h\|).$$

Using standard coordinates, $Df(x)$ may be represented by the usual Jacobian matrix

$$Df(x) = \left[\frac{\partial f_i}{\partial x_j}\right]_{\substack{i=1,\ldots,K \\ j=1,\ldots,n}}$$

The tangent space of M at x, denoted by T_xM, which may be constructed by methods of ordinary calculus, can be given by means of the equation

$$T_xM = D\Phi(x)(R^n),$$

where now Φ^{-1} is a chart of M at x.

Definition 1.9

(a) Given a smooth map $f : U \subseteq R^n \to M \subseteq R^K$, let $x \in U$ with $y = f(x) \in M$. Then f is called *submersive* at x, provided that the derivative $Df(x) : R^n \to T_yM \subseteq R^K$ is a surjective map. If the map f is submersive at each $x \in U$, then f is said to be a *submersion*.

(b) Given $y \in R^K$, if f is submersive at every x such that $y = f(x)$ then y is called a *regular value* of f. Otherwise, y is a *critical value* of f.

(c) If $y = f(x)$ is a regular value of f then x is said to be a *regular point* of f. Otherwise x is called a *critical point* of f.

Several results that will be used in later chapters are listed below. Proofs which are readily available in many standard text books, such as Guillemin and Pollack [23], Hirsch [28], and Milnor [41], are omitted.

Local Submersion Theorem 1.10

Let M and N be two manifolds and $m = \dim(M) \geq \dim(N) = n$. Suppose $f : M \to N$ is a map that is submersive at

$x \in M$ and $y = f(x)$. Then there exists local charts (Ψ,U) and (Φ,V) around x and y respectively such that for the map h defined by $h = \Phi f \Psi^{-1}$ and $h(x_1,x_2,x_3,\ldots,x_m) = (x_1,x_2,x_3,\ldots,x_n)$.

That is, h is the canonical projection near x.

For the proof of this standard result of differential topology, the reader may wish to consult the textbook literature (e.g., Guillemin and Pollack [23], p. 20).

Preimage Theorem 1.11

Let M and N be two manifolds with $\dim(M) \geq \dim(N)$. Suppose y is a regular value of the C^r map $f : M \rightarrow N$, then the preimage $f^{-1}(y)$ is a C^r submanifold of M, and

$$\dim(f^{-1}(y)) = \dim(M) - \dim(N).$$

Proof: See Hirsch [28], page 22.

As a consequence of the Preimage Theorem, the following corollary is obtained:

Corollary 1.12

Let $f : M \rightarrow N$ be a C^r map, $y = f(x) \in N$ be a regular value of f, and let $Z = f^{-1}(y)$, then the kernel of Df(x), denoted by ker(Df(x)), where $Df(x) : T_xM \rightarrow T_yN$ at any $x \in Z$, is precisely the tangent space to Z, T_xZ.

The concept of *transversality* is of central importance for differential topology and in particular in this study. A definition of this concept follows.

Definition 1.13 (Transversality)

Let M, N be two manifolds, and L is a submanifold of N. Then the C^r map $f : M \to N$ is said to be transversal to L, denoted in symbols by $f \pitchfork L$, if the following condition holds:

$$Df(x)(T_xM) + T_yL = T_yN, \tag{1.11}$$

whenever $y = f(x) \in L$, $x \in M$. This means that the tangent space to N at y is generated by the tangent space to L at y and the image under Df(x) of the tangent space to M at x. Note that a direct sum in (1.11) is not required..

Remark: Observe, in case $L = \{y\}$, L is 0-dimensional, then f is submersive at all x with $f(x) = y$ iff $f \pitchfork L$.

Definition 1.14

If L is a submanifold of N, then the codimension of L, denoted by codim(L), is given by the equation Codim(L) = dim(N) - dim(L).

The next result relates the concepts in the previous two definitions.

Transversality Theorem 1.15

Let $f : M \to N$ be a C^r map, and L be a submanifold of N. If $f \pitchfork L$, then $f^{-1}(L)$ is a C^r submanifold of M. Furthermore, $\text{codim}(f^{-1}(L)) = \text{codim}(L)$.

Proof: See Hirsch [28], page 22.

Remark: Observe, in case $L = \{y\}$, L is 0-dimensional, then the Transversality Theorem reduces to the Preimage Theorem.

The next three theorems play a central part in establishing existence theorems in this study.

Classification Theorem of One-dimensional Manifold 1.16

Any C^1, connected one-dimensional manifold is diffeomorphic to S^1, the unit circle, or to some interval of the real numbers.

Proof: See Milnor [41], page 55.

Remark: It should be noted here that the interval mentioned in the theorem can be bounded, unbounded, closed, half-closed, or open.

Sard's Theorem 1.17

Let $U \subseteq R^n$ be an open subset, $f : U \to R^m$ be a C^r map with $r > \max(0, n-m)$. Let $C = \{x \in U : \text{rank}(Df(x)) < m\}$. Then $f(C)$ has m-dimensional Lebesgue measure zero.

Proof: See Milnor [41], page 16.

Parametrized Sard's Theorem (Parametric Transversality Theorem) 1.18

Let V, U be open subsets of R^q and R^m respectively, and $H: V \times U \to R^p$ be a C^r map with $r > \max(0,m-p)$. Define the map $H_a : R^m \to R^p$ by $H_a(x) = H(a,x)$ for all $a \in V$, $x \in U$. If 0 is a regular value of H, then for almost every $a \in V$, in the Lebesque measure sense, 0 is a regular value of H_a.

Proof: See Hirsch [28], page 79.

Finally, this section is concluded by stating two existence theorems from the theory of ordinary differential equations.

Theorem 1.19

Let U be an open subset of a finite dimensional normed linear space E, $f : U \to E$ a C^1 map, and $x_0 \in U$. There is a maximal open interval (α, β), $\alpha < x_o < \beta$ $x : (\alpha, \beta) \to U$ of the IVP

$$\frac{dx}{dt} = f(x) \text{ with } x(0) = x_0. \qquad (1.12)$$

Proof: See Hirsch and Smale [27], page 163.

Theorem 1.20

Let U, E and f as in the previous theorem. Let y(t) be a solution of the differential equation

$$\frac{dx}{dt} = f(x)$$

on the maximal open interval $J = (\alpha,\beta) \subseteq R$ with $\beta < \infty$. Then given any compact set $K \subseteq U$, there is some $t \in (\alpha,\beta)$ such that $y(t) \notin K$.

Proof: See Hirsch and Smale [27], page 172.

Next, the notion of an *ω-limit* point is defined.

Definition 1.21

Let x(t) be a solution of the IVP (1.12), and $Y \in R^n$. If there exists a sequence $\{t_n\}$ of real numbers with $\lim_{n\to\infty} t_n = \beta$, $\alpha < t_n < \beta$ such that $\lim_{n\to\infty} x(t_n) = y$, then y is called an ω-limit point of x(t).

CHAPTER II

CONVERGENCE OF THE CONTINUOUS NEWTON METHOD

In this chapter, following Hirsch and Smale [29], a proof of a convergence theorem is given. This theorem states that under certain conditions the paths defined by the continuous Newton method converge to a zero of the given map from almost all initial points.

In 2.1, a definition of a certain unit vector field $\phi(x)$ is given. This vector field, considered the equivalent of a differential equation by means of the equation

$$\frac{dx}{dt} = \phi(x), \qquad (*)$$

has integral curves which are the paths of the continuous Newton method. In Chapter V, numerical methods relating to the practical implementation of this method are discussed. Also, in 2.1, the projection map

$$g = f/\|f\|,$$

which maps R^n to S^{n-1} and is associated with the nonlinear map f whose zeros are being sought to compute is introduced.

A characterization of the set Reg(g) of regular points of the map g is given. It will turn out that Reg(f) may be a proper subset of Reg(g).

This is, incidentally, one major advantage of the continuous Newton method of the present chapter over the ordinary (classical, discrete) local Newton method defined in 1.1, equation (1.2), which breaks down when $\det(Df(x)) = 0$.

In 2.2, another definition of the vector field $\phi(x)$ which was given by Smale [49], is stated. This second definition, which is in terms of an explicit formula, has the advantage of being easier to understand.

The main emphasis of this chapter is on the convergence theorem for the continuous Newton method which was given by Smale [49] in 1976 and in fuller form by Hirsch and Smale [29] in their 1979 paper. Under certain conditions the solutions of the differential equation (*) converge to a zero of the map f for almost all initial points. This result represents a major milestone of the area of mathematics to which this thesis is devoted. Curiously, the paper has so far remained a monolith that has little relation to other work in the area. This phenomenon may be due in part to the fact that other ideas have evolved [8, 9, 34] which have certain advantages over those presented in this chapter. These ideas are discussed in succeeding parts of this thesis.

The convergence a.e. of the continuous Newton method under the conditions stated in 2.3 implies also the existence of zeros of the map f. Thus, a *convergence theorem* for a numerical method perhaps not unexpectedly also yields an *existence theorem* for the solution of an equation.

2.1 Hirsch and Smale's Definition of the Vector Field $\phi(x)$

Hirsch and Smale's definition of a vector field, given in [29], was rather brief and not defined by an explicit formula. The importance of this vector field is its essential role of defining an IVP whose solution curve is followed to a zero of the map f.

In this section a detailed construction of Hirsch and Smale's definition of this vector is given. First, however, it is necessary to lay down some notations and establish a few results.

Let $f : R^n \to R^n$ be a C^r map, and assume that R^n is equipped with the usual 2-norm and dot product. Also, let us denote the determinant of the Jacobian matrix Df(x) by J(x) or by det(Df(x)) and $S^{n-1} = \{x \in R^n : \|x\| = 1\}$, the unit sphere in R^n.

Let the set of regular points of f be denoted by

$$\text{Reg}(f) = \{x \in R^n : \text{rank}(Df(x)) = n\},$$

the set of critial points by

$$\text{Crit}(f) = R^n \backslash \text{Reg}(f).$$

(Cf. Definition 1.9). The set of zeros of f is $E = f^{-1}(0)$.

Next, associate with f the projection map

$$g : R^n \backslash E \to S^{n-1}$$

Which is defined by

$$g(x) = \frac{f(x)}{\|f(x)\|}. \tag{2.1}$$

Using the same notation as above, let Reg(g) be the set of regular points of g. It is well to remember that according to Definition 1.9, if $x \in Reg(g)$ and $y = g(x)$ then $rank(Dg(z)) = n-1$ for every z such that $g(z) = y$.

Next, let

$$Crit(g) = (R^n \backslash E) \backslash Reg(g).$$

The set Reg(g) may be viewed in a different manner as the proof of the following result shows:

Lemma 2.1

Let the map g be defined as in (2.1), then the set Reg(g) is open.

Proof:

Let $x \in Reg(g)$, then $rank(Dg(x)) = n-1$. This implies that there exists a subscript j_o, say, such that

$$\Psi_{j_o}(x) = \det \left[\frac{\partial g_i}{\partial x_j} \right]_{j \neq j_o} \neq 0.$$

Because det(.) is a continuous function, then

$$\text{Reg}(g) = \bigcup_{j_o=1}^{n} \{x \in R^n : \Psi_{j_o}(x) \neq 0\} \text{ is open.}$$

If $x \in \text{Reg}(g)$, what kind of a geometric configuration is obtained for the preimage $g^{-1}(g(x))$? The answer to this question is given by the next result.

Proposition 2.2

Let the map g be defined as in (2.1), $x \in \text{Reg}(g)$, and define the set A(x) by

$$A(x) = g^{-1}(g(x)).$$

Then A(x) is a C^r one-dimensional submanifold closed in Reg(g). Furthermore, let $\mathcal{C}(x)$ denote the connected component through x in A(x), then $\mathcal{C}(x)$ is a C^r one-dimensional manifold diffeomorphic to S^1 or R.

Proof:

Since $x \in \text{Reg}(g)$, that is, g(x) is a regular value of g, then, by the Preimage Theorem 1.11, the set A(x) $= g^{-1}(g(x))$ is a C^r submanifold of Reg(g). With dim(A(x)) $= \dim(R^n \backslash E) - \dim(S^{n-1}) = 1$. Also, becauses $\{g(x)\}$ is closed in S^{n-1}, then A(x) is closed in Reg(g).

Now, since $C(x)$ is a connected component in $A(x)$, by the Classification Theorem of One-dimensional Manifolds 1.16 $C(x)$ is diffeomorphic to S^1 or to an interval.

But, $C(x)$ is a manifold (without boundary), so $C(x)$ cannot be diffeomorphic either to a closed interval or to a half-closed interval. Hence, either $C(x) \approx S^1$ or $C(x) \approx R$.

Next, a proof is given for the following useful proposition, which shows that Dg is parallel to the orthogonal projection of Df perpendicular to f or g. The reader may recall that the matrix of the orthogonal projection P onto the span of the unit column-vector u can be written as $P = uu^t$. The orthogonal projection perpendicular to u is then $I - uu^t$. This occurs below with $u = g(x)$.

Proposition 2.3

If the map g is defined as in (2.1), then

$$Dg(x) = \frac{1}{\|f(x)\|} \{I - g(x)g(x)^t\} Df(x). \qquad (2.2)$$

In particular, $\text{range}(Dg(x)) \subseteq [g(x)]^{\perp}$, where "$\perp$" indicates the orthogonal complement.

Proof:

Let $g(x)\|f(x)\| - f(x) = 0$. Differentiate this equation with respect to x to get

$$Dg(x)\|f(x)\| + g(x)D_x\|f(x)\| - Df(x) = 0. \qquad (2.3)$$

Since $\|f(x)\| = \sqrt{f_1^2(x) + f_2^2(x) + \ldots + f_n^2(x)}$, then

$$\frac{\partial}{\partial x_i} \|f(x)\| = \sum_{k=1}^{n} f_k(x) \frac{\partial}{\partial x_i} f_k(x)/\|f(x)\|$$

$$= \frac{1}{\|f(x)\|} \{f^t(x)Df(x)\}_i.$$

Thus,

$$D_x\|f(x)\| = \frac{1}{\|f(x)\|} f(x)^t Df(x). \qquad (2.4)$$

Substitute (2.4) in (2.3) and collect terms to obtain

$$Dg(x) = \frac{Df(x) - g(x)f(x)^t Df(x)/\|f(x)\|}{\|f(x)\|}$$

$$= \frac{1}{\|f(x)\|} \{(I - g(x)g(x)^t\}Df(x).$$

The second part follows from noting that range$(Dg(x)) \subseteq$ range$(I - g(x)g(x)^t)$. But, ker$(I - g(x)g(x)^t) = [g(x)]$. Hence, range$(Dg(x)) \subseteq [g(x)]^{\perp}$.

One should note that if $x \in Reg(g)$, then ker$(Dg(x))$ is one-dimensional. By Corollary 1.12 of the Preimage Theorem 1.11 the tangent line to $C(x)$ at x is parallel to the linear space ker$(Dg(x))$.

Now the unit vector field $\phi(x)$ may be defined. For each $x \in Reg(g)$ let $\phi(x) \in$ ker$(Dg(x))$ with $\|\phi(x)\| = 1$ so

that $\phi(x)$ is tangent to $C(x)$. To define $\phi(x)$, since $x \in$ Reg(g), the rank(Dg(x)) = n-1, an ordered basis, say, $\{e_1, e_2, \ldots, e_{n-1}\}$ can be picked for the space

$$U = [\ker(Dg(x))]^{\perp} = \text{the row space of } Dg(x),$$

in such a way that the ordered basis

$$B = \{g(x), Dg(x)e_1, Dg(x)e_2, \ldots, Dg(x)e_{n-1}\}$$

defines the positive orientation of R^n; that is, the determinant of the matrix of their coordinates is positive.

In particular, $Dg(x)e_1, Dg(x)e_2, \ldots, Dg(x)e_{n-1}$ are linearly independent. Namely, if

$$\sum_{i=1}^{n-1} \lambda_i \, Dg(x)e_i = 0$$

for some scalars λ_i, then

$$\sum_{i=1}^{n-1} \lambda_i \, e_i \in \ker(Dg(x)) \cap [\ker(Dg(x))]^{\perp} = \{0\}. \quad \text{So,}$$

$$\sum_{i=1}^{n-1} \lambda_i \, e_i = 0, \text{ and } \lambda_i = 0, \text{ as claimed.}$$

Also, claim B is linearly independent, for otherwise

$$g(x) = \sum_{i=1}^{n-1} \lambda_i \, Dg(x)e_i \in [g(x)]^{\perp},$$

from Proposition 2.2, a contradiction, as $\|g(x)\| = 1$. Therefore, B is an ordered basis for R^n.

Next, choose a sign on $\phi(x)$ such that $\phi(x) \in \ker(Dg(x))$ and such that the ordered basis $\{\phi(x), e_1, e_2, \ldots, e_{n-1}\}$ defines the negative orientation of R^n. By the Implicit Function Theorem: locally in Reg(g), a nonvanishing unit tangent vector $\theta(x) \in \ker(Dg(x)$ can be found. This is possible because $\ker(Dg(x))$ is one-dimensional. Also, if f is a C^r map, then $\theta(x)$ is a C^{r-1}. Thus,

$$\phi(x) = \pm \theta(x)$$

Now give the curves $C(x)$ an orientation by $\phi(x)$.

Lemma 2.4

Let f be a C^r map and for $x \in \text{Reg}(g)$ let $\phi(x)$ be defined as above, then

$$Df(x)\phi(x) = \lambda(x)f(x). \qquad (2.5)$$

Furthermore, $\lambda(x)$ and $J(x)$ have opposite signs, and $\lambda(x) = 0$ iff $J(x) = 0$.

Proof:

By definition

$$\phi(x) \in \ker(Dg(x)) = \ker[(I - g(x)g(x)^t)Df(x)].$$

Then $Df(x)\phi(x) \in \ker(I - g(x)g(x)^t) = \text{range}(g(x)g(x)^t)$. But $\text{range}(g(x)g(x)^t) = \lambda(x)f(x)$, because

$$g(x)g(x)^t(\lambda(x)f(x)) = \frac{f(x)}{\|f(x)\|}\frac{f(x)^t}{\|f(x)\|}(\lambda(x)f(x))$$

$$= \lambda(x)f(x).$$

Hence, the claim.

To show $\lambda(x)$ and $J(x)$ have opposite signs, and $\lambda(x)' = 0$ iff $J(x) = 0$, consider the following two cases.

Case I: $J(x) = 0$

By (2.5) $\lambda(x) = 0$ iff $\phi(x) \in \ker(Df(x))$, but this is true iff $J(x) = 0$.

Case II: $J(x) \neq 0$

Let A be the coordinate matrix of the ordered basis $B' = \{\phi(x), e_1, e_2, \ldots, e_{n-1}\}$. When $Df(x)$ is applied to A and using (2.5), then

$$Df(x)A = (\lambda(x)f(x), Df(x)e_1, Df(x)e_2, \ldots, Df(x)e_{n-1}). \quad (2.6)$$

The definition of $\phi(x)$ shows that $\det(A) < 0$, but

$$\det(Df(x)A) = \det(Df(x))\det(A).$$

Therefore, an orientation reversal occurs iff $J(x) < 0$.

Now apply

$$\frac{1}{\|f(x)\|}(I - g(x)g(x)^t) \text{ to } Df(x)e_i, \text{ to get}$$

$$(\lambda(x)f(x), Dg(x)e_1, Dg(x)e_2, \ldots, Dg(x)e_{n-1}) \quad (2.7)$$

Claim that going from (2.6) to (2.7) does not change orientation. To show this let $e' = Df(x)e_i$. Because $Df(x)$ is invertable, then $e_i = [Df(x)]^{-1}e'$. Consequently

$$Dg(x)e_i = e_i'.$$

This is because $(I - g(x)g(x)^t)$ is a projection map and $e_i' \in \text{range}(I - g(x)g(x)^t)$, otherwise, $e' \in \ker(I - g(x)g(x)^t)$, but this would contradict e_i''s being linearly independent, hence the claim.

2.2 Definition to the Vector Field $\phi(x)$ by Means of the Classical Adjoint

In this section a second definition of the vector field $\phi(x)$ is given. This definition, which was used by Smale in his initial paper [49], has the advantage that it is given by an explicit formula, and hence is easier to understand than the more abstract definition given by Hirsch and Smale [29]. Theorem 2.8 shows that the vector field defined above is also replaced by the elementary formula

$$\phi(x) = - \beta(x)\text{adj}(Df(x))f(x),$$

where $\beta(x)$ is a certain scalar. Also, this explicit formula for $\phi(x)$ certainly makes it easier to think about practical algorithms when implementing the convergence theorem of this chapter. It is shown in this section that the vector field $\phi(x)$, given by the above formula, shares all the basic

properties required for the proof in 2.3. In most cases it is easy to verify that the two vector fields are indeed the same.

For $f(x) \neq 0$ let $L = \{\alpha.f(x) : x \in R^n, \alpha > 0\}$, that is, L is a ray in R^n. Recall that in the proof of Lemma 2.4, it was shown that L is the range of the projection map given by $G(x) = g(x)g(x)^t$. But, range(G(x)) = ker(I - G(x)), and ker(G(x)) = range(I - G(x)). Thus, the orthogonal complement of L, is $L^{\perp}$ = ker(G(x)) = range(I - G(x)). Hence, a translation of $L^{\perp}$ is the tangent space to S^{n-1} at g(x), as shown in Figure 1.

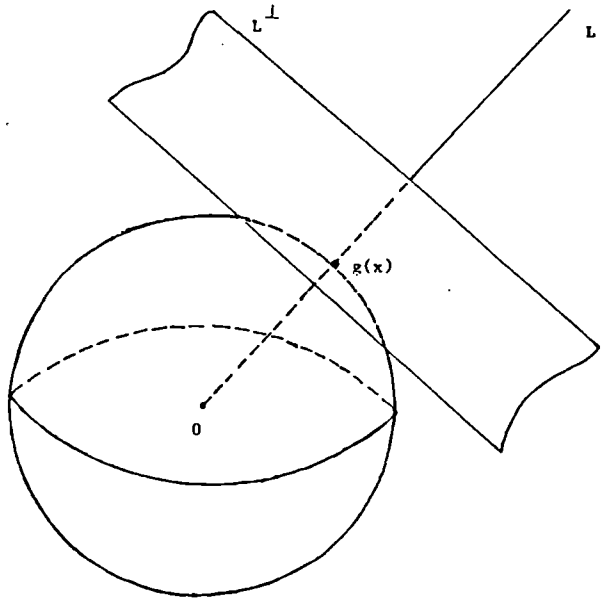

Figure 1. A Tangent Space to S^{n-1} at g(x)

The next result characterizes the regular points of the map $g(x)$.

Theorem 2.5

Let the map g be defined as in (2.1), then $x \in \text{Reg}(g)$ iff one of the following two conditions is satisfied:

(i) $\text{rank}(Df(x)) = n$, or

(ii) $\text{rank}(Df(x)) = n-1$, and $\text{range}(Df(x)) \cap L = \{0\}$.

Proof:

Necessity: Let $x \in \text{Reg}(g)$. Recall from linear algebra if A and B are matrices such that their product is defined, then $\text{rank}(AB) \leq \min(\text{rank}(A), \text{rank}(B))$. By proposition 2.3

$$Dg(x) = \frac{1}{\|f(x)\|} [(I - g(x)g(x)^t)DF(x)],$$

then by the regularity of g, $\text{rank}(Dg(x)) = n-1$. Hence $\text{rank}(I - g(x)g(x)^t) \geq n-1$ and $\text{rank}(Df(x)) \geq n-1$.

Case I: Suppose the rank of $Df(x) = n$. Then condition (i) holds.

Case II: Suppose the $\text{rank}(Df(x)) = n-1$. Claim that condition (ii) holds, i.e., $\text{range}(Df(x)) \cap L = \{0\}$. If not, since L is one dimensional, then $L \subseteq \text{range}(Df(x))$. This implies $g(x) \in \text{range}(Df(x))$, and hence there exists a nonzero $u_1 \in R^n$ such that $Df(x)u_1 = g(x)$. Also, since

rank(Df(x)) = n-1, there exists $u_2 \in \ker(Df(x))$. Then both $u_1, u_2 \in \ker(Dg(x))$.

Next, note that u_1 and u_2 are linearly independent, as $Df(x)u_1 = g(x) \neq 0$, $Df(x)u_2 = 0$ by assumption, while both u_1 and u_2 are nonzero.

Sufficiency: Consider the following two cases:

Case I: Condition (i) holds.

Suppose condition (i) holds, that is, for $x \in R^n$, rank(Df(x)) = n. To compute the kernel of Dg(x), let $u \in \ker(Dg(x))$. Then by Proposition 2.2,

$$\frac{1}{\|f(x)\|} (I - g(x)g(x)^t)Df(x)u = 0.$$

Let $v = Df(x)u$. Thus,

$$v \in \ker(I - g(x)g(x)^t) = \text{range}(g(x)g(x)^t) = L.$$

Hence, $Df(x)u = tg(x)$ for $t \in R$. Therefore, $u = t[Df(x)]^{-1}(g(x))$. This makes it evident that the nullity of Dg(x) = 1. Thus, $x \in Reg(g)$.

Case II: Condition (ii) holds.

Again, compute the kernal of Dg(x). Observe that from the preceeding computation, $u \in \ker(Dg(x))$ if and only if $Df(x)u = tg(x)$, where $t = g(x)^t Df(x)u$. Because condition (ii) holds, then t = 0 and Df(x)u = 0 follow necessarily. Hence the kernels of Df(x) and Dg(x) agree.

Therefore, it follows that nullity(Dg(x)) = 1. Consequently, rank(Dg(x)) = n-1, and hence, in Case II, then $x \in Reg(g)$.

The next two propositions are essential for the alternative definition of the vector field $\phi(x)$. Let the classical adjoint of an n×n matrix A be denoted by adj(A).

Proposition 2.6

Let A be an n×n matrix. If rank(A) = n-1, then rank(adj(A)) = 1. Moreover, range(adj(A)) = ker(A), and ker(adj(A)) = range(A).

Proof:

By assumption rank(A) = n-1, then det(A) = 0, and there exists a submatrix of A of order n-1 whose determinant is not zero. Thus, adj(A) ≠ 0. Now by a familiar equation

$$Aadj(A) = 0, \qquad (*)$$

then $range(adj(A)) \subseteq ker(A)$.

But, nullity(A) = 1, then rank(adj(A)) = 1. Also, since

$$adj(A)A = 0, \qquad (**)$$

then $range(A) \subseteq ker(adj(A))$.

But, rank(A) = n-1, and nullity(adj(A)) = n-1, then range(A) = ker(adj(A)). By (*) and (**) range(adj(A)) = ker(A).

Now, denote the span of the vector u by [u].

Proposition 2.7

Let $x \in Reg(g)$, then the $\ker Dg(x) = [adj(Df(x))f(x)]$.

Proof:

Case I: $\operatorname{rank}(Df(x)) = n$.

In the proof of Theorem 2.5, it is shown that if $\operatorname{rank}(Df(x)) = n$, then $u \in \ker(Dg(x))$ iff

$u = t[Df(x)]^{-1}(g(x)$. But,

$$[Df(x)]^{-1} = \frac{1}{J(x)} adj(Df(x)),$$

then $u = \theta(x)adj(Df(x))f(x)$, where

$\theta(x) = \frac{t\alpha}{J(x)\|f(x)\|}$, and because $x \in Reg(g)$, then $\ker(Dg(x))$ is one-dimensional. Therefore,

$$\ker(Dg(x)) = [adj(Df(x))f(x)].$$

Case II: $\operatorname{rank}(Df(x)) = n-1$.

Suppose $x \in Reg(g)$, $\operatorname{rank}(Df(x)) = n-1$, and $L \not\subset \operatorname{range}(Df(x))$; that is, $g(x) \notin \operatorname{range}(Df(x))$. Then, $0 \neq u \in \ker(Dg(x))$ iff $u \in \ker(Df(x))$.

Let $v = adj(Df(x))f(x)$, then by Proposition 2.6 since $\ker(Df(x)) = \operatorname{range}(adj(Df(x)))$, $v \in \ker(Df(x))$. Thus, $v \in$

$\ker(Dg(x))$. But the $\text{nullity}(Dg(x)) = 1$, then v is parallel to $\ker(Dg(x))$; that is, $\ker(Dg(x)) = [v]$. Therefore, $\ker(Dg(x)) = [\text{adj}(Df(x))f(x)]$.

Note that $v \neq 0$, because by assumption $\alpha.f(x) = g(x) \notin \text{range}(Df(x)) = \ker(\text{adj}(Df(x))$.

The vector field $\phi(x)$ can now be defined.

Theorem 2.8

Let f be a C^r map and $x \in \text{Reg}(g)$. Define a unit vector $\phi(x)$ by

$$\phi(x) = -\beta(x)\text{adj}(Df(x))f(x), \tag{2.8}$$

where $\beta(x) = \dfrac{1}{\|\text{adj}(Df(x)f(x)\|}$.

Then, $\phi(x)$ has the following properties:

(i) $\phi(x)$ is of class C^{r-1},

(ii) $\phi(x) \in \ker(Dg(x))$, and

(iii) $\phi(x) \neq 0$.

Proof:

The proof of (i) follows from noting that f is C^r, then $Df(x)$ and consequently $\text{adj}(Df(x)$ is of class C^{r-1}. By (2.8) $\phi(x)$ is of class C^{r-1}.

To proof (ii), note that Proposition 2.7 implies that any vector in $\ker(Dg(x))$ is a constant multiple of the

vector adj(Df(x))f(x). From the definition of $\phi(x)$ it is immediate that $\phi(x) \in \ker(Dg(x))$.

For the proof of (iii), suppose that $\phi(x) = 0$, then adj(Df(x))f(x) = 0, and Proposition 2.6 implies that $f(x) \in \ker(\text{adj}(Df(x))) = \text{range}(Df(x))$. But this contradicts Theorem 2.5 since $x \in \text{Reg}(g)$.

Corollary 2.9

Let $x \in \text{Reg}(g)$, define $\lambda(x) : R^n \to R$ by

$$\lambda(x) = -\beta(x)J(x),$$

where $\beta(x)$ is defined as in (2.8), and J(x) is the Jacobian determinant. Then,

$$Df(x)\phi(x) = \lambda(x)f(x),$$

$\lambda(x)$, and J(x) are opposite in signs. Furthermore, $\lambda(x) = 0$ iff $J(x) = 0$.

Proof:

By the definition of $\phi(x)$

$$Df(x)\phi(x) = Df(x)[-\beta(x)\text{adj}(Df(x))f(x)]$$

$$= -\beta(x)[J(x)f(x)]$$

Thus, $Df(x)\phi(x) = \lambda(x)f(x)$.

Note that $\lambda(x)J(x) = -\beta(x)J^2(x)$. But by definition $\beta(x) > 0$ and hence, $\lambda(x)J(x) < 0$. Hence, $\lambda(x)$ and $J(x)$ have opposite signs. Also, $\lambda(x) = 0$ iff $J(x) = 0$.

2.3 The Hirsch and Smale's Convergence Theorem

In this section detailed proofs of two convergence theorems due to Hirsch and Smale [29] are given. The proofs of these theorems depend on following certain solution curves of an IVP. To drive this IVP, let $x_0 \in \text{Reg}(g)$ and $C(x_0)$ be the component in $A(x_0)$ through x_0. By Proposition 2.2 let $\xi(t)$ be a parametrization of $C(x_0)$, with $\xi(t_0) = x_0$. For any $x \in C(x_0)$

$$g(x) = g(x_0),$$

differentiating the above equation with respect to t,

$$Dg(\xi(t)) \frac{d\xi}{dt} = 0.$$

Hence, $\frac{dx}{dt}$ is in the $\ker(Dg(x))$, but $\frac{dx}{dt} = \frac{d\xi}{dt}$. Also, from Propositions 2.7 and 2.8, it was known that $\ker(Dg(x))$ is generated by $\phi(x)$, therefore, provided that t is arc length

$$\frac{d\xi}{dt} = \phi(\xi(t)), \text{ with } \xi(t_0) = x_0. \tag{2.9}$$

By Theorem 1.19 (the existence and uniqueness theorem of IVP) $\xi(t)$ is the unique solution of (2.9).

Interestingly enough, by means of numerical methods one approximates the solution curve $\xi(t)$ and follows it until a zero of the map f is reached. This subject is pursued in some depth in Chapter V.

Next, it is shown that the solution curves of the IVP in (2.9) cannot be periodic; that is, $\xi(t)$ cannot be diffeomorphic to a circle. To show this, it is necessary to establish several lemmas.

Lemma 2.10

Let f be defined as before, then $\|f(x)\|$ is nonincreasing along the curve $C(x)$ in every open set where $J(x) \geq 0$ and $\|f(x)\|$ is strictly decreasing where $J(x) > 0$.

Proof:

Let $h(t) = \|f(\xi(t))\|$, where $x(t) = \xi(t)$. By differentiating h(t) with respect to t:

$$\frac{dh}{dt} = D_x\|f(\xi(t))\| \quad \frac{d\xi}{dt}$$

but, from (2.4) $D_x\|f(x)\| = \frac{1}{\|f(x)\|} f(x)^t Df(x)$, then

$$\frac{dh}{dt} = \frac{1}{\|f(x)\|} f(x)^t \, Df(x) \, \frac{d\xi}{dt}$$

Again, from (2.9) and by Corollary 2.8 the following is obtained:

$$\frac{dh}{dt} = \frac{1}{\|f(x)\|} f(x)^t Df(x)\ \phi(x) = \frac{1}{\|f(x)\|} f(x)^t \lambda(x) f(x)$$

$$= \lambda(x)\ \|f(x)\|.$$

Since $J(x) \geq 0$; then by Corollary 2.9 $\lambda(x) \leq 0$. Thus, $\frac{dh}{dt} \leq 0$; hence, $\|f(x)\|$ is nonincreasing along $C(x)$ in every neighborhood where $J(x) \geq 0$. In a similar way it can be shown that in a neighborhood where $J(x) > 0$, $\|f(x)\|$ is strictly decreasing.

In the remainder of this section, the following notation will be used: Let $0 \leq a \leq b$, define

$$E[a,b] = \{x \in R^n : a \leq \|f(x)\| \leq b\}.$$

If $s > 0$, define

$$E(s) = \{x \in R^n : \|f(x)\| = s\}.$$

$$E_+(s) = \{x \in R^n : \|f(x)\| \geq s\}.$$

Finally, define

$$R_+ = \{x \in R : x > 0\}.$$

The next lemma gives conditions which guarantee that $C(x) \pitchfork E(s)$.

Lemma 2.11

Let U be an open subset of Reg(g) with $E(s) \subseteq U$, $\|f\| : U \to R_+$. Suppose s is a regular value of $\|f(x)\|$, $J(x) \neq 0$, then E(S) is a C^r closed submanifold in Reg(g), and

$$C(x) \pitchfork E(s).$$

Proof:

Since s is a regular value of $\|f(x)\|$, then by the Preimage Theorem 1.11 E(s) is a C^r submanifold of Reg(g) and $\dim(E(s)) = n-1$. Moreover, E(s) is closed in Reg(g).

Claim $T_x(C(x)) + T_x(E(s)) = R^n$. Recall that, $D_x\|f(x)\| = \frac{1}{\|f(x)\|} f(x)^t Df(x)$; then $s = \|f(x)\|$ for some $x \in Reg(g)$ is a regular value of $\|f(x)\|$ if $f(x)^t Df(x) \neq 0$. By assumption s is a regular value of $\|f(x)\|$, then by Corollary 2.8 $D_x\|f(x)\|\phi(x) = \lambda(x)\|f(x)\|$. Also, since $J(x) \neq 0$, then $D_x\|f(x)\|\phi(x) \neq 0$. Thus, $\phi(x) \notin \ker(D_x\|f(x)\|)$ and consequently, $[\phi(x)] + [f(x)^t Df(x)]^{\perp} = R^n$.

This implies that $C(x) \pitchfork E(x)$.

The following assumptions are made in the next four propositions:

(I) (i) $\|f(x_0)\| = s_0 > 0$,

(ii) $J(x_0) > 0$,

(iii) $J(x) \geq 0$ in a neighborhood of $E(s_0)$.

Recall that in Proposition (2.2), it was proven that

$$C(x) \approx S^1 \text{ or } C(x) \approx R.$$

In the next result, it is shown that $C(x)$ cannot be diffeomorphic to S^1.

Proposition 2.12

Let $f : R^n \to R^n$ be a C^r map satisfying the conditions in I, then

$$C(x_0) \cap E(s_0) = \{x_0\}, \text{ and } C(x_0) \approx R.$$

Proof:

Let $h(t) = \|f(\xi(t))\|$. By assumption (iii) above since $J(x) \geq 0$, and as result of Lemma 2.10 $h'(t) \leq 0$, where "'" stands for $\frac{dh}{dt}$, for all $\xi(t)$ in a neighborhood of $E(s_0)$.

Suppose $C(x_0) \approx S^1$; then there exists t_0 and t_1 with $t_0 \neq t_1$ and $h(t_0) = s_0 = h(t_1)$. By assumption (ii) $J(x_0) > 0$, then $h'(t_0) < 0$. Therefore, there exists $\delta > 0$ and $\epsilon > 0$ such that $h'(t) < 0$ on $[t_0-\delta, t_0+\delta]$ with

$$h(t_0-\delta) \geq s_0 + \epsilon$$

$$h(t_0+\delta) \leq s_0 - \epsilon \qquad (2.10)$$

Case I: $t_1 < t_0-\delta$

Suppose $t_1 < t_0-\delta$. Since $h(t_1) = s_0 > 0$ by assumption, then $h'(t) \leq 0$ for all t in a neighborhood of t_1 (Figure 2).

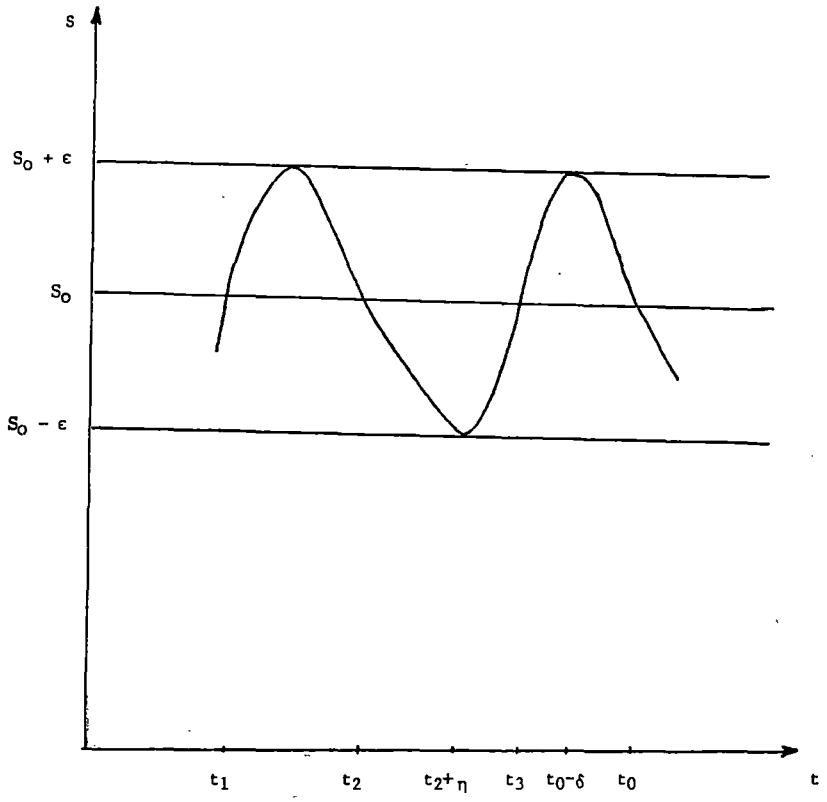

Figure 2. The Function $h(t) = \|f(x(t))\|$ in a Neighborhood of t_1 and t_2

Let $t_2 = \text{Sup}\{t : t_1 \leq t \leq t_0-\delta, h(t) = s_0\}$, then $t_2 \leq t_0-\delta$.

But, $h(t_2) = s_0$, then $h'(t) \leq 0$ in a neighborhood of t_2; that is, there exists an $\eta > 0$ such that $h(t) \leq s_0$ for all $t \in [t_2, t_2+\eta]$ (Figure 2).

But, $h(t0-\delta) \geq s + \epsilon$; then by the Intermediate Value Theorem there exists $t_3 \in (t_2, t_0-\delta)$ such that $h(t_3) = s_0$. This contradicts the definition of t_2. Hence, no such t_1 exists.

Case II: $t_1 > t_0+\delta$

In this case one defines $t_4 = \inf\{t : t_0+\delta \leq t \leq t_1, h(t) = s_0\}$. By a similar argument to that of Case I, one arrives to another contradiction. Therefore, $C(x_0)$ cannot be diffeomorphic to S^1, and hence $C(x_0) \approx R$.

It remains to show that $C(x_0) \cap E(s_0) = \{x_0\}$. For this purpose, it is shown that x_0 disconnects $C(x_0)$. Let $V = \{x : \|f(x)\| < s_0\}$, and $W = \{x : \|f(x)\| > s_0\}$. It is clear that both V and W are open.

Next, it is shown that $V \cap C(x_0)$, $W \cap C(x_0)$ are nonempty. From (2.10) there exist $t_1 \in (t_0-\delta,t_0)$, and $t_2 \in (t_0,t_0+\delta)$ with $\xi(t_1) = x_1$, and $\xi(t_2) = x_2$. Then $\|f(x_1)\| > s_0$, and $\|f(x_2)\| < s_0$. Hence, the claim. But this says that $C(x_0)\backslash\{x_0\} = [C(x_0) \cap V] \cap [C(x_0) \cap W]$.

Therefore, x_0 disconnect $C(x_0)$. By Lemma 2.10 since $C(x_0) \overline{\cap} E(s_0)$, then $C(x_0) \cap E(s_0) = \{x_0\}$.

It is shown in Proposition 2.12 that x disconnects $C(x)$ into two components; each is diffeomorphic to R. Let us denote the closure of these two components by $C_+(x)$, and $C_-(x)$, where the vector field $\phi(x)$ points toward $C_+(x)$, the forward orbit (the solution curve $\xi(t)$) associated with the vector field $\phi(x)$.

The following corollary is a conquence of Lemma 2.10 and Proposition 2.12:

Corollary 2.13

Let f be defined as in the proposition, then

$$\|f(y)\| < s_0 \text{ for all } y \in C_+(x_0)\backslash\{x_0\}.$$

Proof:

Note that from the hypothesis (i) above $\|f(x_0)\| = s_0$, $J(x) \geq 0$ in a neighborhood of $E(s_0)$, then Lemma 2.10 implies $\|f(y)\|$ is nonincreasing along $C(x_0)$. Also, Proposition 2.11 implies that for $y \in C_+(x_0)\backslash\{x_0\}$, $\|f(y)\| < s_0$.

Let $\xi : R \to C(x)$ be a parametrization of $C(x)$, which is given by $x = \xi(t)$ and $\xi([0, \infty)) = C_+(x)$. If y is a ω-limit point of $C_+(x)$, what is the connection between this ω-limit point and the maps f and g ? The answer to this question is given by the next proposition.

Proposition 2.14

If y is an ω-limit point of $C_+(x)$, then either y is a critical point of g or a zero of f.

Proof:

Let y be an ω-limit point of $C_+(x)$, suppose $f(y) \neq 0$, and $y \notin \text{Crit}(g)$. This implies $y \in \text{Reg}(g)$. Claim that $C(y) \subseteq A(x)$. Since y is an ω-limit point of $C_+(x)$, there exists a sequence of real numbers $\{t_m\}$ and a diffeomrphism $\xi : [0, \infty) \to C_+(x)$ such that $\lim_{m\to\infty} \xi(t_m) = y$, also, $\xi(t_m) = g(x)$. By the continuoutity of g, $\lim_{m\to\infty} g(\xi(t_m))$

$= g(\lim_{m\to\infty} \xi(t_m)) = g(y)$. Hence, $g(y) = g(x)$ and $y \in A(x)$. Therefore, $C(y) \subset A(x)$.

Claim, $C(x) = C(y)$. Since $y \in \bar{C}(x)$, then by hypothesis $C(x) \cup C(y)$ is connected. Suppose $C(x) \neq C(y)$; then because $C(x)$ and $C(y)$ are components of $A(x)$, there exists open sets $U, V \subseteq R^n$ such that $C(x) \subseteq (U \cap A(x))$, and $C(y) \subseteq (V \cap A(x))$. Moreover, $\xi(t_m) \in C(y)$, this implies that $\xi(t_m) \in V$.

Now, $U \cap V \cap A(x) = \emptyset$. But because $\lim_{m\to\infty} \xi(t_m) = y$, there exists and $\epsilon > 0$ and $N > 0$ such that $\xi(t_m) \in B(y,\epsilon) \subseteq U$ for all $m \geq N$. Therefore, $\xi(t_m) \in U \cap V \cap A(x)$, but this is a contradiction. Hence, the claim.

The next result is the last proposition required for the establishment of the convergence theorems of this chapter.

Proposition 2.15

In addition to the assumptions (i-iii) in (I) suppose $0 < q < s_0$ and the following two more conditions hold:

a) $E[q,s_0]$ is compact,

b) $g(x_0)$ is a regular value of $g|_{E[q,s_0]}$.

Then $C_+(x_0) \cap E(q) \neq \emptyset$.

Proof:

Let $x \in C_+(x_0)$, then by Corollary 2.13 $\|f(x)\| \leq s_0$. Suppose $C_+(x_0) \cap E(q) = \emptyset$, then $q < \|f(x)\|$ and $C_+(x_0) \subseteq$

$E[q,s_0]\backslash E(q)$, by connectedness. By hypothesis $E[q,s_0]$ is compact; then $C_+(x_0)$ has an ω-limit point $y \in E[q, s_0]$ and as consequence of Proposition 2.15 either $f(y) = 0$ or $y \in Crit(g)$. But, $\|f(y)\| > q > 0$, and $\lim_{m\to\infty} g(\xi(t_m)) = g(\lim_{m\to\infty} \xi(t_m)) = g(y)$. Also, $g(\xi(t_m)) = g(x_0)$, then $g(y) = g(x_0)$.

Once more by hypothesis, since $g(x_0)$ is a regular value of $g|_{E[q,s_0]}$, then $y \notin Crit(g)$. This is a contradiction to y being an ω-limit point of $C_+(x_0)$. Hence, $C_+(x_0) \cap E(q) \neq \emptyset$.

It should be noted here that the above proposition affirms the statement of Theorem 1.20 in that the solution curve of an IVP, which is defined on a maximal open interval, leaves every compact subset of the domain.

Recall also that if W_1 is a subset of W and $W\backslash W_1$ has measure zero, then W_1 is said to have *full measure*.

Now the first convergence theorem of this chapter can be stated and proved.

Theorem 2.16 (Hirsch and Smale's)

Let $f : R^n \to R^n$ and $\alpha > 0$ satisfy the following conditions:

(i) f is a C^2 and proper,

(ii) $J^{-1}(0)$ has measure zero, and

(iii) $J(x) \geq 0$ if $\|x\| \geq \alpha$.

Let $0 < \epsilon < \alpha$. Then there exists a subset

$$W(\epsilon) \subseteq E_+(\alpha)$$

which is open and of full measure, such that if $x_0 \in W(\epsilon)$, then $C(x_0) \approx R$ and $C_+(x)$ contains a point y with $\|f(y)\| = \epsilon$.

Proof:

For the sake of clarity, the proof will be divided into five major steps. To begin with, for each $\beta > \alpha$ define

$$B(\epsilon, \beta) = g(Crit(g) \cap E[\epsilon, \beta])$$

First, claim that $B(\epsilon, \beta)$ is compact in S^{n-1}. Let $A = \{f(x) : \epsilon \leq \|f(x)\| \leq \beta\}$; then $f^{-1}(A) = E[\epsilon, \beta]$. Since f is proper, and A is compact, then $E[\epsilon, \beta]$ is compact. Also, since Crit(g) is closed, then $Crit(g) \cap E[\epsilon, \beta]$ is compact and hence, $B(\epsilon, \beta)$ is compact supset of S^{n-1} by the continuity of g. As a consequence of Sard's Theorem 1.18 $B(\epsilon, \beta)$ has measure zero. Therefore, $S^{n-1}\backslash B(\epsilon, \beta)$ has full measure and open in S^{n-1}.

Secondly, claim that Reg(g) has full measure in $R^n\backslash E$. By hypothesis $J^{-1}(0)$ has measure zero, then Reg(f) $= R^n\backslash J^{-1}(0)$ has full measure in R^n. But $Reg(f) \subseteq Reg(g)$, then $[Reg(g)]^c \subseteq [Reg(f)]^c = J^{-1}(0)$. Thus, Reg(g) has full measure in $R^n\backslash E$.

Thirdly, claim $g^{-1}(S^{n-1}\backslash B(\epsilon, \beta))$ has full measure in $R^n\backslash E$. To show this, it suffices to check it at points in Reg(g). Let $x \in Reg(g)$, then Dg(x) is serjective and hence g is a submersive at x. Let $y = g(x)$. By the Local Submersion Theorem 1.10 there exist local charts (Ψ,U) and (Φ,V)

around x and y respectively, such that $\pi = \Phi \, g \, \Psi^{-1}$ is the standard projection, from R^n onto R^{n-1}.

It is shown that π^{-1} takes a full measurable subset of R^{n-1} into a full measurable subset of R^n. For this purpose, let $D \subseteq R^{n-1}$ and $\mu_{n-1}(D) = 0$, where μ_{n-1} stands for Lebesgue measure in R^{n-1}. Also, let $F = \pi^{-1}(D)$, then $F = D \times R$.

If $z \in R^{n-1}$, then $\pi^{-1}(z) = z \times R$ and F can be rewritten as $F = D \times R = D \times [\bigcup_{k=1}^{\infty} (-k, k)] = \bigcup_{k=1}^{\infty} [D \times (-k, k)]$. Then,

$$\mu_n(F) = \mu_n(\bigcup_{k=1}^{\infty} D \times (-k, k)) \leq \sum_{k=1}^{\infty} \mu_n(D \times (-k, k))$$

$$\leq \sum_{k=1}^{\infty} \mu_{n-1}(D) . \mu_1(-k, k) = 0.$$

Thus π^{-1} carries subset of full measure in R^{n-1} into full measurable subsets of R^n.

Fourthly, let $M = \{x \in R^n : \alpha < \|f(x)\| < \beta\}$, and

$$W(\epsilon, \beta) = M \cap g^{-1}(S^{n-1} \backslash B(\epsilon, \beta)) \cap J^{-1}(R_+).$$

It should be shown that $W(\epsilon, \beta)$ is open in R^n and has full measure in $E[\alpha, \beta]$. Note first that, $M \subseteq E[\alpha, \beta]$, also, since every point in $S^{n-1} \backslash B(\epsilon, \beta)$ is regular value of $g|_{E[\epsilon, \beta]}$, then $N = M \cap g^{-1}(S^{n-1} \backslash B(\epsilon, \beta))$ has full measure in $E[\epsilon, \beta]$. In particular, since $\epsilon < \alpha$, then $W(\epsilon, \beta)$ has a full

measure in $E[\alpha, \beta]$. The openness of $W(\epsilon, \beta)$ follows from the fact that every set of the sets involved is open in R^n.

Finally, define $W(\epsilon) = \bigcap_{\beta>\alpha} W(\epsilon, \beta)$,

claim $W(\epsilon)$ is open in R^n and has full measure in $E_+(\alpha)$.

Clearly, $W(\epsilon)$ is open because each $W(\epsilon, \beta)$ is. Note also $[W(\epsilon)]^c = \cap\, W^c(\epsilon, \beta) \subseteq [W(\epsilon, \beta)]^c$, which has measure zero, for each ϵ, α, and β. Hence, the claim.

Let $x_0 \in W(\epsilon)$, then $x_0 \in W(\epsilon, \beta)$ for some β with $0 < \epsilon < \|f(x_0)\| < \beta$. Put $\|f(x_0)\| = s_0$, then by Proposition 2.12 $C(x_0) \cap E(\epsilon) \neq \emptyset$, this implies that there exists $y \in C_+(x_0)$ such that $\|f(y)\| = \epsilon$.

As a consequence of the proof of the theorem and Proposition 2.15, it may be concluded that $C_+(x_0)$ has no ω-limit points in $E[\epsilon, \alpha]$.

The above remark will be used to establish the main convergence theorem. Recall that a *Baire subset* of $X \subseteq R^n$ is the intersection of countably many open dense subsets of X.

Theorem 2.17 (Hirsch and Smale's)

Suppose the hypotheses of Theorem 2.16 hold, then there exists a Baire subset W of full measure in $E_+(\alpha)$ such that if $x_0 \in W$, then $C(x_0) \approx R$. Furthermore, if $\{t_m\}$ is a sequence of real numbers in $[0, \infty)$ with $\lim_{m\to\infty} t_m = \infty$ and $\xi : R \to C(x_0)$ is a diffeomorphism with $\xi(0) = x_0$ and

$\xi[0,\infty) = C_+(x_0)$, then $\lim_{m\to\infty} \xi(t_m) \in E$ for all $x_0 \in W$, and in particular the set $E \neq \emptyset$.

Proof:

Let $W(\epsilon)$ be defined as in Theorem 2.16 and put

$$W = \cap \{W(\tfrac{1}{n}) : 1, 2, 3, \ldots\}.$$

Since $W(\frac{1}{n})$ is open and of full measure in $E_+(\alpha)$; then $W(\frac{1}{n})$ is a dense subset of $E_+(\alpha)$. Therefore, W is a Baire subset and it has a full measure in $E_+(\alpha)$.

Let $x_0 \in W$, $\|f(x_0)\| = s_0$; then by Theorem 2.16 $C(x_0) \approx R$, and for all ϵ such that $0 < \epsilon < s_0$ then, $C_+(x_0) \cap E(\epsilon) \neq \emptyset$. According to the remark following the proof of the preceding theorem, $C_+(x_0)$ has no ω-limit points in $E[\epsilon,s_0]$.

Choose a sequence $\{\epsilon_n\}$ where $\epsilon_n = \frac{1}{n}$. Again, by Theorem 2.16, correspond to each ϵ_n, an $x_n \in C_+(x_0)$ can be chosen, such that $\|f(x_n)\| \leq \frac{1}{n}$. An ω-limit point for $C_+(x_0)$ needs to be obtained out of the sequence $\{x_n\}$.

To this end, claim that $E[0,s_0]$ is compact. To show this, let $A = \{y \in R^n : 0 \leq \|y\| \leq s_0\}$. Since $\|.\|$ is a continuous function, then A is closed set. Also, A is bounded, therefore, A is compact. By the properness of the map f, $f^{-1}(A)$ is compact. Furthermore, since f is continuous, then $B = f(f^{-1}(A))$ is compact. Note that $B \subseteq A$, once more,

the properness of the map f implies that $f^{-1}(B) = E[0,s_0]$ is a compact set.

Now, $\{x_n\}$ is a sequence in the compact set $E[0,s_0]$ which is sequentially compact, that is, $\{x_n\}$ has a convergence subsequence $\{x_m\}$, say.

Let y be the ω-limit point of $C_+(x_0)$ obtained from taking the limit of $\{x_m\}$. Because f is continuous, then $0 = \lim_{m\to\infty} \|f(x_m)\| = \|f(\lim_{m\to\infty} x_m)\| = \|f(y)\|$. Therefore, $f(y) = 0$. Hence, the result.

In both Theorems 2.16 and 2.17 the nonlinear map f is assumed to be proper. As a conclusion to this chapter, equivalent conditions to the properness assumption are stated. To do so, the following definition should be recalled:

Definition 18

Let $f : R^n \to R^n$ be a nonlinear map, then f is said to be *coercive* if $\lim_{\|x\|\to\infty} \|f(x)\| = \infty$. Next, these equivalent conditions are stated.

Theorem 2.19

Let f $R^n \to R^n$ be a continuous map. Then the following are equivelant:

(i) f is proper,

(ii) f is a closed mapping and the solution set $S_p = \{x \in R^n, f(x) = p\}$ is compact for any fixed p,

and

(iii) f is coercive.

Proof:

Only a sketch to the proof of the theorem is given; however, the details can be found in Berger [7].

(i) $\Rightarrow$ (ii): The compactness of S_p follows from the properness of f and {p} being compact. To show f is closed, pick a sequence of points in a closed subset of the domain, say, $\{x_n\} \in K$ with $y_n = f(x_n)$, again by the properness of f and passing to a subsequence, if necessary, it can be shown that the limit of the sequence $\{x_n\}$, say $\bar{x}$, belongs to K, and as a consequence $\{y_n\}$ converges to $f(\bar{x})$.

(ii) $\Rightarrow$ (i): Let C be a compact subset of the range of f, claim that $f^{-1}(C)$ is compact. To this end, pick a collection of closed subsets of the domain that has the finite intersection property and covers $f^{-1}(C)$, then show that the intersection of this collection is not empty.

(ii) $\Rightarrow$ (iii): Suppose f is proper, then the inverse image of a bounded subset of the range is a bounded subset of the domain. But this implies that f is coercive.

(iii) $\Rightarrow$ (ii): if f is coercive and C is a compact subset of the image, then $f^{-1}(C)$ is bounded and so relatively compact in the domain.

CHAPTER III

HOMOTOPY EXISTENCE THEOREMS

Even though Brouwer's and Leray-Schauder's fixed point theorems have been established for many years, proofs for these theorems were nonconstructive in character, in the sense that the techniques used in those proofs did not provide means to calculate such fixed points.

Since the introduction of Scarf's algorithm, many constructive proofs of Brouwer's fixed point theorem under various hypothesis have appeared.

The objectives of this chapter are two fold. First, to give a constructive proof of Brouwer's fixed point theorem following Chow et al. [8]. The term *constructive proof* means that a practical numerical method for locating the fixed point emerges as part and for the purpose of proving its existence. Moreover, using the same technique in proving Brouwer's fixed point theorem, a constructive proof of the Leray-Schauder's theorem is given.

Once more, by using a similar proof method, the second objective of this chapter is reached by giving a constructive proof of an existence theorem of a zero of a map satisfying certain conditions.

3.1 C^2 Maps Fixed Point Theorems

Let F, G : $R^n \to R^n$ nonlinear maps and define the homotopy

$$H : R^n \times I \to R^n \text{ by}$$

$$H(x, t) = tF(x) + (1-t)G(x), \tag{3.1}$$

where H(x,0) = G(x), H(x,1) = F(x).

As pointed out in Chapter I, the map G is usually chosen such that the equation G(x) = 0 has a trivial solution or it can be easily obtained. For certain purposes G will be taken to be either G(x) = x - a or G(x) = F(x) - $F(x_0)$, x, x_0, and a $\in R^n$.

A natural question that arises here is how freely can a be chosen and at the same time guarantee that 0 is a regular value of H. An answer to this question is provided by the Parametric Transversality Theorem 1.18 of Chapter I.

Suppose f is C^2 nonlinear map and f : K $\to$ K, where K is a convex and compact subset of R^n.

Choose a $\in$ int(K) and let the maps G and F in (3.1) be defined by

$$G(x) = x - a, \; F(x) = x - f(x), \tag{3.2}$$

where int(.) stands for the interior of a set.

Define the homotopy H : int(K)$\times$(0,1)$\times$int(K) $\to R^n$, by

$$H(a,t,x) = t\,(x - f(x)) + (1 - t)\,(x - a). \tag{3.3}$$

Finally, define the map $H_a : (0,1)\times int(K) \rightarrow R^n$ by

$$H_a(t,x) = H(a,t,x). \tag{3.4}$$

It was pointed out earlier in Chapter I that finding a fixed point or a zero of a map by means of analytic homotopy essentially reduced to following a solution curve of an IVP. Moreover, the new homotopy approach differs from the Davidenko's approach in one basic thing; that is, the latter uses the variable t of the homotopy map H(t,x) as the independent variable while the new homotopy approach introduces arc length, say s, as an independent variable to the homotopy map H(t(s),x(s)).

Thus, even if the matrix $D_xH_a(t,x)$ becomes singular on the solution curve of the IVP to be defined later, this causes no serious difficulty to the new homotopy approach as it does to the Davidenko's case.

Differentiating the equation $H_a(t(s),x(s)) = 0$ with respect to s, the following IVP is obtained:

$$\begin{aligned} &d/ds\ H_a(t(s),x(s)) = 0 \\ &|dt/ds|^2 + \|dx/ds\|^2 = 1 \\ &\text{with } t(0) = 0,\ x(0) = a \end{aligned} \tag{3.5}$$

From (3.5)

$$[I - t(s)Df(x(s))]\ dx/ds + [a - f(x(s))]\ dt/ds = 0$$

Let $\dot{Y} = (dx/ds, dt/ds)^t$, the above equation can be written in the compact form:

$$DH_a(t,x)\ \dot{Y} = 0$$

where $DH_a(t,x) = (I - tDf(x), a - f(x))$. Thus, solving the IVP in (3.5) is equivalent to finding $\dot{Y}$ and hence Y. But $\dot{Y}$ can be obtained by finding the kernel of the matrix $DH_a(t,x)$.

The existence of the solution curve of the above IVP will now be established by first proving the following important lemma.

Lemma 3.1

Let the maps f, H, H_a be given as in (3.2) - (3.4), and 0 be a regular value of H_a. Then $C(a)$, the component of $H_a^{-1}(0)$ through (0,a), is diffeomorphic to an interval.

Proof:

By the Preimage Theorem 1.11, since 0 is a regular value of H_a, then $C(a)$ is a C^2 one-dimensional submanifold of $H^{-1}(0)$. As a consequence of the Classification Theorem of one-dimensional Manifold 1.16, $C(a)$ is diffeomorphic to a circle or an open interval. It needs to be shown that $C(a)$ is not diffeomorphic to a circle. To this end, consider the map H_a of equation (3.4) to be defined on the larger domain $(-\infty,1)\times int(K)$.

Since $H_a(0,a) = 0$, $D_xH_a(t,x) = t(I-Df(x)) + (1-t)I$, where I is the identity $n\times n$ matrix.

Note $D_xH_a(0,x) = I$, so by the Implicit Function Theorem, in the neighborhood of $(0,a)$. There is an open interval J with $0 \in J$ and a neighborhood W of $(0,a)$ such that for each $t \in J$, there exists a unique C^1 map $g : J \to R^n$ with $(t,g(t)) \in W$ and $H_a(t,g(t)) = 0$, where $g(0) = a$. Thus every solution of $H_a(t,x) = 0$ must be of the form $x = g(t)$, $t \in L = [0,1] \cap J$.

Now, suppose $C(a)$ is diffeomorphic to a circle, and $T : [0,1] \to (0,1)\times int(K)$ be a parametrization of $C(a)$ so that $t = T(s)$ and let $h(s) = g(T(s))$, $s \in [0,1]$.

By assumption $C(a)$ is diffeomorphic to a circle, then

$$(T(0),h(0)) = (T(1),h(1)) = (0,a),$$

$$H_a(T(s),h(s) = 0, \tag{3.6}$$

$$\text{with } |T'(s)|^2 + \|h'(s)\|^2 \neq 0,$$

where "'" stands for d/ds. Also, since 0 is a minimum value of T, then $T'(0) = 0$. Differentiate (3.6) with respect to s one gets

$$\frac{\partial}{\partial t} H_a(T(s),g(s))\ T'(s) + D_xH_a(t(s),h(s))\ h'(s) = 0.$$

At $t = 0$ it is known $T(0) = T'(0) = 0$, $h(0) = a$, $D_xH_a(0,a) = I$ to get $h'(0) = 0$. But this is a contradiction to (3.6). Hence $C(a)$ is diffeomorphic to an open interval.

Note here that the above lemma says that $C(a)$ cannot be diffeomorphic to any of the components Γ_1, Γ_2, and Γ_3 shown in Figure 3, but rather to a component such as Γ.

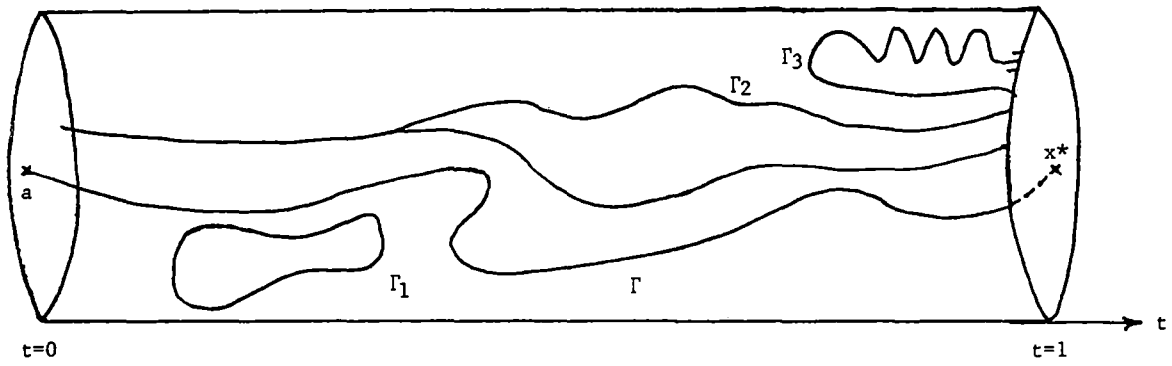

Figure 3. Components of $H_a^{-1}(0)$

Brouwer's fixed point theorem for C^2 maps can now be stated and proved.

Theorem 3.2

Let the maps f, H, H_a be defined as in (3.2) - (3.4); and $C(a)$ be the component of $H_a^{-1}(0)$ through (0,a) in $(0,1)\times$ int(K); $(0,a) \in \bar{C}(a)$.

Then

(i) 0 is a regular value of H,

(ii) for almost every $a \in \text{int}(K)$, in the sense of n-dimensional Lebesgue measure, $C(a)$ is C^2 one-dimensional manifold in $(0,1)\times\text{int}(K)$ joining $(0,a)$ to a fixed point of f (or to a set of fixed points) at $t = 1$.

Proof:

Let $(\hat{a},\hat{t},\hat{x}) \in \text{int}(K)\times(0,1)\times\text{int}(K)$ and $H(\hat{a},\hat{t},\hat{x}) = 0$. Since $D_aH(\hat{a},\hat{t},\hat{x}) = (1-\hat{t})\ (-I) = (\hat{t}-1)\ I$, then for $\hat{t} \neq 1$ $\text{range}(DH(\hat{a},\hat{t},\hat{x}) \supseteq \text{range}(D_aH(\hat{a},\hat{t},\hat{x}) = R^n$. Hence 0 is a regular value of H; this proves (i).

By the Parametric Transversality Theorem 1.18, for almost every $a \in \text{int}(K)$, 0 is a regular value of H_a. Also, by Lemma 3.1 $C(a)$ is a C^2 one-dimensional manifold in $(0,1)\times\text{int}(K)$ and is diffeomorphic to an open interval.

To complete the proof it needs to be shown that $C(a)$ does not have a limit point on the surface of the cylinder $(0,1)\times\partial K$, where ∂K denotes the boundary of K. To show this, let $0 < t < 1$ and suppose (t,x) is a limit point of $C(a)$; thus $H_a(t,x) = 0$; hence, $t(x - f(x)) + (1-t)\ (x - a) = 0$; obtained from this is

$$x = tf(x) + (1 - t)a \qquad 0 < t < 1.$$

By assumption $a \in \text{int}(K)$, $f(x) \in K$, and K is a convex set, then $x \in \text{int}(K)$.

Consequently, $\mathcal{C}(a)$ has no limit point on $(0,1)\times\partial K$. Furthermore, any limit point of $\mathcal{C}(a)$ is in $H_a^{-1}(0)$. Moreover, because $\mathcal{C}(a)$ is diffeomorphic to an open interval, $(0,a)$ is at one end of $\mathcal{C}(a)$; also, by the compactness of $[0,1]\times K$, there is at least one more limit point of $\mathcal{C}(a)$ at $\{1\}\times\text{int}(K)$. If $(1,x_*)$ is one such a limit point, then from (3.3) $f(x_*) = x_*$. Thus, x_* is a fixed point of f.

Corollary 3.3

Suppose the assumptions of the theorem hold. If at every fixed point of the map f the matrix I-Df(x) is nonsingular, then $\mathcal{C}(a)$ has a finite arc length.

Proof:

The proof follows from the fact that $\mathcal{C}(a) \subseteq (0,1)\times\text{int}(K)$ and $[0,1]\times K$ is compact, then $\mathcal{C}(a)$ is bounded and hence has a finite arc length.

The next result gives a constructive proof of a version of Leray-Schauder's fixed point theorem for C^2 maps.

Theorem 3.4

Let U be an open, bounded subset of R^n, and $f : U \to R^n$ is a C^2 map. Suppose there is an $a \in U$ such that $f(x) \neq sx + (1-s)a$, $s > 1$, whenever $x \in \partial U$. Then f has a fixed point in $\bar{U}$.

Proof:

Let the maps H, H_a be defined as in (3.3) and (3.4). Let $C(a)$ be the component of $H^{-1}(0)$ through (0,a) in $(0,1)\times U$, and $(0,a) \in C(a)$. Then by a similar argument to that in the proof of Theorem 3.2, one shows that for almost every $a \in U$, $C(a)$ is a C^2 one-dimensional manifold in $(0,1)\times U$, and $C(a)$ is diffeomorphic to a open interval. One needs only to prove that $C(a)$ can be continued from (0,a) to a fixed point of f.

To do so, it needs to be shown that $C(a)$ has no limit point on $(0,1)\times\partial U$. To this end, let $(t,x) \in (0,1)\times\partial U$ then

$$H_a(t,x) = (1- t)(x - a) + t(x - f(x)) \qquad (3.7)$$

Let $s = 1/t$, then $s \in (1,\infty)$ and (3.7) becomes

$$H_a(s,x) = (1- 1/s)(- a) + 1/s(x - f(x))$$

$$= 1/s\,[sx + (1-s)a - f(x)].$$

By assumption $f(x) \neq sx + (1-s)a$ for $x \in \partial U$, $s > 1$; therefore, $H_a(s,x) \neq 0$. Hence, $C(a)$ has no limit point on $(0,1)\times\partial U$. Because $C(a)$ is diffeomorphic to an open interval, (0,a) at one end of $C(a)$, and since $[0,1]\times U$ is compact, there must exist at least one limit point of $C(a)$ at $\{1\}\times U$ say $(1,x_*)$. Therefore, from (3.7) $f(x_*) = x_*$.

3.2 Existence Theorem of Zeros of Maps

Recall that, if $f : [a,b] \to R$ is a continuous function satisfying $f(a) \leq 0$ and $f(b) \geq 0$, then there exists an $x \in [a,b]$ such that $f(x) = 0$. These conditions can be rewritten in the following form. For $x_0 \in (a,b)$,

$$(x-x_0)f(x) \geq 0.$$

The above fact has been extended to n-dimension, a proof of which may be found in Ortega and Rheinboldt [42]. The objective of this section is to give a constructive proof of the result in its most general setting for C^2 maps (Chow et al. [8]).

Theorem 3.5

Let U be an open, bounded subset of R^n and assume that $f : U \to R^n$ is a C^2 map which satisfies

$$(x-a)^t f(x) \geq 0 \quad \text{for some } a \in U \text{ and all } x \in \partial U. \tag{3.8}$$

Then there exists an $x_* \in \bar{U}$ such that $f(x_*) = 0$.

Proof:

Define a homotopy $H : U \times (0,1) \times U \to R^n$ by

$$H(a,t,x) = (1-t)(x - a) + tf(x).$$

Let the map $H_a : (0,1) \times U \to R^n$ be defined by

$$H_a(t,x) = H(a,t,x).$$

By applying the same argument that was used to prove Theorem 3.2 , it can be shown that for almost every $a \in U$, $\mathcal{C}(a)$, the component of $H_a^{-1}(0)$ through $(0,a)$, is a C^2 one-dimensional manifold in $(0,1)\times U$ diffeomorphic to an open interval. If it can be shown that $\mathcal{C}(a)$ has no limit point on the cylinder $(0,1)\times\partial U$, the proof will be completed. Because $\mathcal{C}(a)$ starts at one end at $(0,a)$ and ends at $(1,x_*)$, a limit point of $\mathcal{C}(a)$ at $\{1\}\times U$. Thus, $f(x_*) = 0$.

To show $\mathcal{C}(a)$ has no limit point on $(0,1)\times\partial U$, suppose there is $t \in (0,1)$ and $x \in \partial U$ such that $H_a(t,x) = 0$; that is

$$(1-t)\ (x-a) + tf(x) = 0. \tag{3.9}$$

The following is obtained by taking the dot product of (3.9) with $(x-a)^t$

$$(1-t)\ (x-a)^t(x-a) + t(x-a)^t f(x) = 0.$$

From (3.8) $(x-a)^t(x-a) + t(x-a)^t f(x) = 0$. $(x-a)^t\ (x-a) \leq 0$ must be obtained. But this is a contradiction. Hence, $\mathcal{C}(a)$ has no limit point on $(0,1)\times\partial U$.

Finally, the following corollary, which was given without proof by Allgower [4], is established.

Corollary 3.6

Let f, U as in the theorem. Suppose $a \in U$ and if for every $x \in \partial U$ there is a nonzero vector $v_x \in R^n$ which satisfies:

$$v_x^t f(x) > 0 \text{ and } v_x^t (x-a) > 0, \tag{3.10}$$

then there exists an $x_* \in U$ such that $f(x_*) = 0$.

Proof:

The proof is the same as in the proof of the theorem except in proving that $\mathcal{C}(a)$ has no limit point on the cylinder $(0,1)\times\partial U$. But this follows from noting that for $t \in (0,1)$, $x \in \partial U$ and using (3.10) the following is obtained

$$v_x^t H_a(t,x) = (1-t)\, v_x^t (x-a) + v_x^t f(x) > 0.$$

Hence, $\mathcal{C}(a)$ has no limit point on $(0,1)\times\partial U$. Therefore, the result.

CHAPTER IV

THE RELATION BETWEEN GLOBAL NEWTON AND GLOBAL HOMOTOPY METHODS

Since the introduction of the *global Newton* method by Smale [49] in 1976, several extensions of Smale's results have been published. In 1979, Keller [34] used the so-called *global homotopy* to extend Smale's results. Also, Garcia and Gould in [18], and Gould and Schmidt in [22] obtained similar extensions.

The aims of this chapter are, first, in 4.1, on the one hand, to give a detailed proof of Smale's theorems, and on the other hand, to extend these theorems so that they can be applied to a wider class of maps.

Secondly, in 4.2, an extension of Smale's results due to Keller is given. The advantage of the global homotopy method is that one can find several zeros of a map using a single solution curve of an IVP.

Thirdly, in 4.3, the relation between the global Newton and the global homotopy methods is studied.

4.1 Global Newton Method

Let $\Omega \subseteq R^n$ be a compact domain with a smooth boundary $\partial\Omega$, that is, a C^1 submanifold of R^n of dimension n-1.

Let $f : \Omega \to R^n$ be a C^2 nonlinear map. Associate with f, just as in Chapter II, a map $g : \Omega \backslash E \to S^{n-1}$ which is defined by

$$g(x) = \frac{f(x)}{\|f(x)\|}.$$

where $E = f^{-1}(0)$.

Recall from Chapter II that the unit vector field $\phi(x)$ satisfies the following differential equation:

$$Df(x)\phi(x) = \lambda(x)f(x), \tag{4.1}$$

where $\lambda(x) = \dfrac{\overline{+}\, J\ (x)}{\|adj(Df(x))f(x)\|}$.

Smale in [49] refers to (4.1) as the "Global Newton Equation". The name seems to be originated from the fact that if one uses Euler's method to approximate equation (4.1) with step size h, assuming that Df(x) is nonsingular, one gets the different equation

$$\xi_{n+1} = \xi_n - h\ \lambda(\xi_n)[Df(\xi_n]^{-1}f(\xi_n). \tag{4.2}$$

Of course, equation (4.2) resembles the well known local Newton method; in fact, if h is chosen to be $1/\lambda$, then (4.2) reduced to Newton method.

To ensure the existence of zeros of the system

$$f(x) = 0\ , \tag{4.3}$$

Smale in [49] formulated the following boundary conditions:

(a) $Df(x)$ is nonsingular for all $x \in \partial\Omega$,

(b) there is a sign choice for λ, as defined by (4.1), so that $\phi(x)$ *points into* Ω for all $\partial \in \Omega$.

The term points into Ω should be understood in the following sense:

Definition 4.1

Let $N(x)$ be a unit normal vector at $x \in \partial\Omega$, then $N(x)$ is said to be inward pointing if there exists an $\epsilon > 0$ such that for all $t \in (o, \epsilon)$, $x+tN(x) \in \Omega$.

Definition 4.2

Let $x \in \partial\Omega$, $\phi(x)$ is said to point into Ω if $\phi(x) . N(X) > 0$.

The main result of this section may now be stated.

Theorem 4.3 (Smale's)

Let Ω be a compact domain with a smooth boundary $\partial\Omega$ in R^n and $f : \Omega \to R^n$ be a C^2 map satisfying the boundary conditions (a) and (b). Then (4.1) has a unique C^1 solution $\xi : [t_0, t_1) \to \Omega$ starting at x_0, that means, $\xi(t_0) = x_0$, with the properties $\|d\xi/dt\| = 1$, the interval $[t_0, t_1)$ is maximal, and $t_1 \leq \infty$. Furthermore, $\lim_{t \to t_1} \xi(t) = \bar{y}$, an ω-limit point of $\xi(t)$.

Proof:

Let $x_0 \in \partial\Omega$, and $y_0 = g(x_0)$. By boundary condition (a) and Theorem 2.5 of Chapter II, y_0 is a regular value of g. Therefore, by the Preimage Theorem 1.11 $g^{-1}(y_0)$ is a one-dimensional submanifold in Ω/E.

Let $C(x_0)$ be the component of $g^{-1}(y_0)$ starting at x_0. By the Classification Theorem of One-Dimensional Manifold 1.16 $C(x_0)$ is diffeomorphic to a circle or an interval.

Claim $C(x_0)$ is not diffeomorphic to a circle. Suppose it is, then $C(x_0)$ would be a loop in Ω/E, and hence it would meet $\partial\Omega$ once more at x_0, where it started, but this says that $\phi(x)$ would be tangent to $\partial\Omega$ at x_0 a contradiction to boundary condition (b). Hence, $C(x_0)$ is not diffeomorphic to a circle.

Thus, the only other choice for $C(x_0)$ is to be diffeomorphic to an interval (open, half-closed or closed).

The first choice cannot happen, because $C(x_0)$ has a boundary point, namely, $x_0 \in \partial\Omega$. Also, claim the third choice cannot be true either. Without loss of generality, suppose on the contrary $C(x_0)$ is diffeomorphic to the closed interval $[t_0, t_1]$. Since $C(x_0)$ is the solution of an IVP and Ω is compact set, then by Theorem 1.20 (the Maximal Interval Theorem) $C(x_0)$ must "leave" Ω. Thus, $C(x_0)$ must have another boundary point, say, x_2 such that $\xi(t_2) = x_2 \in \partial\Omega$, $t_2 < t_1$. Hence, at $t = t_2$, $\phi(x_2)$ must point out of Ω. But, this contradicts boundary condition

(b). Therefore, $C(x_0)$ is not diffeomorphic to a closed interval. Consequently, $C(x_0)$ is diffeomorphic to a half-closed interval; thus, there exists a diffeomorphism ξ : $[t_0, t_1) \to C(x_0)$. In fact, ξ is a parametrization of $C(x_0)$ by arc length. This follows from noting that $d\xi/dt$ is tangent to $C(x_0)$ at $\xi(t_0)$; also, by Theorem 2.8 of Chapter II the tangent to $C(x_0)$ is the unit vector $\phi(x)$ which spans the kernel of $Dg(x)$. Thus,

$$\frac{d\xi}{dt} = \phi(\xi(t)), \ \xi(t_0) = x_0$$

As a consequence of Theorem 1.19 (the Existence and Uniqueness Theorem of an IVP) ξ is a unique C^1 solution of the "Global Newton Equation."

Without loss of generality, one may assume that $[0,+\infty) \approx C(x_0)$, $\xi(0) = x_0$.

To complete the proof it needs to be shown that $\lim_{t\to\infty} \xi(t) = y$ is an ω-limit point of $C(x_0)$.

Since Ω is compact and $C(x_0) \subseteq \Omega$, then $C(x_0)$ must have a ω-limit point $y \in \Omega$, say. Let $\{t_n\}$ be a sequence of real numbers such that $\lim_{n\to\infty} t_n = \infty$ and $\xi(t_n) = x_n \in C(x_0)$, then by the sequential compactness of Ω there exists a subsequence, say, $\{x_m\}$ such that $\lim_{m\to\infty} x_m = y$.

By a variant of Lemma 2.15 of Chapter II, y is either a critical point of g or it is a zero of f.

Next, the following important hypothesis is introduced:

Genericity Hypothesis (G.H.):

Suppose f is defined as before. If $x \in E$, then $Df(x)$ is nonsingular.

As a consequence of the G.H. the preceding theorem becomes:

Theorem 4.4

If $f : \Omega \to R^n$ is a C^r map, satisfying the boundary conditions (a) and (b) and the G.H.; then $\lim_{t \to t_1} \xi(t) = x_*$ with $f(x_*) = 0$; that is, the solution curve $\xi(t)$ converges to a single zero of f.

Proof:

The proof is the same as in the previous theorem except for showing the solution $\xi(t)$ converges to a single zero of f.

It needs to be shown that the set E is finite. To this end, since f satisfies the G.H., then for each $x \in E$, one can find a small open ball B_x around x so that if $y \in E$, $y \neq x$, then $y \notin B_x$. But E is closed and $E \subseteq \Omega$, which is compact, then there are finite number of these balls covering E and as a consequence of this finitely many of these balls cover E, hence E is finite. By Theorem 4.3 the solution curve $\xi(t)$ of the IVP given by (4.1) converge to E, but the zeros of f are isolated. Thus, $\xi(t)$ converge to a single zero f.

In Smale's existence theorems the first boundary condition; that is Df(x), is nonsingular for all $x \in \partial\Omega$, seems too strong as the following example shows:

Example:

Let $f : R^2 \to R^2$ defined by

$$f(x, y) = \begin{bmatrix} x^2 + y^2 - x \\ x^2 - y^2 - y \end{bmatrix}$$

$$Df(x, y) = \begin{bmatrix} 2x-1 & 2y \\ 2x & -2y-1 \end{bmatrix}$$

Note that $\det(Df(x)) = -(2x-1)(2y+1) - 4xy$. The $\det(Df(x)) = 0 \Longleftrightarrow y = \frac{2x - 1}{2 - 8x}$.

Now, let Ω be a ball with radius greater than one and center at (1/4, -1/4), say. Then Df(x, y) have four singularity points on $\partial\Omega$ as can easily be seen from Figure 4.

Therefore, Smale's Theorems do not hold in this particular example. As a consequence of this, one should pose the following question: Is it possible to weaken Smale's boundary conditions without changing the conclusions of the theorems for this section? The answer to this question is affirmative; in fact, Smale mentioned the possibility of relaxing this boundary conditions, but he did not give a clear formulation.

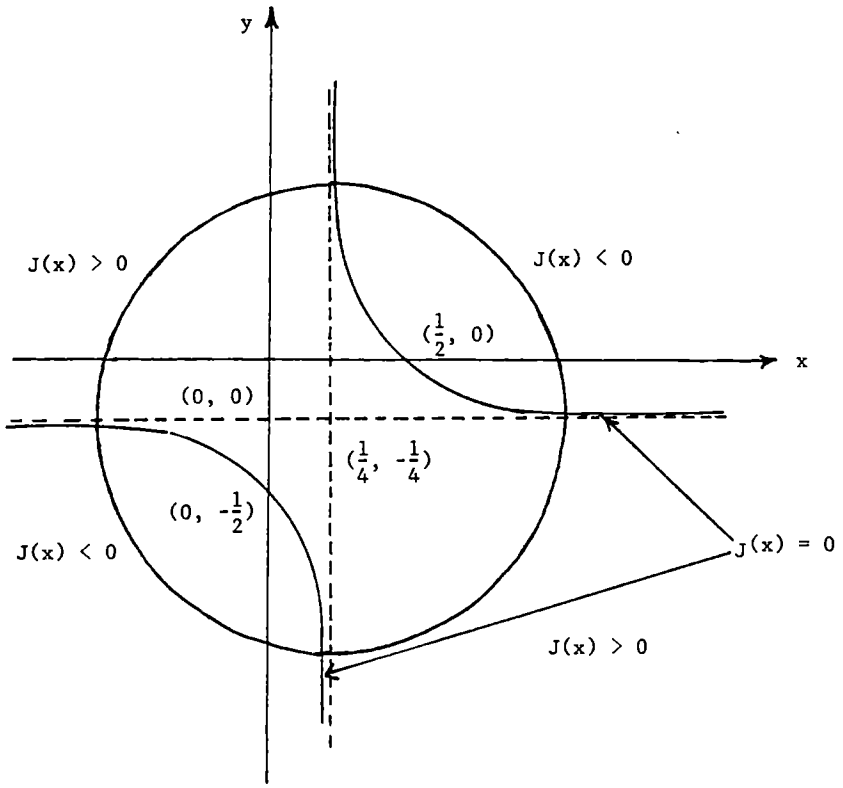

Figure 4. A Region Ω Where $J(x) = 0$ on $\partial\Omega$

Now, Smale's boundary conditions (a) may be replaced by the following:

(aa) for all $x \in \partial\Omega$, $g(x)$ is a regular value of g and the set $C = \{x \in \partial\Omega : J(x) = 0\}$ has measure zero in $\partial\Omega$.

Note that condition (aa) implies Smale's boundary condition (a). By Theorem 2.5 of Chapter II if x is a regular point of g, then

(i) $Df(x)$ is nonsingular for all $x \in \partial\Omega$ (Smale's),

or

(ii) $\text{rank}(Df(x)) = n-1$, and $\text{range}(Df(x)) \cap L = \{0\}$.

where $L = \{\alpha.y \in R^n : y = f(x),\ x \in \Omega,\ \alpha > 0\}$.

The whole point in Smale's first boundary condition is to guarantee the starting point at $\partial\Omega$ is a regular point for the map g.

Now, an extension to Smale's results may be stated as follows:

Theorem 4.5

Let $f : \Omega \to R^n$ satisfies the boundary conditions (aa) and (b); then the conclusions of both Theorems 4.3 and 4.4 hold.

Proof:

The proof of the theorem is exactly the same as in Theorems 4.3 and 4.4.

4.2 Global Homotopy Method

Let $\Omega \subseteq R^n$ be a compact domain with smooth boundary $\partial\Omega$, $f : \Omega \to R^n$ be a C^2 map. For a fixed $x_0 \in \partial\Omega$ define the Newton homotopy $H : \Omega \times R \to R^n$ by

$$H(u, \theta) = f(u) - \theta\, f(u_0). \tag{4.6}$$

For the time being it may be assumed that u and θ are functions of another variable, say, s. Differentiating the identity $H(u(s), \theta(s)) = 0$ with respect to s

$$Df(u)\ du/ds - d\theta/ds\ f(u_0) = 0. \tag{4.7}$$

On the one hand by (4.6), (4.7) becomes

$$Df(u)\ du/ds = \frac{d\theta/ds}{\theta}\ f(u). \tag{4.8}$$

On the other hand (4.7) can be rewritten in the form

$$[Df(u), - f(u_0)] \begin{bmatrix} \frac{du}{ds} \\ \\ \frac{d\theta}{ds} \end{bmatrix} = 0.$$

Hence, $(du/ds, d\theta/ds)^t$ is in the kernel of $DH(u, \theta) = (Df(u), - f(u_0))$. Therefore, by normalizing the above vector gives

$$\|du/ds\|^2 + |d\theta/ds|^2 = 1. \tag{4.9}$$

The identity in (4.9) makes s an arc length parameter.

Let the *ith* component of du/ds and $DH(u, \theta)$ be denoted by $\dot{u}_i$ and $H_i(u)$, respectively, and let $\dot{u}^i$, $H^i(u)$ denote the remaining components of du/ds and $DH(u, \theta)$.

To establish the main result of this section, the following two lemmas, whose proofs are due to Garcia and Gould [17], need to be proven.

Lemma 4.6

Let 0 be a regular value of the homotopy map $H : R^{n+1} \to R^n$ defined as in (4.6) and let $C(v)$ be the component of $H^{-1}(0)$ through v and ξ is parametrization of $C(v)$ such that $H(v(s)) = 0$, where $v(s) = (u(s), \theta(s)) = \xi(s)$. Then

$$\dot{v}_i = 0 \iff \det(H^i(v)) = 0.$$

Proof:

Differentiate $H(v(t)) = 0$ with respect to s to get

$$DH(v)\ dv/ds = 0$$

Since 0 is a regular value of H, that is, rank(DH(u)) = n, then a $1 \uparrow n+1$ vector $e_j = (0,\ldots,0,1,0,\ldots,0)$ can be chosen so that the $n+1 \uparrow n+1$ matrix defined by

$$A = \begin{bmatrix} DH(v) \\ e_j \end{bmatrix}$$

is nonsingular. Then

$$A\ dv/ds = \begin{bmatrix} 0 \\ \dot{v}_j \end{bmatrix}$$

By Cramer's rule for i = 1, 2, 3, ..., n+1

$$\dot{v}_i = \frac{(-1)^{n+1+i}\ \dot{v}_j\ \det(H^i)}{(-1)^{n+1+j}\ \det(H^j)} = \frac{(-1)^{i-j}\ \dot{v}_j\ \det(H^i)}{\det(H^j)}.$$

Since dv/ds is a tangent vector to $C(v)$ at v, then $dv/dt \neq 0$. Thus, there exists some j such that $\dot{v}_j \neq 0$. Therefore,

$$\dot{v}_i = 0 \Leftrightarrow \det(H^i) = 0.$$

Lemma 4.7

Suppose the hypotheses of the previous lemma hold, then $\operatorname{sgn}(\dot{v}_i(s)) = \operatorname{sgn}(\det(H^i(v(s))$ for all s

or

$$\operatorname{sgn}(\dot{v}_i(s)) = -\operatorname{sgn}(\det(H^i(v(s))) \text{ for all } s$$

Where $\operatorname{sgn}(0) \equiv 0$.

Proof:

$$\text{Let } A(s) = \begin{bmatrix} H^i(v(s)) & H_i(v(s)) \\ [\dot{v}^i(s)]^t & \dot{v}_i(s) \end{bmatrix}$$

$$B(s) = \begin{bmatrix} H^i(v(s)) & \dot{v}^i(s) \\ 0 & \dot{v}_i(s) \end{bmatrix}$$

Since $DH(v)\, dv/ds = 0$, then $\dot{v}(s)$ is orthogonal to $DH(v)$ and consequently, $\operatorname{rank}(A(s)) = n+1$ for all s. Therefore, $\det(A(s)) \neq 0$. Thus, $\det(A(s)) > 0$ or $\det(A(s)) < 0$. But,

$$AB = \begin{bmatrix} H^iH^i & 0 \\ [\dot{v}^i]^t H^i & \dot{v}^t\dot{v} \end{bmatrix}$$

Hence, $\det(AB) = \dot{v}^t\dot{v}\,[\det(H^i)]^2$. By the previous lemma since $\dot{v}_i \neq 0$; then $\det(H^i) \neq 0$. Also, since $\det(AB) = \det A \det B > 0$, then $\det(A)$ and $\det(B)$ have the same sign for

all s. But, because $\det B = \dot{v}^i \det(H^i)$, then $\dot{v}_i \det(H^i) > 0$ or $\dot{v}_i \det(H^i) < 0$.

Let $v = (u_1, u_2, \ldots, u_a, \theta)$, and define H by $H(v) = f(u) - \theta f(u_0)$ where $f : R^n \to R^n$, then the conclusion of the above lemma takes the special form.

Corollary 4.8

Let f, H be defined as above and satisfy the hypotheses of the lemma, then

$\operatorname{sgn}(\dot{\theta}) = \operatorname{sgn}(\det Df(u))$ for all s, or

$\operatorname{sgn}(\dot{\theta}) = -\operatorname{sgn}(\det Df(u))$ for all s.

Proof: Follows immediately from the lemma.

Next, the statement and proof of Keller's theorem is given.

Theorem 4.9 (Keller's)

Let Ω be a compact domain in R^n and $f : \Omega \to R^n$ be a C^2 nonlinear map. Define the homotopy map H as in (4.6). Also, Suppose the map f satisfies Smale's boundary conditions (a) and (b). Then for any $u_0 \in \partial\Omega$ for which 0 is a regular value of H, there is a C^1 solution $(u(s), \theta(s))$ of (4.7) and (4.9) over the interval $[0, S_F]$ starting at

$$(u(0), \theta(0)) = (u_0, 1), \tag{4.10}$$

and terminating at $(u(S_F), \theta(S_F))$ where:

$$u(S_F) \in \partial\Omega, \ |\theta(S_F)| < L \text{ and} \tag{4.11}$$

$$L \equiv \underset{x\in\Omega}{\text{Max}} \|f(x)\| / \underset{y\in\partial\Omega}{\text{Min}} \|f(y)\|.$$

Furthermore, for an odd number of points $S_\nu \in (0, S_F)$

$$\theta(s_\nu) = 0, \text{ and } f(u(S_\nu)) = 0. \tag{4.12}$$

Proof:

Consider the cylinder $K = \Omega \times [-L, L]$, where L is given by (4.11). Fix $u_0 \in \partial\Omega$ and claim $H(u, \theta) \neq 0$ on the bases of the cylinder K; that is, where $\theta = \pm L$, $x \in \Omega$. This follows from noting that $L >> 1$. On the surface of the cylinder K there exists at least one zero of H, namely $(u_0, 1)$ (Figure 5).

Since 0 is a regular value of H, by the Preimage Theorem 1.11 $H^{-1}(0)$ is a C^2 one-dimensional manifold in $\Omega \times R$. Let $\mathcal{C}(v_0)$ be the component of $H^{-1}(0)$ that contains $v_0 = (u_0, 1)$.

By the Classification Theorem of One-Dimensional Manifold 1.16 $\mathcal{C}(v_0)$ cannot be diffeomorphic to a circle because this would contradict Smale's boundary condition (b). Also, since v_0 is a boundary point of the indicated component; then $\mathcal{C}(v_0)$ is not diffeomorphic to an open interval. Thus, two choices are left to be checked.

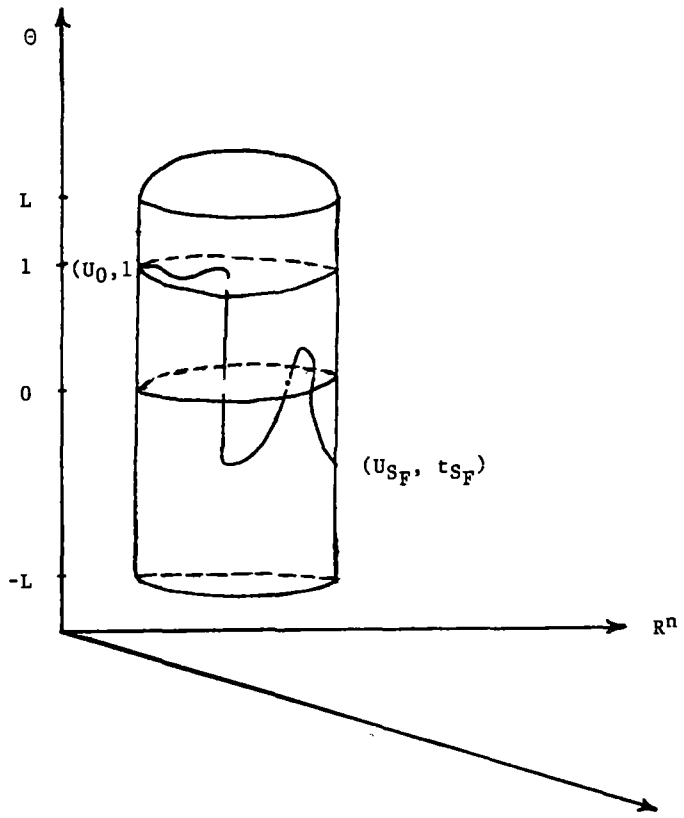

Figure 5. The Cylinder $K = \Omega \times [-L,L]$

The first choice for $C(v_0)$ is to be diffeomorphic to a half-closed interval, but this cannot happen because if it does, then $C(v_0)$ would terminate at an interior point of the cylinder K. But then since $C(v_0)$ consists of regular points, by the Implicit Function Theorem it could be continued beyond the indicated interior point of K.

The second choice, $C(v_0)$ is to be diffeomorphic to a closed interval. It may be assumed that this closed interval is $[0,S_F]$. Hence, there exists a diffeomorphism ξ : $[0,S_F] \rightarrow C(v_0)$ so that $\frac{d\xi}{ds} = \left[\frac{du}{ds}, \frac{d\theta}{ds}\right]$ is a tangent vector to $C(v_0)$ at v_0 with $\xi(0) = (u(0), \theta(0) = v_0$ and $\xi(S_F) = (u(S_F), \theta(S_F)) = (u_F, \theta_F) \in \partial\Omega$.

Without loss of generality, it may be assumed that at $(u_0,1)$, the vector du/ds has the Newton direction, that is, du/ds points into Ω, so that by equation (4.8) $\frac{\dot{\theta}}{\theta} < 0$, but $\theta(0)=1$ hence $\dot{\theta}(0) < 0$. By Corollary 4.8 $\dot{\theta}(s) < 0$ for all $s \in (0,s_F)$, in particular, $\dot{\theta}(S_F) < 0$. Because the solution $C(v_0)$ leaves the cylinder K; then $d\xi/ds$ cannot point into K. This says that du/ds is the negative Newton direction.

Consequently, $\frac{\dot{\theta}(S_F)}{\theta(S_F)} > 0$, thus, $\theta(S_F) < 0$. Therefore, it has been shown that $\theta(0) = 1 > 0$, $\theta(s_F) < 0$, then by the Intermediate Value Theorem there exists at least one $s_\nu \in (0, S_F)$ such that $\theta(s_\nu) = 0$, that is $\theta(s)$ has an odd number of zeros. But, then from (4.6) we get $H(u(s_\nu)) = f(u(s_\nu)) - \theta(s_\nu)\ f(u_0) = 0$. Hence, $f(u(s_\nu)) = 0$.

For the sake of completeness of the discussion at hand, it should be noted that the hypothesis of Keller's Theorem assumes that for any $x_0 \in \partial\Omega$, 0 is a regular value of H. This assumption holds for a large class of maps. In fact, Percell in [44] showed that for almost any starting point $x \in \partial\Omega$, 0 is a regular value of H. To be more precise, Percell's result is stated next.

Theorem 4.10 (Percell's)

Let M be a C^2 n-dimensional manifold with boundary and let $V \subseteq M$ be a C^2 (n-1)-dimensional submanifold without boundary (that is, $V = \partial M$). Let $f : M \to R^n$ be a C^2 map such that the following conditions do hold:

(i) $\operatorname{rank}(Df(x)|_V) = n-1$ for all $v \in V$,

(ii) $f(v)\ (Df(x)|_V)(T_vV) \subseteq R^n$ for all $v \in V$,

(iii) $\operatorname{rank}(Df(x)) \geq n-1$ whenever $f(x) = 0$, and

(iv) $f(x) = 0$ for at most countably many $x \in M$.

For $v \in V$, define $H_v : M \times R \to R^n$ by

$$H_v(x, \theta) = f(x) - \theta f(v).$$

Then $0 \in R^n$ is a regular value of H_v for almost all $v \in V$.

Proof: See Percell [44].

4.3 The Relation Between the Solution Curves of the Global Newton and Global Homotopy Methods

To facilitate the comparison between the solution curves of both the global Newton and global homotopy methods, let their solution curves be denoted by $\gamma(t)$, $\Gamma(s)$, respectively. Let $x = \xi(t)$, $(u,\theta) = \eta(s)$ be their parametrization.

Claim $\gamma(t)$ is a particular instance of $\Gamma(s)$. In fact, by a change of variable and projecting $\Gamma(s)$ onto R^n it is

shown $x(t) = u(s)$. Thus, starting at the boundary point $x_0 = u_0$, both $x(t)$, $u(s)$ define the same curve in R^n leading to the first zero of the map f (Figure 6).

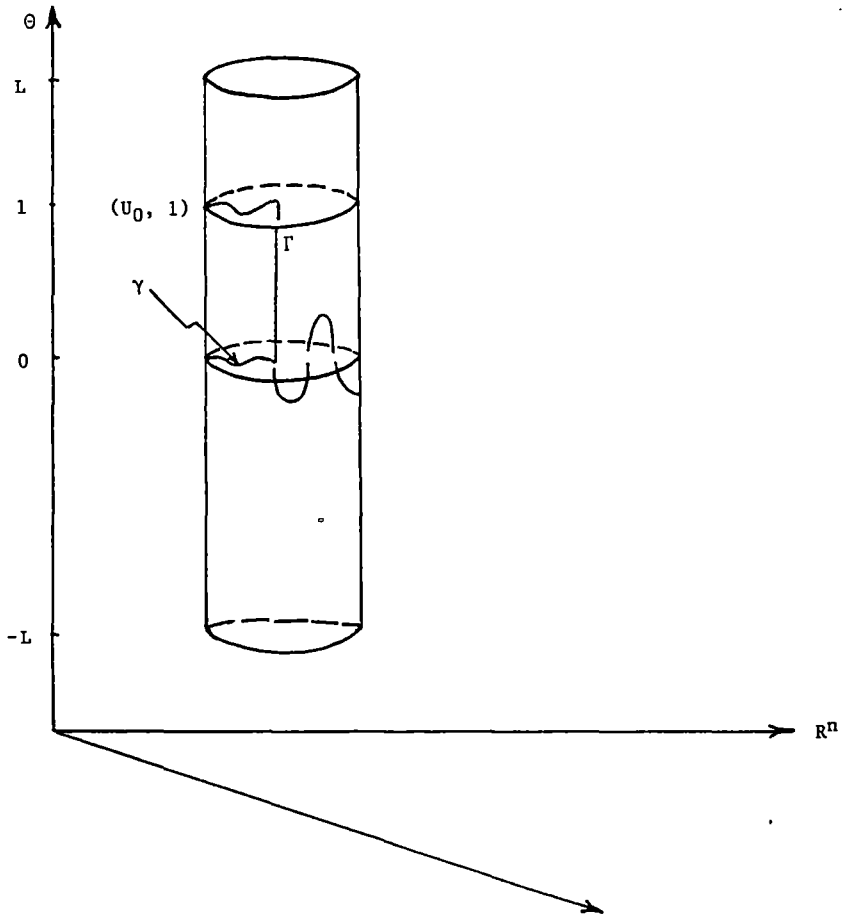

Figure 6. The Solution Curves γ and Γ

To prove the claim, recall that the associate map g is defined by

$$g(x) = \frac{f(x)}{\|f(x)\|}. \tag{4.13}$$

Let $x_0 \in \partial\Omega$ be a regular point of g, and let $\alpha(t)$ the solution curve of the IVP:

$$\frac{d\xi}{dt} = \phi(x),\ x(t) = \xi(t) \text{ and } \xi(0) = x_0 = u_0. \tag{4.14}$$

It was also proved in 4.1 that

$$Df(x)\frac{dx}{dt} = \lambda(x)f(x). \tag{4.15}$$

Where $\lambda(x) = \dfrac{\mp J(x)}{\|adj(Df(x)f(x)\|}$.

Since $g(x(t)) = g(x_0) = g(u_0)$. Then from (4.14) we get

$$f(x(t)) = \|f(x(t))\| \frac{f(u_0)}{\|f(u0)\|}.$$

hence, (4.15) becomes

$$Df(x(t))\frac{dx}{dt} = \lambda(x(t))\ \|f(x(t))\| \frac{f(u_0)}{\|f(u_0)\|}. \tag{4.16}$$

Now, by making the change of variable s = s(t) such that s satisfies

$$\frac{d\theta}{dt} = \frac{d\theta}{ds}\frac{ds}{dt} = \frac{\lambda(x(t))\ \|f(x(t))\|}{\|f(u_0)\|},\ s(0) = 0.$$

It needs to be proven that s is monotone, and hence one-to-one. But this follows from the definition of λ and Corollary (4.8) that both λ and $\frac{d\theta}{ds}$ vanish at the same t, namely when det(Df(x)) = 0, and change sign together. Then (4.16) becomes:

$$Df(x(t))\frac{dx}{dt} = f(u_0)\frac{d\theta}{ds}\frac{ds}{dt}$$

$$= f(u_0)\frac{d\theta}{dt}$$

From (4.7)

$$Df(x(t))\frac{dx}{dt} = Df(u(s))\frac{du}{dt}. \qquad (4.17)$$

This implies that for $t \in [1, t_1]$, $x(t) = u(s(t))$, where $x(t_1)$ is the first zero of f, which was the goal of this section.

As mentioned earlier, the advantage of the global homotopy method is in its ability of finding several zeros of the map f by following a single solution curve. In Figure 7, it is shown a possible solution curve, $C(s)$, of the global homotopy method, where the part of this curve from $(x_0, 1)$ to the first zero of the map f is essentially Smale's path.

By Corollary 4.8 it was shown that det(Df(x)) = 0 if $\dot{\theta} = 0$. The graph also shows $\dot{\theta} = 0$ at $x = x_1, x_2, x_4$, and x_6.

Interestingly, even if Df(x) becomes singular along the solution curve of the IVP (4.15), the method still works.

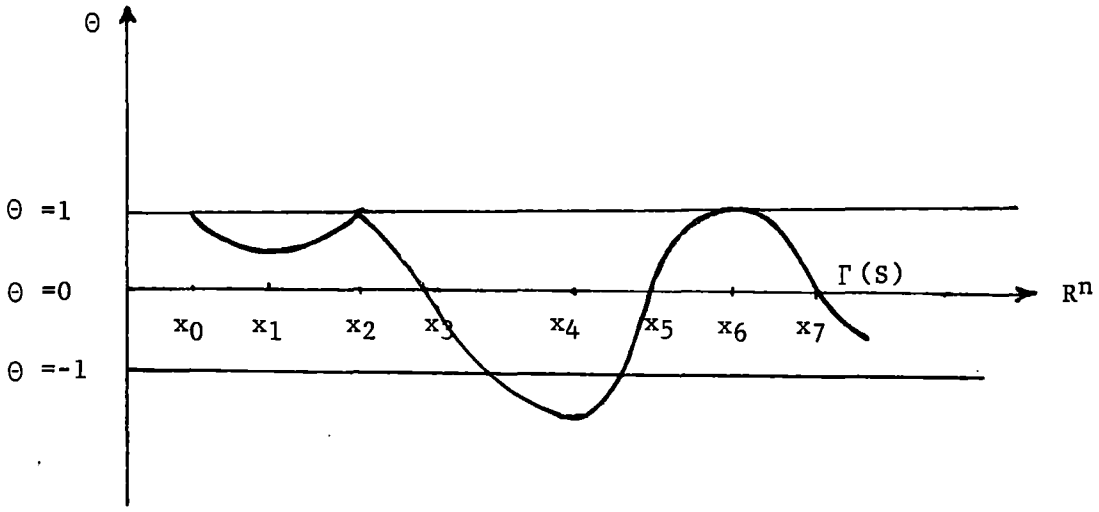

Figure 7. A Solution Curve $\Gamma(s)$ Passing Through Several Zeros of H

CHAPTER V

ALGORITHMS AND COMPUTATIONS

The objectives of this chapter are to describe typical algorithms based on both the continuous Newton method and homotopy methods. In 5.1 a description of three algorithms due to Hirsch and Smale [29] is given. Also, using the alternative definition of Hirsch and Smale's unit vector field, a new algorithm is described. In 5.2 typical homotopy algorithms are reported. To this end, two algorithms are described. The first is due to Watson [50], and the second is due to Li and Yorke [38]. According to Theorems 3.2 and 3.5 of Chapter III, the former finds fixed points of a C^2 map and the latter may be used to find zeros of certain C^2 maps. In 5.3 computational experience about some of these algorithms is reported.

5.1 Algorithms Based on the Continuous Newton Method

All algorithms of this section are based on the continuous Newton method and the theory developed in Chapters II and IV. To begin with, let $f : R^n \to R^n$ be a nonlinear map satisfying certain conditions to be specified shortly. The

basic idea behind all these algorithms is to follow the solution curve, $C(x_0)$, of the IVP

$$\frac{d\xi}{dt} = \phi(\xi(t)) \quad , \quad \xi(0) = x_0, \tag{5.1}$$

where the unit vector field $\phi(x)$, $x = \xi(t)$ satisfies the equation

$$Df(x)\phi(x) = \lambda(x)f(x). \tag{5.2}$$

By following the solution curve, $C(x_0)$, it is meant that a numerical approximation to the solution curve is obtained so that eventually one reaches a zero of the map f.

To describe Hirsch and Smale's algorithms the following definitions and notations are introduced. Let the map f be of class C^r, $r \geq 2$. Suppose a point $x \in R^n$ at which $J(x) \neq 0$. A *Newton vector*, $N(x)$, is defined by

$$N(x) = - \operatorname{sgn}(J(x))[Df(x)]^{-1}f(x).$$

Thus, $N(x)$ is just a scalar multiple of the unit vector $\phi(x)$ defined in Chapter II.

For $\rho > 0$, the *Newton transformation* of length ρ is the C^{r-1} map $T_\rho : \operatorname{Reg}(f) \rightarrow R^n$ defined by

$$T_\rho(x) = x + tN(x), \; t > 0, \; \|tN(x)\| = \rho.$$

A *Newton step of length* ρ from x is defined to be $T_\rho(x)$. Finally, by γ successive Newton steps it is meant to be the

sequence $T_\rho(x)$, $T_\rho^2(x)$, ..., T_ρ^γ if all these are defined.

Now, Hirsch and Smale's first algorithm may be described.

Algorithm A (Hirsch and Smale's)

This algorithm uses Euler's method to integrate the IVP in (5.1). The integration process goes as follows: the algorithm starts at a point x_0 where $J(x_0) > 0$, with step length 1. For $i = 0, 1, 2, \ldots$, the algorithm takes a Newton step and tests the norm condition $\|f(x_i)\| < \epsilon$ for some $\epsilon > 0$. If the norm condition does not hold and the allowable number of steps is reached, that is, 4^k Newton steps for each "cycle" of integration, $k = 0, 1, 2, \ldots$; or the determinant $J(x_i) = 0$, then the integration process is restarted at x_0. Note here that the efficiency of the algorithm is bound to be low.

In each restart of the integration process the step size is cut into half of what it was in the previous cycle. Furthermore, the number of Newton steps increased to four times the number of steps of the preceding cycle, that is, the integration process extends over an interval of length twice that of the preceding cycle.

One should note here that in each cycle of integration the step size is fixed.

The algorithm may be summarized as follows:

1. Start: Choose a set of starting points $\{y_{l,0}\}_{l=0}$, where $J(y_{l,0}) > 0$ and a tolerance $\epsilon > 0$. Set $\rho = 1$, $k = 1$, $i = 0$, $l = 0$.
2. Set $x_0 = y_{l,0}$.
3. If $J(x_i) = 0$ go to (7).
4. Take a Newton step of length 2^{-l} and set $x_{i+1} = T_\rho(x_i)$.
5. If $\|f(x_{i+1})\| < e$ stop.
6. If $i < k-1$, set $i = i+1$ and go to (3).
7. Set $\rho = \frac{1}{2}\rho$. $k = 4k$, $i = 0$, $l = l+1$, and go to (2).

The algorithm is also illustrated by Figure 8.

Next, a theorem concerning the convergence of Algorithm A whose proof can be found in Hirsch and Smale [29] is stated.

Theorem 5.1

Let $f : R^n \to R^n$ be a proper analytic map. Let $\epsilon > 0$ be given. Suppose $J(x) \geq 0$ outside some compact set and $J(x)$ is not identically 0. Also, suppose a number $\alpha_0 \in R$ is known such that $J(x) \geq 0$ if $\|f(x)\| \geq \alpha_0$. Then there is an open subset W^* of full measure of the set $E_+(\alpha_0) = \{ x \in R^n : \|f(x)\| > \alpha_0\}$ such that for every $x_0 \in W^*$, Algorithm A, described above, is defined and it stops at a point x with $\|f(x)\| < \epsilon$.

The discussion about Algorithm A is concluded by giving several remarks. Theoretically speaking, Theorem 5.1

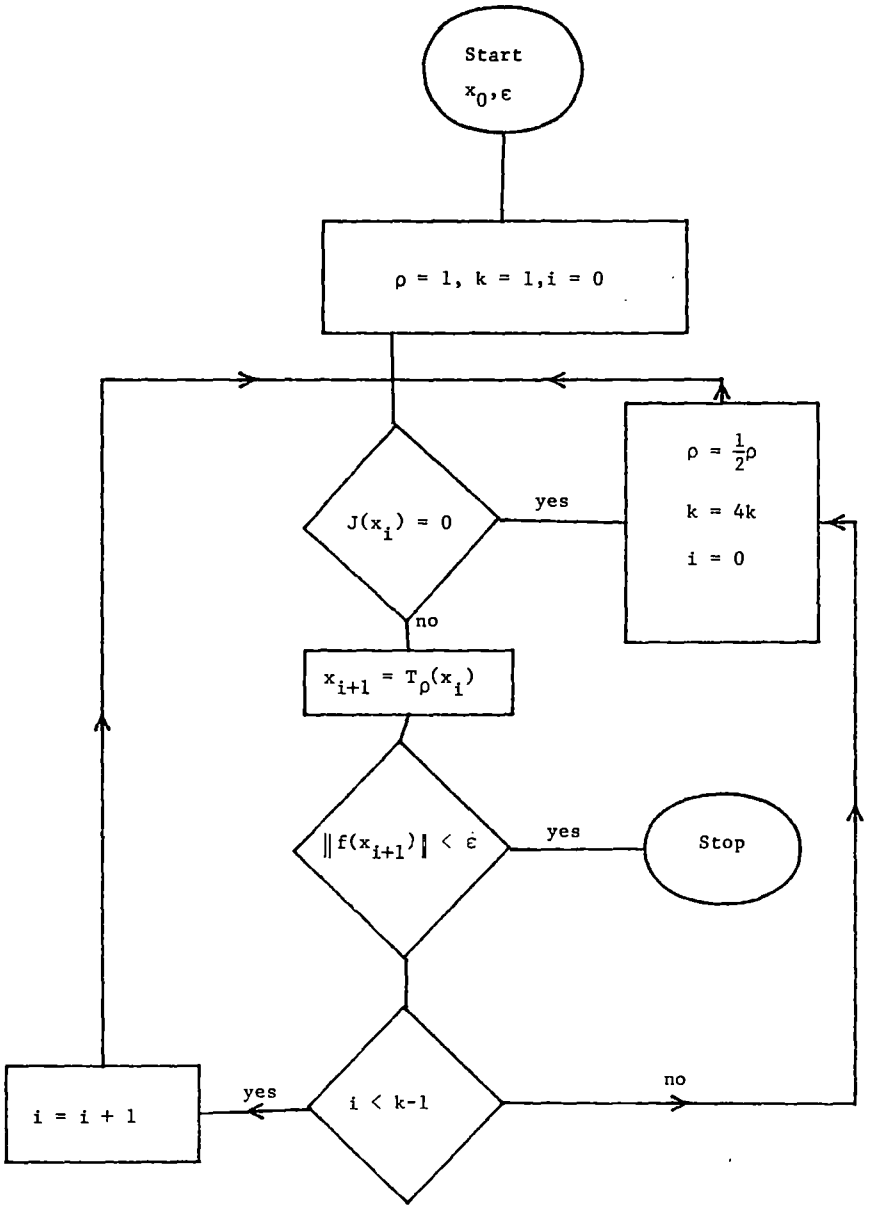

Figure 8. Flowchart of Algorithm A

ensures that after a finite number of Newton steps Algorithm A stops at a point x with $\|f(x)\| < \epsilon$, for some tolerance ϵ.

But, in practice this algorithm is not very useful for many reasons. Perhaps the greatest disadvantage of all is the waste in computing time because of the nature of this algorithm of stopping the integration process as soon as the maximum allowable number of Newton steps for each cycle is reached, even though the integration may have been successful when it stopped.

Another disadvantage of this algorithm lies in the method of integration itself; that is, it is well known that the Euler's method is not an efficient method of integration. Even with the introduction of the strategy of the step length halving so that it stays as closed as possible to solution curve, another problem arises, the problem of rounding error.

Computational experiments with this algorithm will be given in 5.3.

To overcome some of the above mentioned problems, the following algorithm is offered:

Algorithm AA

To describe the algorithm recall the definition of the vector field $\phi(x)$ given in Chapter II. $\phi(x)$ is defined by

$$\phi(x) = -\beta(x)\,\mathrm{adj}(Df(x))f(x), \tag{5.3}$$

where $\beta(x) = \dfrac{1}{\|\mathrm{adj}(Df(x))f(x)\|}$.

Suppose at $x \in \mathrm{Reg}(f)$ and $J(x) \neq 0$, then (5.3) can be rewritten as follows:

$$\phi(x) = - \operatorname{sgn}(J(x)) \frac{[Df(x)]^{-1} f(x)}{\| [Df(x)]^{-1} f(x) \|}. \qquad (5.4)$$

One should note that in practice, one does not actually find the inverse of the Jacobian matrix $Df(x)$, but rather solves the linear system $Df(x)\Psi(x) = f(x)$ and then set

$$\phi(x) = - \operatorname{sgn}(J(x)) \frac{\Psi(x)}{\|\Psi(x)\|}$$

Now, the algorithm may be describe. The basic idea behind this algorithm is to follow the solution curve, $C(x_0)$, of the IVP (5.1). Thus, one needs to approximate the solution curve $C(x_0)$ by means of numerical integration.

To this end, a predictor-corrector method is used. This is the first difference between Algorithms AA and A.

For the sake of simplicity, the Forward Euler's (F.E.) method, that is, the explicit method of integrating an IVP is given by the difference equation

$$X_{n+1} = X_n + h\, f(t_n, X_n), \quad n = 0, 1, 2, \ldots, \qquad (5.5)$$

where $X' = f(t,X)$, and h is the step size.

As pointed out earlier in this section, the Euler's method is not an accurate method for numerical integration, especially when the IVP to be integrated is stiff problem. For this reason the Backward Euler's (B.E.) method is used,

which is better than the F.E. method from the numerical integration point of view, to correct the predicted point. The B.E. is given by the difference equation

$$X_{n+1} = X_n + h\, f(t_{n+1}, X_{n+1}),\ n = 0,\ 1,\ 2, \ldots, \qquad (5.6)$$

The B.E. method has the advantage of handling stiff IVP. Also, because the B.E. is an implicit method and a classical correction process is not effective in the case of stiff IVP, the local Newton method is used in the correction of the function:

$$R(X_{n+1}) = X_{n+1} - X_n - hf(t_{n+1}, X_{n+1}). \qquad (5.7)$$

One should note that in the above equations, $f(t,X) = \phi(X)$.

In the correction process using equation (5.7) one needs the derivative of R(x) and consequently that of the vector field $\phi(x)$, which is very difficult to come by if not impossible to get in an explicit form. One way to overcome this is to get an approximation to the derivative of R(x) by means of the forward finite-difference, that is, an approximation to the (i,j)th component of the Jacobian matrix DR(x) given by the formula

$$\frac{\partial R_i}{\partial x_j} = \frac{R_i(x + he_j) - R_i(x)}{h}$$

where $e_j = (0,\ldots,0,\ 1,\ 0,\ldots,0)$, and h is sufficiently small.

Other methods of approximating the Jacobian matrix can be found in Dennis and Schnabel [12].

Another point of departure in Algorithm AA from that of Hirsch and Smale is the variability of the step size during integration. As pointed out earlier, Algorithm A of Hirsch and Smale does not really have a variable step size during the integration process. Instead, it keeps reducing the step size to half of what it was in the previous cycle if the integration is not successful, and then it continues the integration with the latest fixed step size.

On the contrary, Algorithm AA uses a variable step size by means of the Milne's device. This is achieved by measuring the local error of the integration after the correction process to a predicted point.

Let τ denote the local truncation error of integration, then τ is obtained by the formula:

$$\tau = \frac{1}{2} \| X^{B.E.}_{corr.} - X^{F.E.}_{pred.} \|$$

where $X^{F.E.}_{pred.}$ is the predicted point and $X^{B.E.}_{corr.}$ is the point after correction. An estimate of the new step size can be found from the formula:

$$h_{new} = \sqrt{\frac{\epsilon}{\tau}} \; h_{old}$$

where ϵ is predetermined tolerance.

Furthermore, the algorithm follows the following strategy to control both the local error and the step size:

Given a tolerance $\epsilon > 0$ and constants c_1 and c_2 with $c_1 < c_2$, and set $\epsilon_1 = \epsilon^2$, $\epsilon_2 = c_1*\epsilon$, and $\epsilon_3 = c_2*\epsilon$, the new point is accepted and the integration is continued with the same step size if $\epsilon_2 \leq \tau \leq \epsilon_3$. Otherwise, the new point is rejected and a new step size is calculated as follows:

(i) If $\tau < \epsilon_1$, then $h_{new} = 2h_{old}$, or

(ii) If $\epsilon_1 < \tau < \epsilon_2$ or $\epsilon_3 < \tau$, then the step size is given by (5.8).

Finally, a criterion on which the algorithm will be successfully terminated is described. To do so, note first that the continuous Newton (Hirsch and Smale's) method is itself a homotopy method. To see this, recall that if $x \in C(x_0)$, the solution curve of the IVP (5.1), then $g(x) = g(x_0)$, where $g(x) = \frac{f(x)}{\|f(x)\|}$. Rewrite this to get

$$f(x) = f(x_0) \frac{\|f(x)\|}{\|f(x_0)\|}. \tag{5.9}$$

Define $t : R \to R$ by

$$t = \begin{cases} \dfrac{\|f(x)\|}{\|f(x_0)\|}, & \text{if } f^t(x)f(x_0) \geq 0. \\ -\dfrac{\|f(x)\|}{\|f(x_0)\|}, & \text{if } f^t(x)f(x_0) < 0. \end{cases}$$

Thus, (5.9) becomes $f(x) - tf(x_0) = 0$, but this equation is just the homotopy defined by equation (4.6) in 4.2.

When following the solution curve, $C(x_0)$, the IVP solver has no way of knowing if it is or it is not near a zero of the map f. For this reason, a criterion is needed to prevent the occurrence of an overshooting. The criterion is simply to follow the solution curve by means of integration and at each new point the value of t is checked and as soon as the value of t becomes very closed to zero, say, when $t = 0.05$, then a switch to the local Newton method is made until a zero of f is found.

Figure 9 briefly describes the algorithm:

Next, the other two algorithms of Hirsch and Smale given in [29] are described. Under certain conditions to be given later, the first of these two algorithms does not guarantee to stop, but, produces an infinite sequence $\{X_n\}$ which converges to a zero of the map f. Moreover, there exists an n_0 such that if $n \geq n_0$, the algorithm proceeds by the Newton method.

Algorithm B (Hirsch and Smale's)

First, Algorithm B essentially is a modification of Algorithm A. What is new in this algorithm is the introduction of the local Newton method which is used after each Newton step of the integration process to test if the

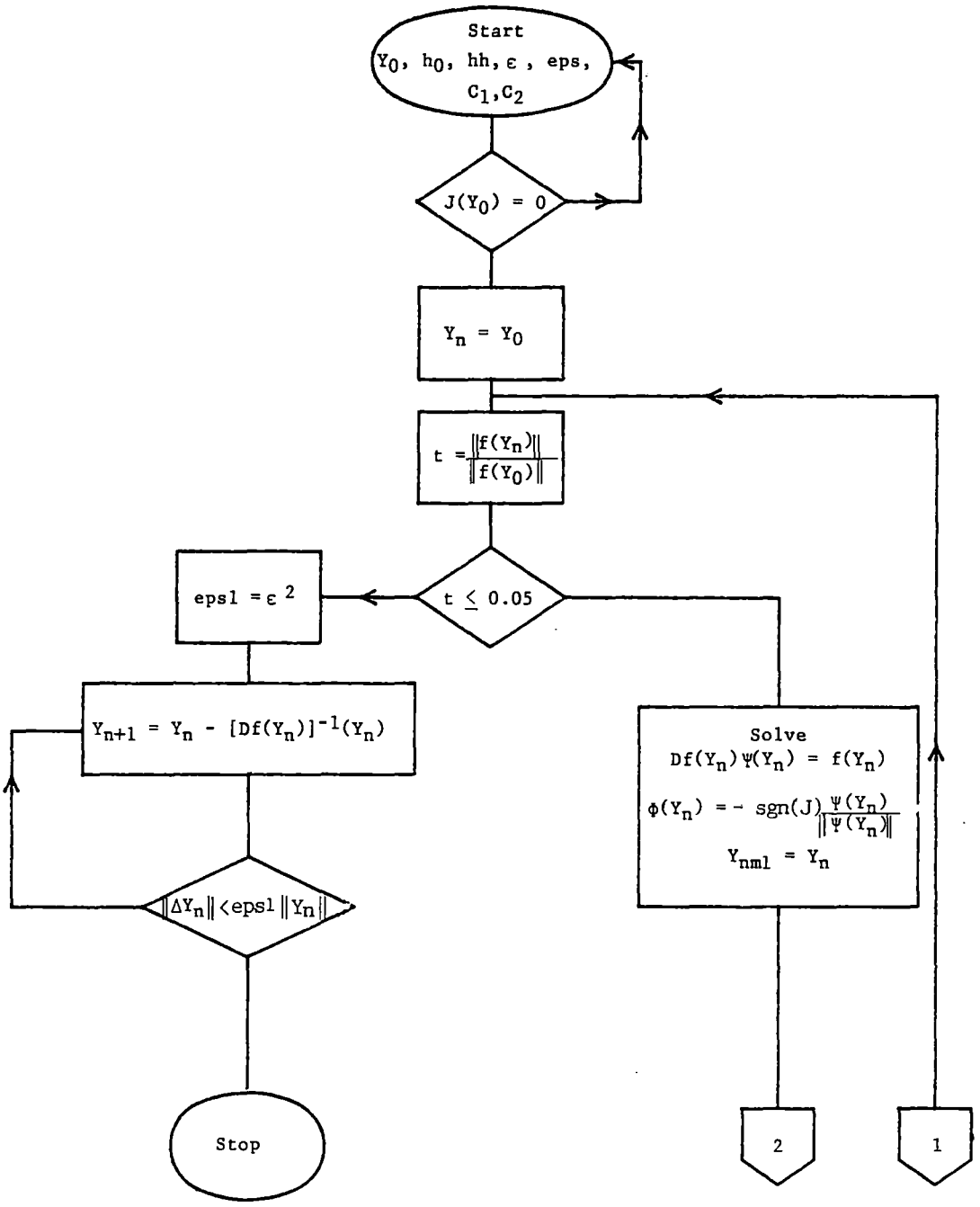

Figure 9. Flowchart of Algorithm AA

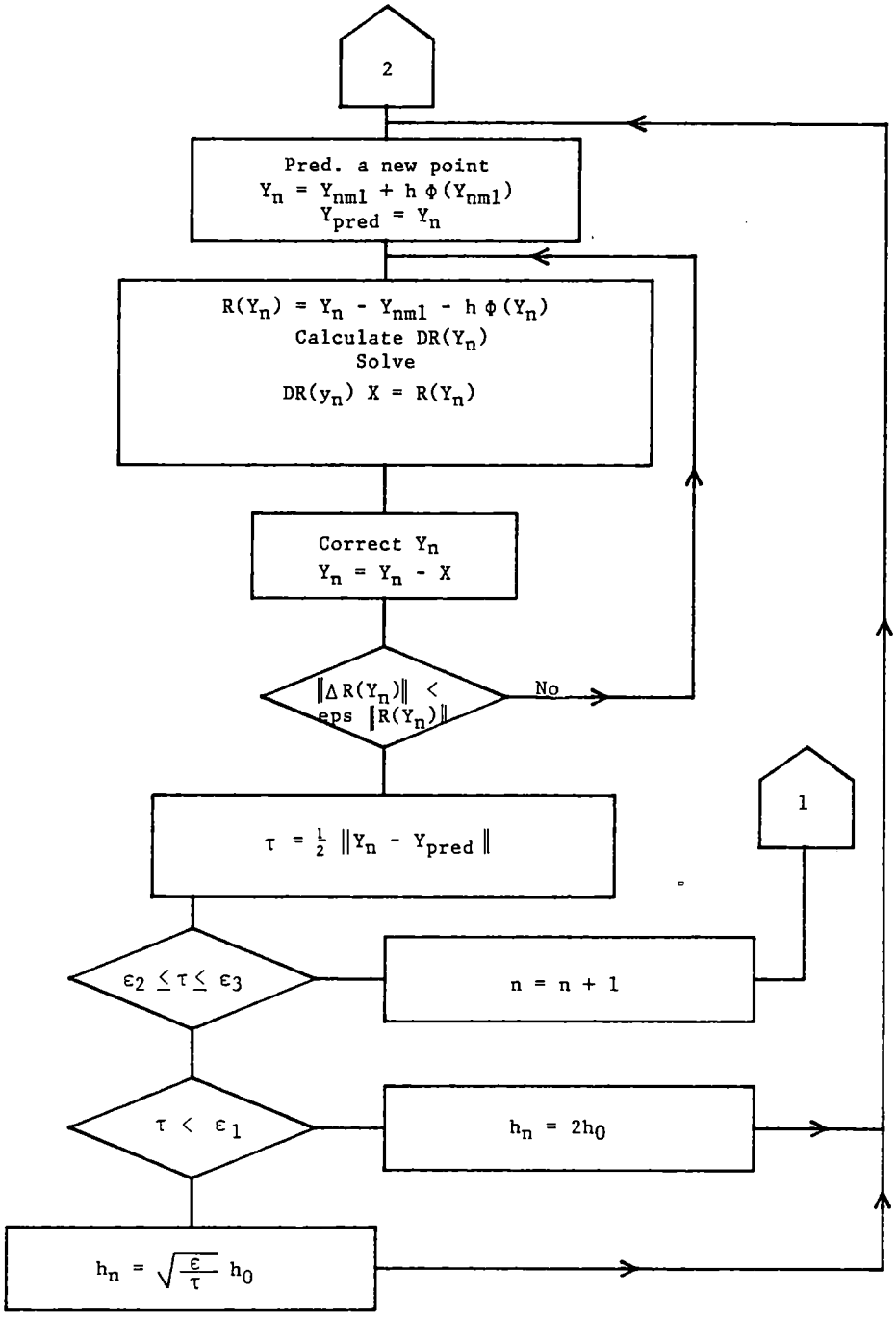

Figure 9 (Continued)

generated sequence by the Euler's method is close to the zero of f. If this is the case, then the algorithm proceeds by the Newton method; otherwise, the integration process is repeated. The following test of closeness to a zero of f is checked:

$$\|f(v)\| \leq \frac{1}{2} \|f(u)\|, \text{ where } v = u - [Df(u)]^{-1}f(u).$$

Figure 10 describes the algorithm.

In order to state a theorem concerning the above algorithm, the following Nondegeneracy (ND) condition is assumed:

(ND)
- (a) (a) The set $E = f^{-1}(0)$ is discrete and $Df(x)$ is nonsingular at each $x \in E$.
- (b) The se $\{J^{-1}(0)\}$ is closed and has measure zero.

Now, the necessary conditions which guarantee the sequence produced by Algorithm B are stated in the following theorem a proof of which can be found in Hirsch and Smale [29].

Theorem 5.2 (Hirsch and Smale's)

Let $f : R^n \to R^n$ be a proper C^2 map satisfying the ND condition. Also, suppose that a number $\alpha_0 \geq 0$ is know such that $J(x) \geq 0$ if $\|f(x)\| \geq \alpha_0$. Then there is an open set W^* of full measure in $E_+(\alpha_0) = \{x \in R^n : \|f(x)\| > \alpha_0\}$ with the

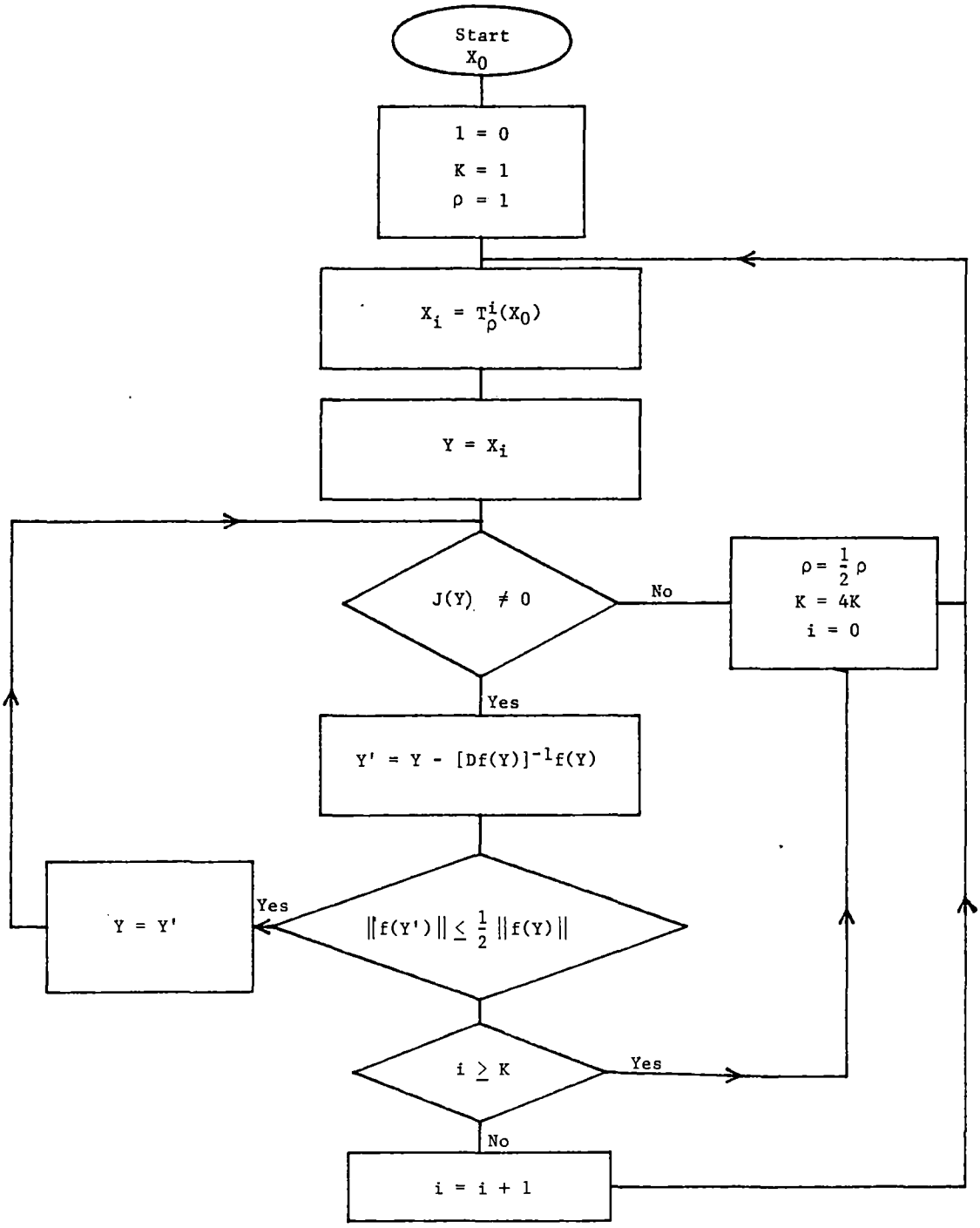

Figure 10. Flowchart of Algorithm B

following properties. When Algorithm B (defined above) is started at any $x_0 \in W^*$, it produces an infinite sequence $\{X_n\}$ which converges to a zero of f. Moreover, there exists an n_0 such that if $n \geq n_0$,

$$X_{n+1} = X_n - [Df(X_n)]^{-1} f(X_n)$$

In other words, eventually and automatically the sequence proceeds by the Newton-Raphson iteration.

This section is concluded by describing Algorithm C of Hirsch and Smale.

Algorithm C (Hirsch and Smale's)

This algorithm is a modification of both Algorithms, A and B. Again, the map f is assumed to satisfy the same conditions stated before, that is, f is C^2, proper, $J(x) \geq 0$ outside a compact set, and J(x) is not identically zero. However, with all the above conditions, the algorithm may fail as reported by Hirsch and Smale in [29].

The algorithm may be summarized by the flowchart shown in Figure 11.

5.2 Algorithms Based on Homotopy Methods

It is shown in Chapter III that there are two types of existence theorems of C^2-nonlinear maps. The first type is about fixed points and the second type is about zeros of maps satisfying certain conditions.

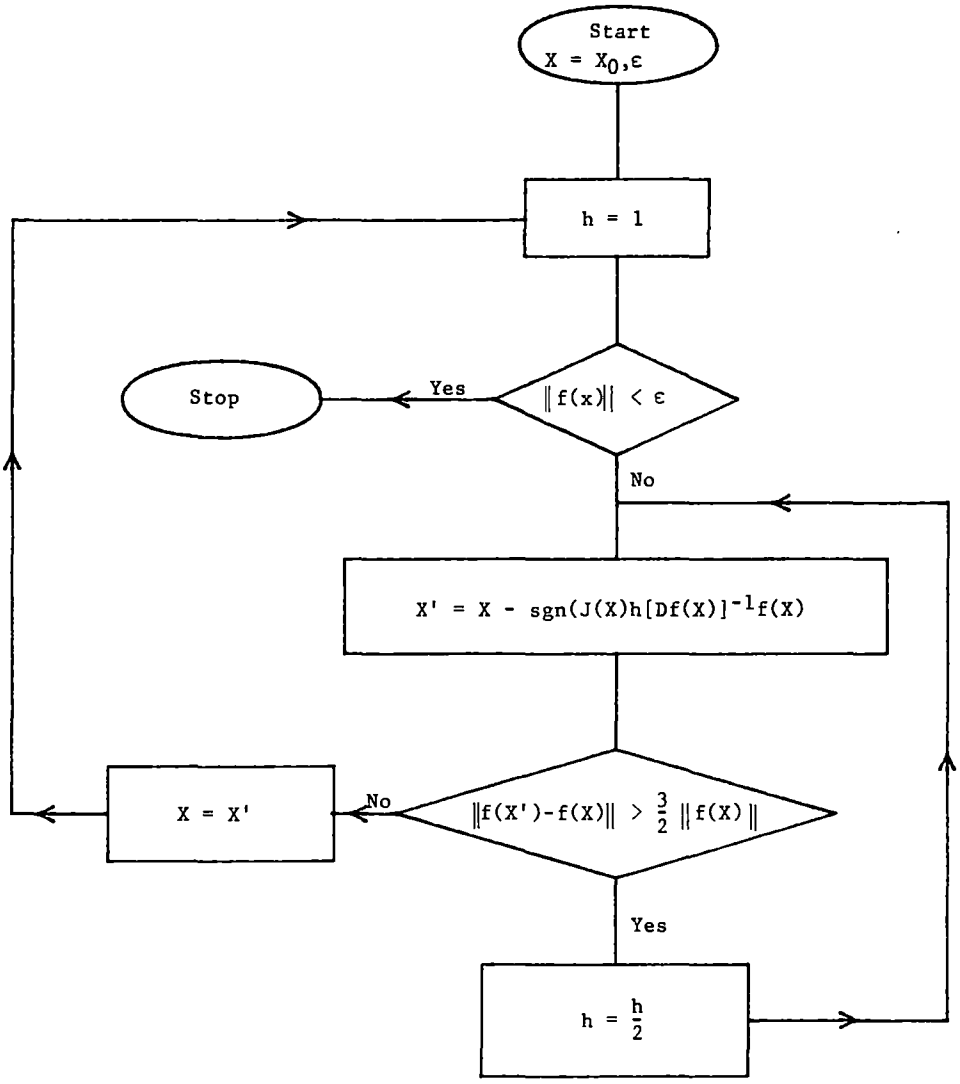

Figure 11. Flowchart of Algorithm C

In this section typical algorithms from each type are reported and some possibilities for improvement in the implementations of these algorithms are also indicated.

A typical algorithm of finding fixed points of C^2 nonlinear maps is Chow-Yorke algorithm given in [8]. This algorithm was implemented and extensively tested by Watson in [50].

Watson's Algorithm

In order to describe Watson's algorithm, first recall some of the facts that were established in Chapter III:

Let $H : \text{int}(K)\times(0,1)\times\text{int}(K) \to R^n$ be defined by

$$H(a,t,x) = t(x-f(x)) + (1-t)\ (x-a), \tag{5.9}$$

where K is a compact convex subset of R^n.

It is also shown in Chapter III that if 0 is regular value of the homotopy H, then 0 is a regular value of the map $H_a : (0,1)\times\text{int}(K) \to R^n$ defined by $H_a(t,x) = H(a,t,x)$.

Differentiating H_a with respect to arc length, say s, and get the IVP

$$\frac{d}{ds} H_a(t(s),x(s)) = 0$$

$$|dt/ds|^2 + \|dx/ds\|^2 = 1,\ t(0) = 0,\ x(0) = a. \tag{5.10}$$

The above IVP can be put in the compact form

$$DH_a(t,x)\dot{Y} = o, \text{ with } Y(0) = (0,a), \|\dot{Y}\| = 1, \qquad (5.11)$$

where $Y = (t,x)$ and $DH_a(t,x) = (I-tDf(x), a-f(x))$.

According to Theorem 3.2, if one starts at $(0,a)$, the solution curve of the above IVP leads to a fixed point at $(1,x_*)$ with $f(x_*) = x_*$. For this, one needs to approximate this solution curve numerically.

To this end, an ODE solver is needed to follow the solution curve emanating from the point (o,a). Watson has suggested the use of the STEP subroutine along with other subroutines written by Shampine and Gordon [48]. The STEP subroutine is based on Adame's predictor-corrector methods with variable step size.

Furthermore, because the IVP at hand is implicit, one needs to find a unit vector field in the kernel of the matrix $DH_a(Y)$ at each point on the solution curve. Also, Watson has recommended the use of Householder's transformation to obtain such a unit vector field.

Since the main goal is to find a fixed point as soon as possible, Watson has advised to follow the solution curve of the IVP in (5.10) rather loosely, except in two particular instances where the curve should be followed very closely.

The first case (when the curve makes "sharp" turns of some sort) when $|dt/ds|$ becomes very small, say, $|dt/ds| < .01$.

This type of measure is to taken to prevent drifting away to another nearby component of $H_a^{-1}(0)$. Figure 12a shows a case where cycling may occur due to such drifting. Also, Figure 12b shows another case in which a misorientation to the solution curve occurred and this may lead back to the beginning.

The second case occurs near a fixed point. Thus, as soon as the value of t becomes closed to 1, say, .99. The process of following the solution curve is restarted by calculating a new starting point $(\bar{t},\bar{a})$ where $\bar{a}$ is obtained by using the following equation:

$$\bar{a} = \frac{\bar{x} - \bar{t}f(\bar{x})}{1 - \bar{t}}. \qquad (5.12)$$

The point $(\bar{t}, \bar{a})$ lies exactly on the new solution curve $C(\bar{a})$ which is followed as accurate as machine precision permits until a fixed point of f(x) is reached or $t > 1$. When the value of t becomes greater than 1, $x(\bar{s})$ is determined, where $x(\bar{s})$ is a fixed point of f(x), and $x(\bar{s})$ corresponds to $t(\bar{s}) = 1$. The value $\bar{s}$ is unknown, but this can be obtained by solving the equation $t(\bar{s}) = 1$ for s using inverse interpolation. Then by Using the available data near the point $(t(\bar{s}),x(\bar{s}))$ to interpolate once more and get $x(\bar{s})$.

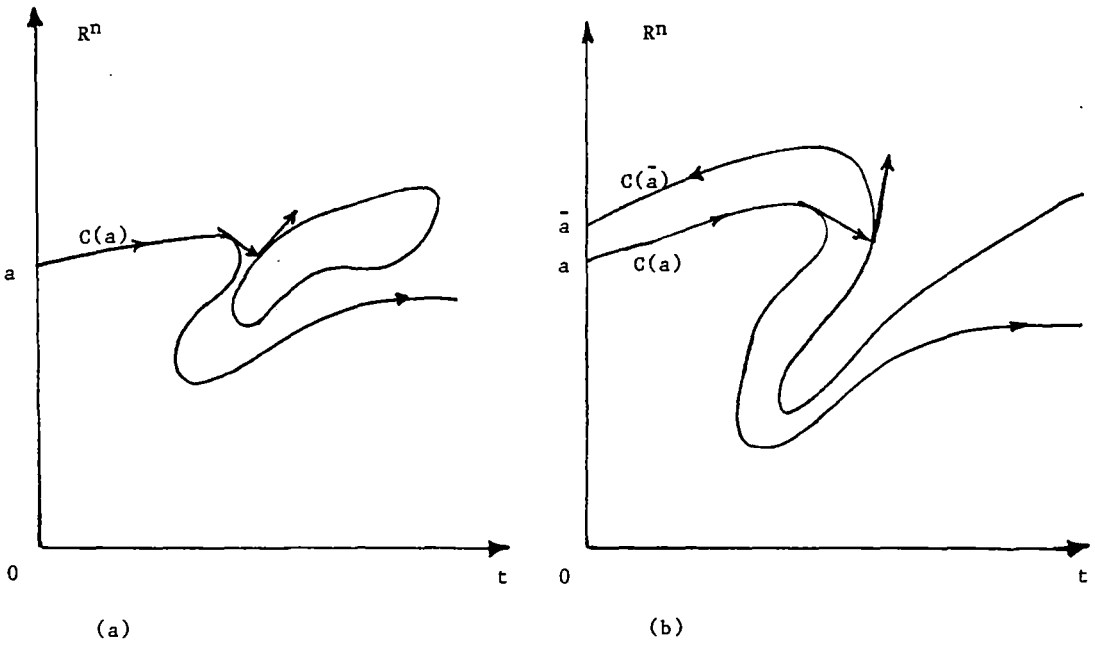

Figure 12. A Cycling or Misorientation in Watson's Algorithm

If the arc length of the solution curve $C(a)$ happen to be very large, then points generated by the ODE solver may lie far away from the actual solution curve. To remedy this problem, Watson suggests the use of equation (5.12) to restart the whole process from the last computed point and get $(\bar{t}, \bar{a})$. Again the new solution curve $C(\bar{a})$ is followed until a fixed point of f(x) is reached. When taking the last measure it might happen that $\bar{a} \notin \text{int}(K)$, but this indicates that the computed solution curve has drifted too far from the original solution curve. A way out of this is to follow the solution curve very closely from the first starting point.

Now, a summary of the previous discussion follows:

Algorithm (Watson's)

1. Start. Choose $a \in \text{int}(K)$, a tolerance δ for normal following the solution curve, and ϵ to be used in case the solution curve has a sharp turn or $t > 0.99$. Usually, choose $\epsilon << \delta$. Also, set $s = 0$, $t(0) = 0$ and $x(0) = a$.
2. Compute a unit vector field $\dot{Y}$.
3. Compute a new point along the solution curve by means of the ODE solver using the tolerance δ.
4. If the ODE solver fails to compute a new point go to (10).
5. If the current arc length is too long or $t \geq 0.99$ restart the following process by computing a new

starting point $(\bar{t}, \bar{a})$ using equation (5.12) above and set a flag to indicate to the ODE solver to follow the new solution curve $C(\bar{a})$.

6. If $|dt/ds| \leq 0.01$ or $t \geq 0.99$ set the tolerance equal to ϵ.
7. If too many steps have been taken without getting closer to a fixed point go to (10).
8. If $t < 1$ go to (2).
9. Use inverse interpolation to find $\bar{s}$ such that $t(\bar{s}) = 1$.
10. Set appropriate flag and stop.

At this point of the discussion one should point out the ODE solver used by Watson was designed essentially to solve nonstiff IVP. If the system obtained as a result of differentiating the homotopy map given by (5.9) is a stiff system, then one should expect some difficulties in following the solution curve $C(a)$.

To remedy this problem, maybe, the use of ODEPACK, which is a software designed by Hindmarsh [23], might help. This software consists of several subroutines, each dealing with a certain type of IVP. Because the problem at hand is implicit, one may use the subroutine LSODI, which is specifically designed to solve this kind of IVP. In this way, one does not need to use the Householder's transformation to get a unit vector field. LSODI has another advantage; that is it determines internally whether a given IVP is stiff and adjusts to that automatically.

Another possible modification to Watson's algorithm is the use of the local Newton method in the final stage of following the solution curve instead of interpolations. To do this, one may keep a record of one point on the approximating curve and as soon as the level t = .99 is reached. This process is continued until the value of t becomes greater than one, then one uses the point just before the last point generated by the ODE solver as a starting point for the local Newton method.

Li and Yorke Algorithm

Now, a typical algorithm of finding zeros of certain nonlinear C^2 maps is described. The algorithm was developed by Li and Yorke [38].

To start the description of this algorithm, some of the facts given in Chapter III should first be recalled. Let $f : R^n \to R^n$ be a C^2 nonlinear map. Define the homotopy map $H : [0,1]\times R^n \to R^n$ by

$$H(t,x) = tf(x) + (1-t)g(x), \tag{5.13}$$

where $H(0,x_o) = g(x_0)$, $H(1,x) = f(x)$, and $g(x_0)$ has a trivial solution.

Suppose that 0 is a regular value of H and $\mathcal{C}(a)$ is a component of $H^{-1}(0)$ through (0,a). Also, let $\xi : [0,b] \to [0,1]\times R^n$ be a parametrization of $\mathcal{C}(a)$ by arc length, that is, $\xi(s) = (t(s),x(s))$ and $\|d\xi/ds\| = 1$. By differentiating $H(x,t) = 0$ with respect to s one gets the IVP

Thus, to find a zero of the map f one needs to follow the solution curve of the above IVP. A discussion of Li and Yorke's algorithm follows:

The algorithm first predicts a point on the solution curve $C(a)$; for this purpose Li and Yorke used a 4th order Runge-Kutta method. In this way, it is unavoidable to make some errors during the integration process. To remedy this problem, the local Newton method is used as a corrector to bring back the predicted point closer to the solution curve.

The correction process goes as follows: let Y_n be the corrected value at the n-th step of integration. One predicts a new point Y_{n+1}, say, starting at Y_n and let $Z_0 = Y_n + \delta\, \Delta Y_n$, where δ is the current step size of the predictor method. Now, Z_0 is used as a starting point for the local Newton method to obtain Z_n on the intersection of the solution curve $C(a)$ and a hyperplane, say N, that is approximately normal to the solution curve Figure 13.

Let $G(Z_k, \Delta y) = \begin{bmatrix} DH(Z_k) \\ \Delta y^t \end{bmatrix}, R(Z_K) = \begin{bmatrix} H(Z_k) \\ 0 \end{bmatrix}$.

To get Z_n the local Newton method is used, that is, one iterates using

$$Z_{k+1} = Z_k - [G(Z_k)]^{-1} R(Z_k),\ k = 0,1,2,... \qquad (5.15)$$

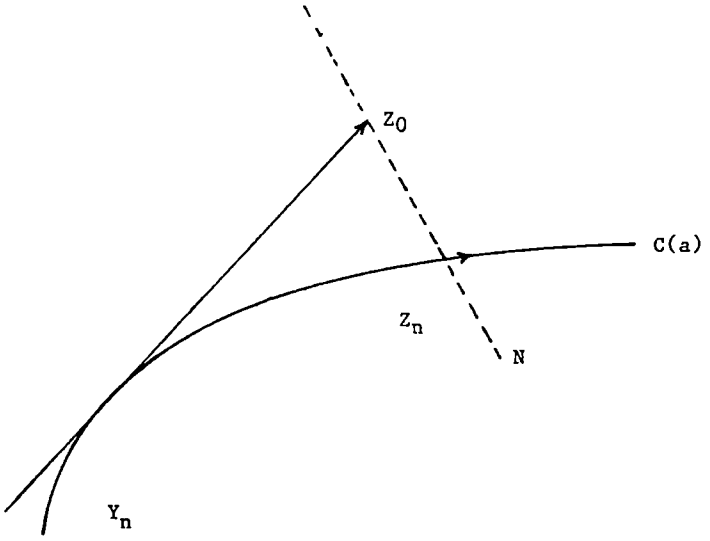

Figure 13. A Normal Plane to the Solution Curve $C(a)$

Depending on the location of Z_0 the Newton method may or may not converge. For this reason, Li and Yorke suggested the use of the following criterion to be checked:

$$\|H(Z_i)\| > 10 \|H(Z_{i+1})\|. \tag{5.16}$$

If the above condition is satisfied then one continues the Newton itergration until $\|\Delta Z_n\| = \|Z_n - Z_{n-1}\| < \epsilon$ for some tolerance ϵ. Then one sets $Y_{n+1} = Z_n$ and continues the integration process. Otherwise, if $\|\Delta Z_n\| > \epsilon$, then the step size of the ODE solver at Y_n, say, δ_n is cut in half and the whole procedure is restarted with the new step size.

Next, an orientation to the solution curve of the IVP (5.14) is needed. To achieve it, one uses a unit vector field, u, obtained from the kernel of $DH(\xi)$. But, then there are two choices of direction, namely, $d\xi/ds = \pm u$. Thus, at each new point on the solution curve the correct sign for the unit vector field needs to be chosen, other wise, a misorientation to the solution curve may lead back to the starting point or a cycling of the integration pro cess may occur.

To prevent a misorientation from happening, Li and Yorke used the following criteria: Let Y_1, Y_2 be two successive points on the solution curve and U_1, U_2 be the corresponding unit vector fields obtained from the kernel of $DH(\xi)$. Then a sign choice of U_2 is made such that

$$< U_1, U_2 > \geq .95, \tag{5.17}$$

where $<.,.>$ stands for the usual inner product. The criterion in (5.17) amounts to saying the angle between U_1, U_2 should always be less than or equal 18°. On the one hand, if the above criterion does not hold, the current step size is cut in half and the whole process is restarted once more. On the other hand, if the criterion does hold, then the current step size is doubled and one continues the integration process.

The discussion of Li and Yorke's algorithm may be closed by briefly mentioning the criterion on which the

algorithm terminates. To this end, it should be first pointed out that according to the theory developed in Chapter III, Li and Yorke's algorithm may not work. To be more specific, the algorithm may fail if the curve that is being followed turns back to the level t = 0 as shown in Figure 14.

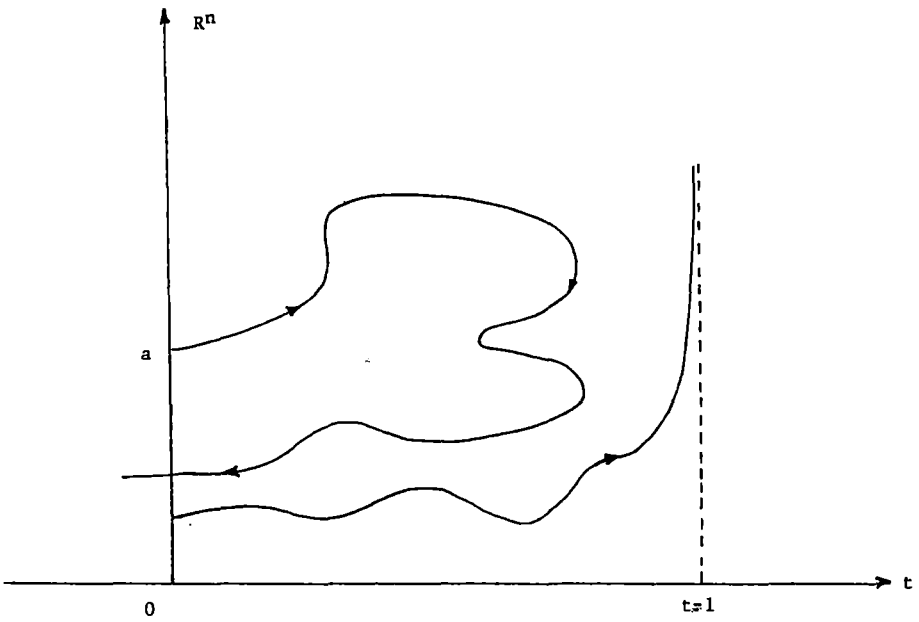

Figure 14. A Solution Curve Turns back to the Level t = 0 or Becomes Unbounded

Thus, it is necessary to take this into consideration; otherwise, the solution curve may wander around in the region where t < 0 and as a result, a lot of computing time may be wasted.

Another situation in which the algorithm may fail is in the case when the solution curve is not bounded, as shown in Figure 14. In this case also, a lot of computing time may be wasted in following a curve which cannot reach the level $t = 1$.

Having introduced some of the problems which may cause Li and Yorke's algorithm to fail, the criteria on which the algorithm terminates with success is now discussed.

Let $A = \{(t, x) \in R^n : |1 - t| < \epsilon\}$, where ϵ is some tolerance. The algorithm is terminated when $(t_{n+1}, x_{n+1}) \in A$. Now, there are two cases to consider. The first case, $t_{n+1} > 1$, then one interpolates t in terms of s to find a new step size δ which gives $\bar{t}_{n+1}(s) \sim 1$, and the corresponding $\bar{x}_{n+1}$ is the zero of $f(x)$.

The second case is when the solution curve changes direction just at $t = 1$ so that it touches the level $t = 1$. This situation is shown in Figure 15.

In this case, suppose $Y_n = (t_n, x_n)$ lies on the solution curve and $t < 1$. Also, let Y^* be the point symmetric to Y_n with respect to $t = 1$, that is, $Y^* = (2-t_n, x_n)$ and $Y_{n+1} = (t_{n+1}, x_{n+1})$, $t_{n+1} < 1$. Suppose also $dt/ds|_{t_{n+1}} < 0$, and if $|Y^*_n - Y_{n-1}| < \delta$, where δ is the current step size. Then, the solution curve must have touched the level $t = 1$.

To find the point of contact, say, $\bar{Y}_{n+1} = (\bar{t}_{n+1}, \bar{x}_{n+1})$ one interpolates $dt/ds|_{t_n}$, $dt/ds|_{t_{n+1}}$ linearly and finds a new δ_0 which makes $dt/ds \sim 0$.

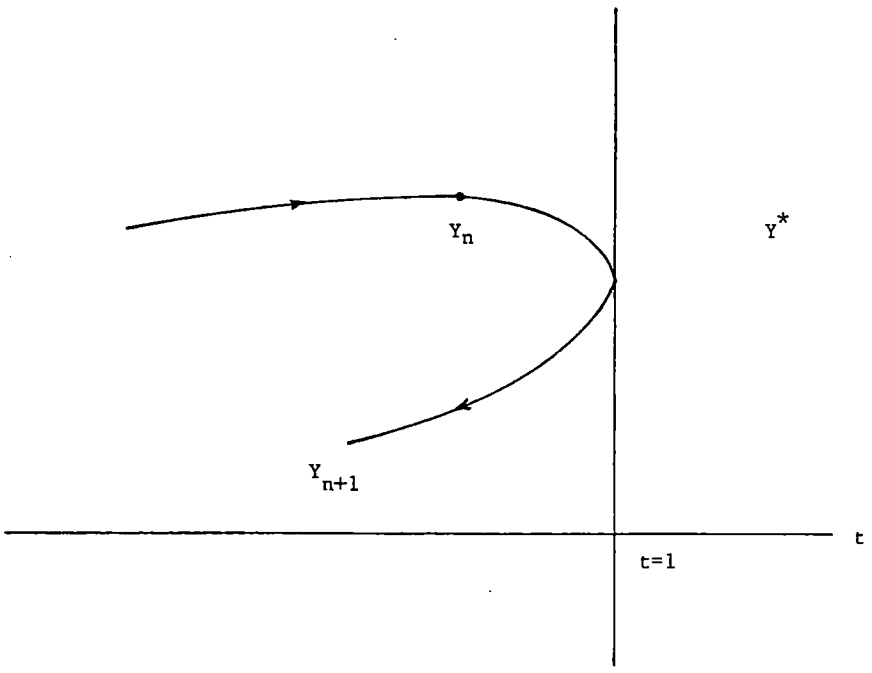

Figure 15. The Solution Curve $C(a)$ Touches the Level t = 1

A final remark about the discussion is about how the unit vector field $d\xi/ds$ is obtained. Even though Li and Yorke did not point out how to get such a unit vector, one may find it by using either Gauss elimination with partial pivoting or the Householder transformation.

In brief, the algorithm is shown in Figure 16.

Next, some of the improvements that might be introduced to Li and Yorke's algorithm are pointed out. On the one

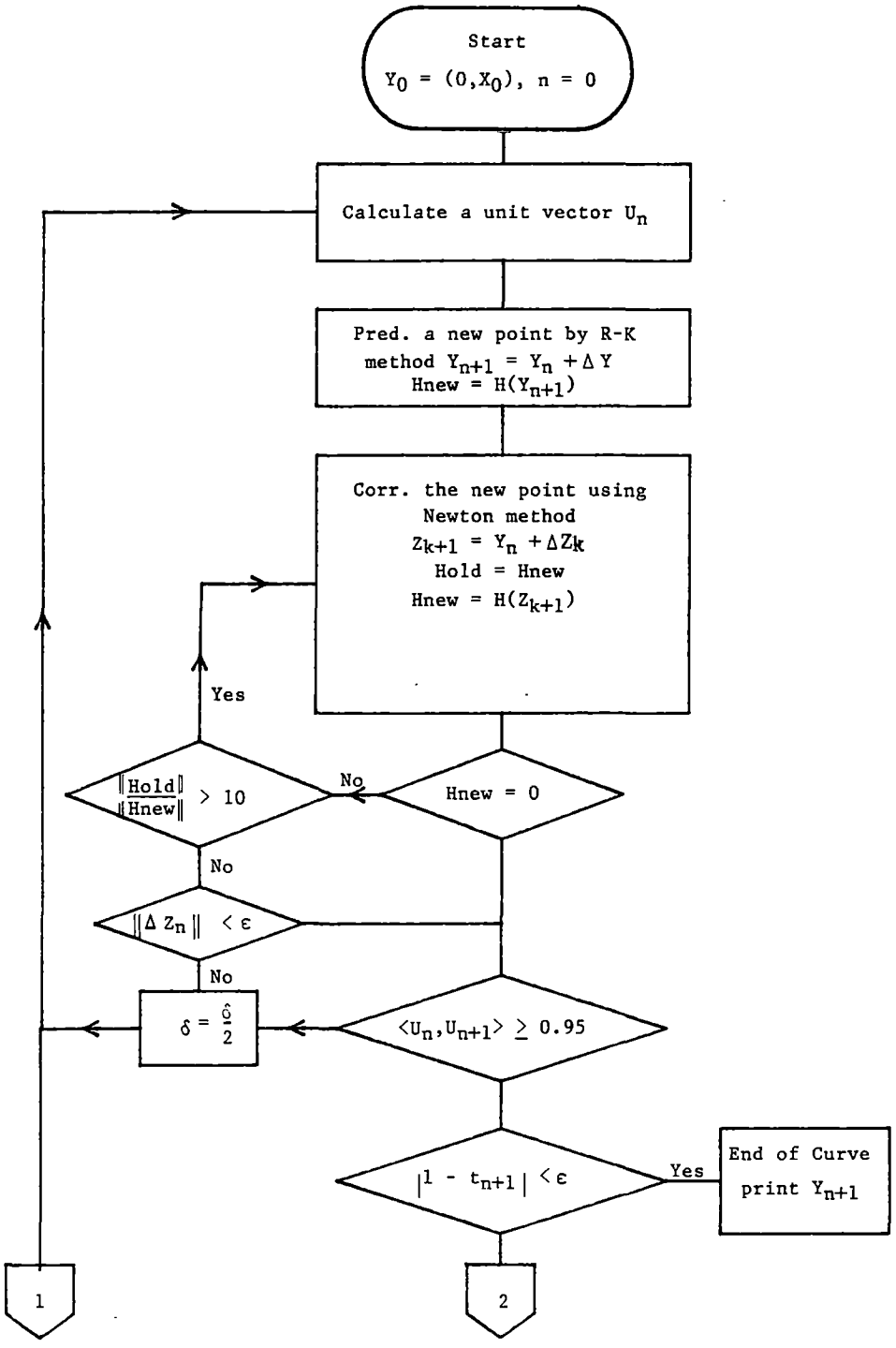

Figure 16. Flowchart of Li and Yorke's Algorithm

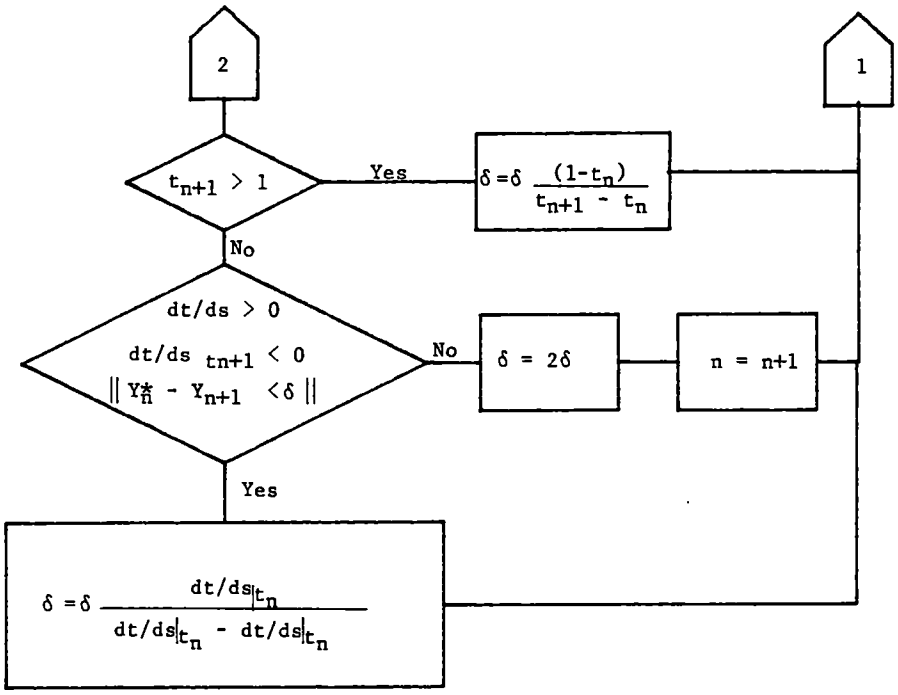

Figure 16 (Continued)

be achieved by following the solution curve very closely as soon as the value of t becomes .95, say. In doing so, one also keeps record of one point on the solution curve; then as soon as t reaches a value greater than 1, one uses the penultimate point as starting point for the Newton method.

At this point of the discussion, one should point out a similar algorithm given by Allgower and Georg in [3]. But they substituted the Runge-Kutta method by the Euler's as a predictor method.

Speaking of other alternatives, an algorithm similar to that which was given in 5.1 may be developed. To be more specific, one may use the forward Euler's method as a predictor and the Backward Euler's method as a corrector. Because the latter method can handle stiff IVP such as those arising from solving systems of polynomials, this subject will not be dealt with here.

In addition, with this algorithm a special form of homotopy that was suggested by Chow et al. [9] may be incorporated. The homotopy map is given by

$$H : C^n \times [0,1] \times C^n \times C^{n^2} \rightarrow C^n$$

with its ith component given by

$$H_i(Z,t,b,a) = (1-t)(Z_i^{d_i} - b_i) + tP_i(Z) + t(1-t)\sum_{j=1}^{n} a_{ji} Z_j^{d_i},$$

where $b \in C^n$, $a \in C$, $t \in [0,1]$, $d_i \geq 1$ is the degree of the ith component, and $P(Z) : C^n \rightarrow C^n$ is a polynomial and the degree of $P_K(Z)$ is d_k.

Also, note here that the extra term

$$R_i(Z) = t(1-t) \sum_j^n a_{ji} Z_j^{d_i},$$

is added to force the solution curves emanating at t = 0 to go all the way to t = 1. In addition, it is also shown by Chow et al. [9] that for almost every $(b,a) \in C^n \times C^{n^2}$, in Lebesque sense, every solution curve starting at the level t = 0 reaches the level t = 1; that is, all solution curves are bounded. This would be a big advantage over Li and Yorke's algorithm.

This section may be closed by briefly mentioning another type of modification to Li and Yorke's algorithm. These types of algorithms are based on the derivative-free (Quasi-Newton) methods for following the solution of an IVP.

In fact, Georg in [19] and Kearfott in [28] developed similar derivative-free path following methods. Their main modification seems to be in the use of a *Least-Change Secant* method for the Jacobian matrix DH(Y). To achieve this, an adoptive controlled predictor step size, and Powell's indexing procedure to preserve linear independence when updating are used.

The derivative-free path following methods have another useful feature. These methods can handle bifurcation

problems, but this subject too is beyond the scope of this study. Further details on this matter can be found in the above mentioned two references.

5.3 Computational Experience

The computational experience reported here is limited to algorithms based on the continuous Newton method.

To be more specific, Hirsch and Smale's three algorithms and Algorithm AA were actually tested. The computations reported here are about five different problems.

The first problem is to find all roots of the polynomial

$$P(x) = x^3 + 1 \tag{5.18}$$

This polynomial has one real root and two complex roots, namely -1.0 and $(1 \mp \sqrt{3}\, i)/2$.

To find all the roots of P(x) numerically, one first complexifies this polynomial, that is to say, write P(x) as a complex polynomial and get

$$P(Z) = Z^3 + 1,$$

then, one separates P(Z) into real and imaginary parts. Let $P_1(x, y)$, and $P_2(x, y)$ be the real and imaginary parts of P(Z), respectively. Thus, the nonlinear system is obtained

$$P_1(x, y) = x^3 - 3xy + 1$$
$$P_2(x, y) = 3x^2y - y^3. \tag{5.19}$$

One should note that the problem of finding the roots of (5.18) is equivalent to determining the zeros of (5.19).

A summary of the results obtained from solving the system (5.19) using Algorithms AA, B, and C are given in Table I.

The solution curves of the system of the IVP that correspond to the system (5.19) obtained by using Algorithms AA and C are also shown in Figures 17 and 18, respectively.

From Table I, one may point out several remarks. The first is about the number of iterations it took each algorithm to converge to a zero of (5.19). Algorithm AA took almost three times the number of iterations taken by both Algorithm B and C, while the last two algorithms took the same number of iterations to converge to a zero of (5.19).

The second remark is about the starting points of these algorithms. When Algorithms AA and C were started at the point (-20., -20.) they did converge to the zero (-1.0, 0.0), while Algorithm B did not converge. But when the starting point was changed to (-20., -15.) Algorithm B converged to the above zero without any difficulty.

The second problem that was used in computations is the following "simple" nonlinear system:

TABLE I

SUMMARY OF THE RESULTS OF THE FIRST PROBLEM

Alg.	Initial Values	No. Iterations	Zeros and Notes
	$\epsilon = 10^{-5}$, $c_1 = .8$, $c_2 = 1.2$		
AA	(20.0, 20.0)	37	(.5, 0.86602)
	(20.0, -20.0)	37	(.5, -.886602)
	(-20.0, -20.0)	39	(-1.0, 0.0)
	$\epsilon = 10^{-6}$		
B	(20.0, 20.0)	13	(.5, 0.86602)
	(20.0, -20.0)	13	(.5, -.86602)
	(-20.0, -15.0)	14	(-1.0, 0.0)
	$\epsilon = 10^{-5}$		
C	(20.0, 20.0)	13	(.5, 0.86602)
	(20.0, -20.0)	13	(.5, -.86602)
	(-20.0, -20.0)	14	(-1.0, 0.0)

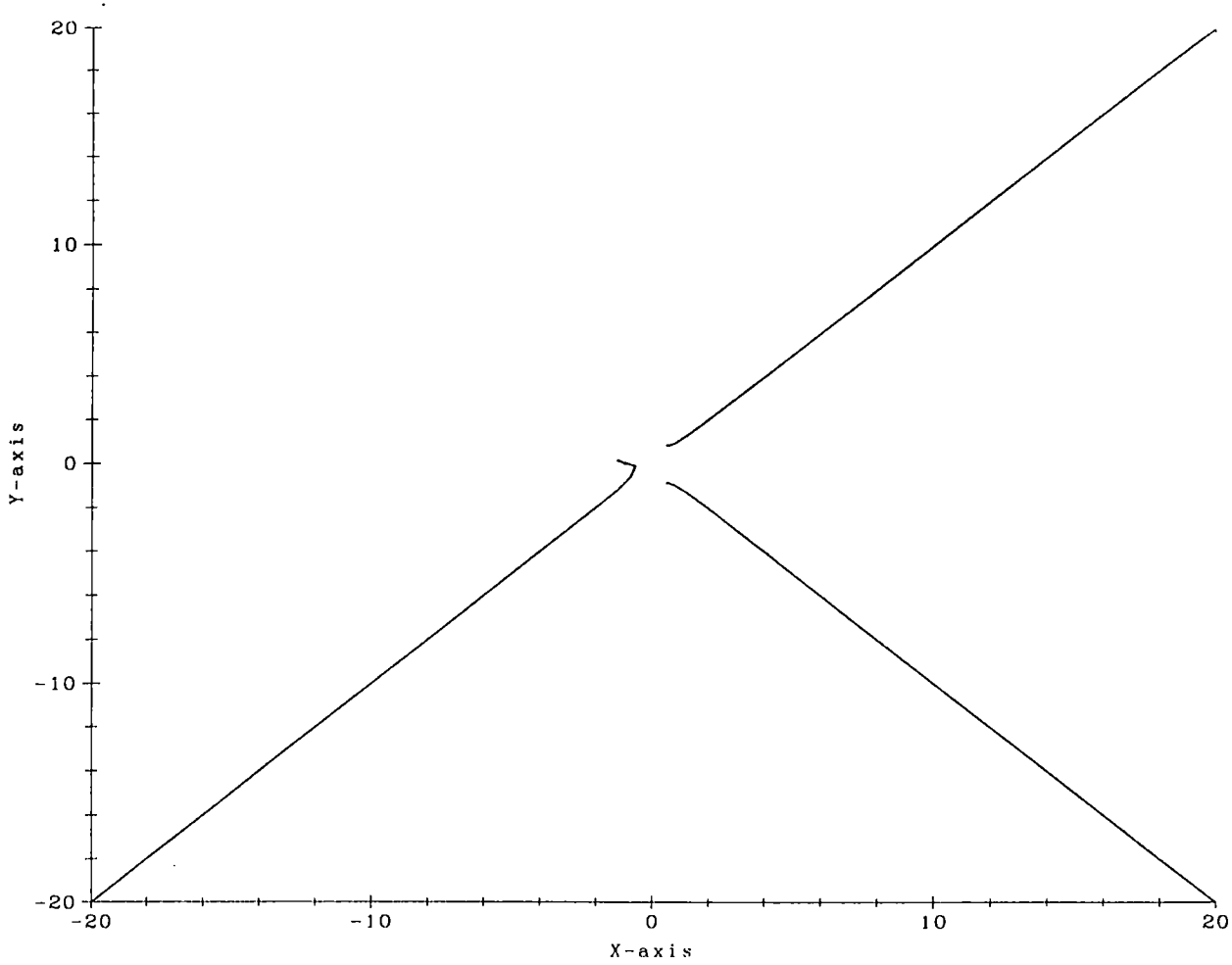

Figure 17. Several Solution Curves of the First Problem Obtained by Algorithm AA

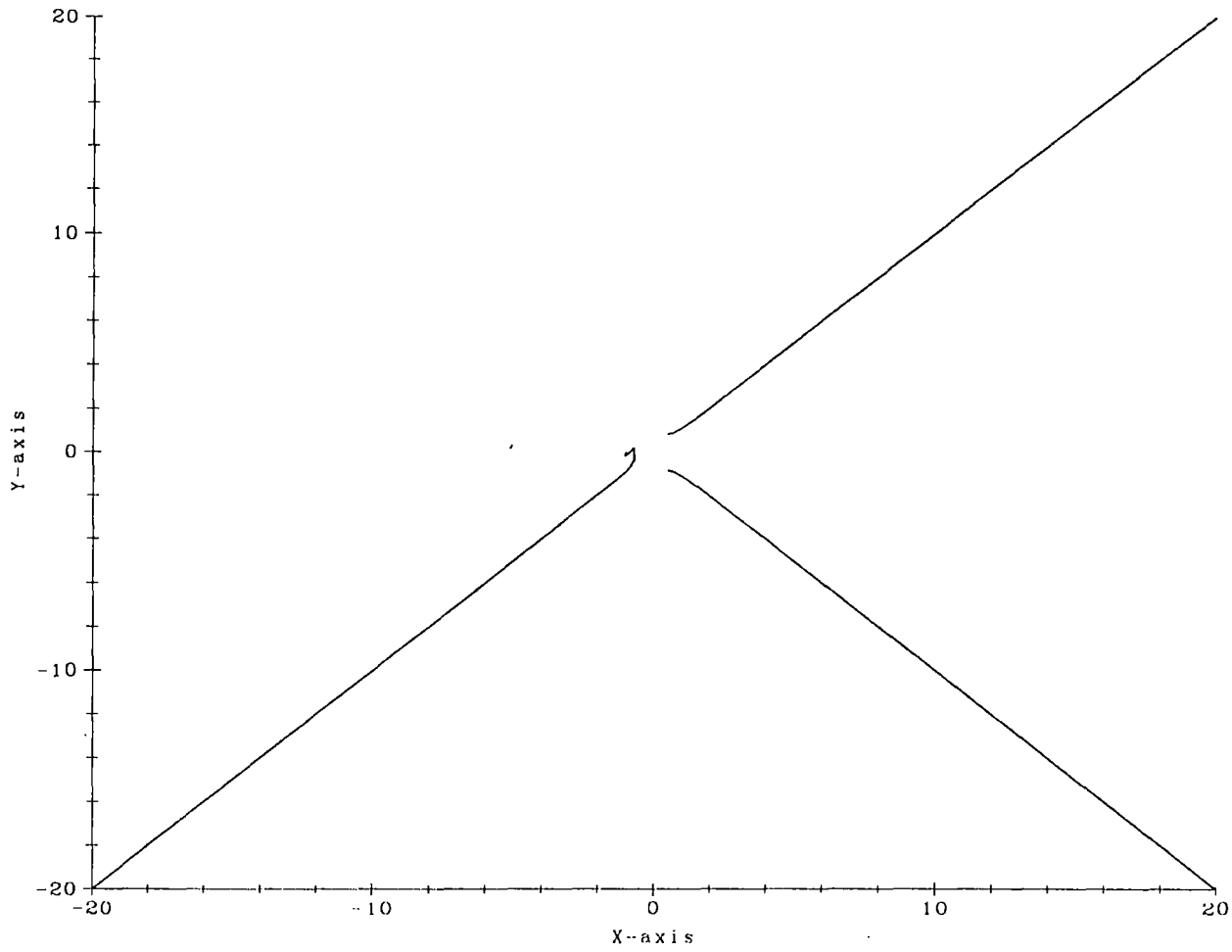

Figure 18. Several Solution Curves of the First Problem Obtained by Algorithm C

$$f_1(x, y) = x - y$$
$$f_2(x, y) = x^2 - y - 2. \tag{5.20}$$

Note that the determinant of this system,

$$J(x) = 2x - 1.$$

Thus, $J(x) > 0$ if $x > 1/2$. Also, according to Theorems 5.1 and 5.2 starting at any point where $J(x) > 0$, both Algorithms B and C converge to a zero of the system (5.20). In fact, this system has two zeros, namely, (-1., -1.) where $J(x) < 0$, and (2., 2.) where $J(x) > 0$.

The computational results obtained from solving system (5.20) using all four algorithms are shown in Table II.

It is also shown in Figures 19 and 20 some of the solution curves of system (5.20) obtained by using Algorithm AA.

From Table II one may note the following:

(i) Algorithm A when started at the point (3.0, 4.0) did not converge even after 500 iterations. Also, one can see from Figure 21 how this algorithm overshoots beyond the zero (2.0, 2.0).

(ii) When Algorithms AA, B, and C are started at points where $J(x) > 0$, they do converge to the zero (2.0, 2.0) with almost the same number of iterations for both Algorithms B and C, while Algorithm AA took more iterations to converge to the above mentioned zero.

TABLE II

SUMMARY OF THE RESULTS OF THE SECOND PROBLEM

Alg.	Initial Values	No. Iterations	Zeros and Notes
	$\epsilon\ 10^{-3}$		
A	(3., 4.)	500	(1.9938, 1.9885) no conv.
	$\epsilon = 10^{-6}$		
	(-0.9, -0.8)	4	(-1.0, -1.0)
	(-0.5, -0.6)	5	(-1.0, -1.0)
B	(-200., 1000.)	11	(-1.0, -1.0)
	(300., 200.)	12	(2.0, 2.0)
	(-0.4, -1.0)	100	no conv.
	$\epsilon = 10^{-5}$		
	(-0.9, -0.8)	9	(2.0, 2.0)
	(-0.4, -1.0)	9	(2.0, 2.0)
C	(5.0, 70.0)	6	(2.0, 2.0)
	(200.0, 300.0)	12	(2.0, 2.0)
	(-1.1, -0.9)	25	(-11610.9, -6699281) div.
	$\epsilon = 10^{-4}$, $c_1 = .8$, $c_2 = 1.2$		
	(-0.9, -0.8)	136	(2.0, 2.0)
	(-0.5, -0.6)	77	(2.0, 2.0)
	(-0.2, -1.0)	38	(2.0, 2.0)
AA	$\epsilon = 10^{-3}$, $c_1 = .8$, $c_2 = 1.2$		
	(5., 70.)	12	(2.0, 2.0)
	(20., 0.0)	15	(2.0, 2.0)
	(50., 80.)	13	(2.0, 2.0)

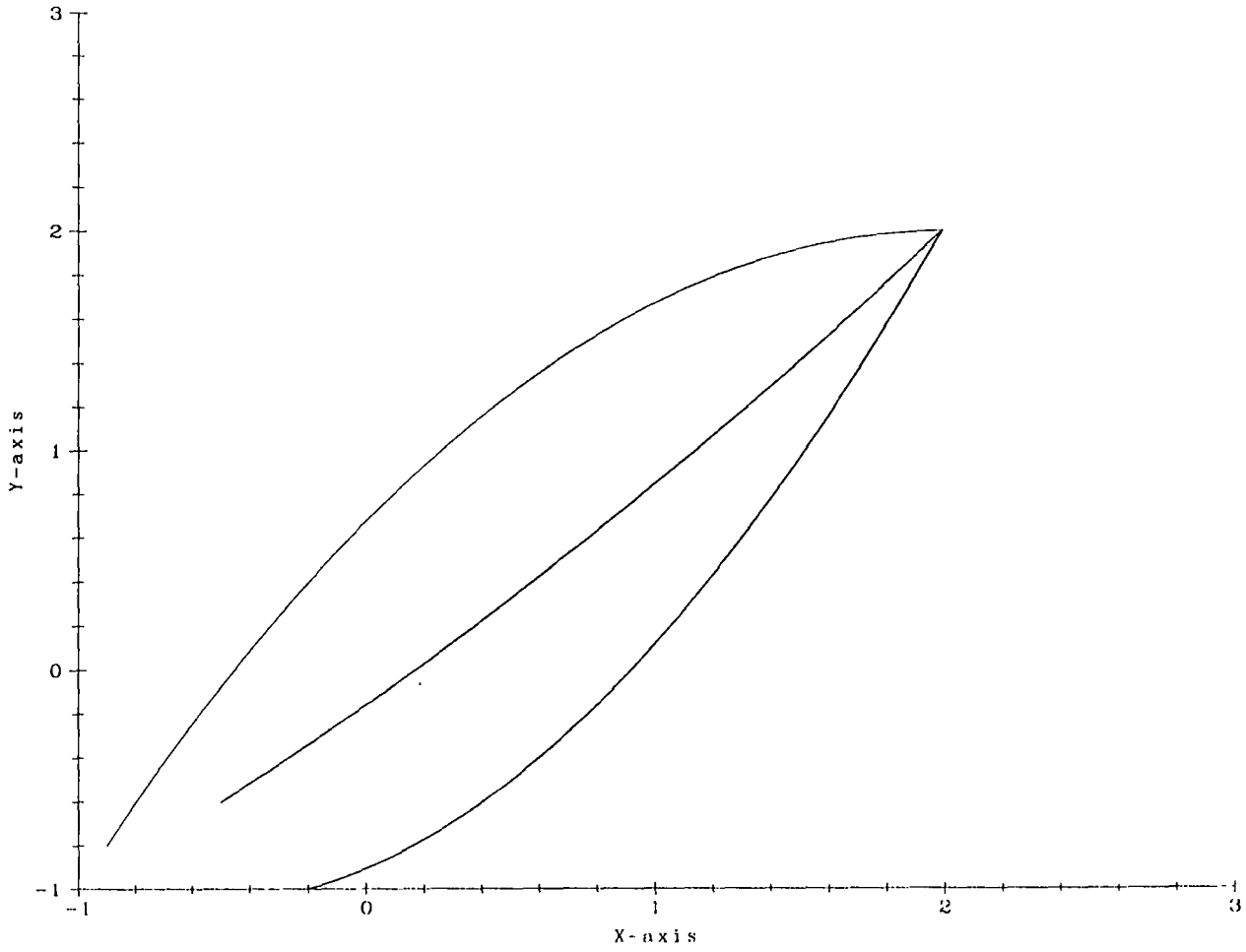

Figure 19. Several Solution Curves of the Second Problem That Crosses the Line x = 1/2 where J(x) = 0 Obtained by Algorithm AA

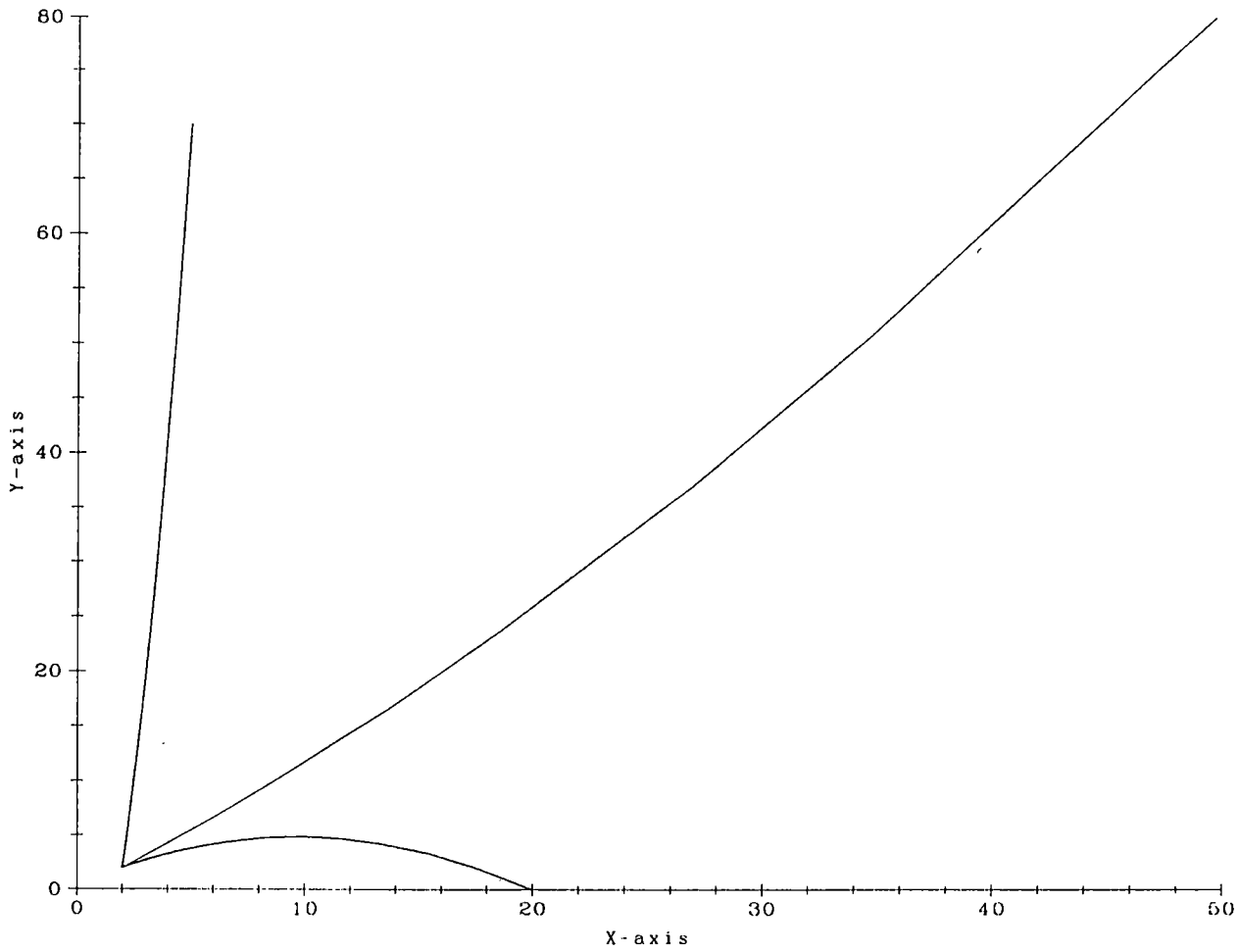

Figure 20. Several Solution Curves of the Second Problem With Starting Points Where J(x) > 0 Obtained by Algorithm AA

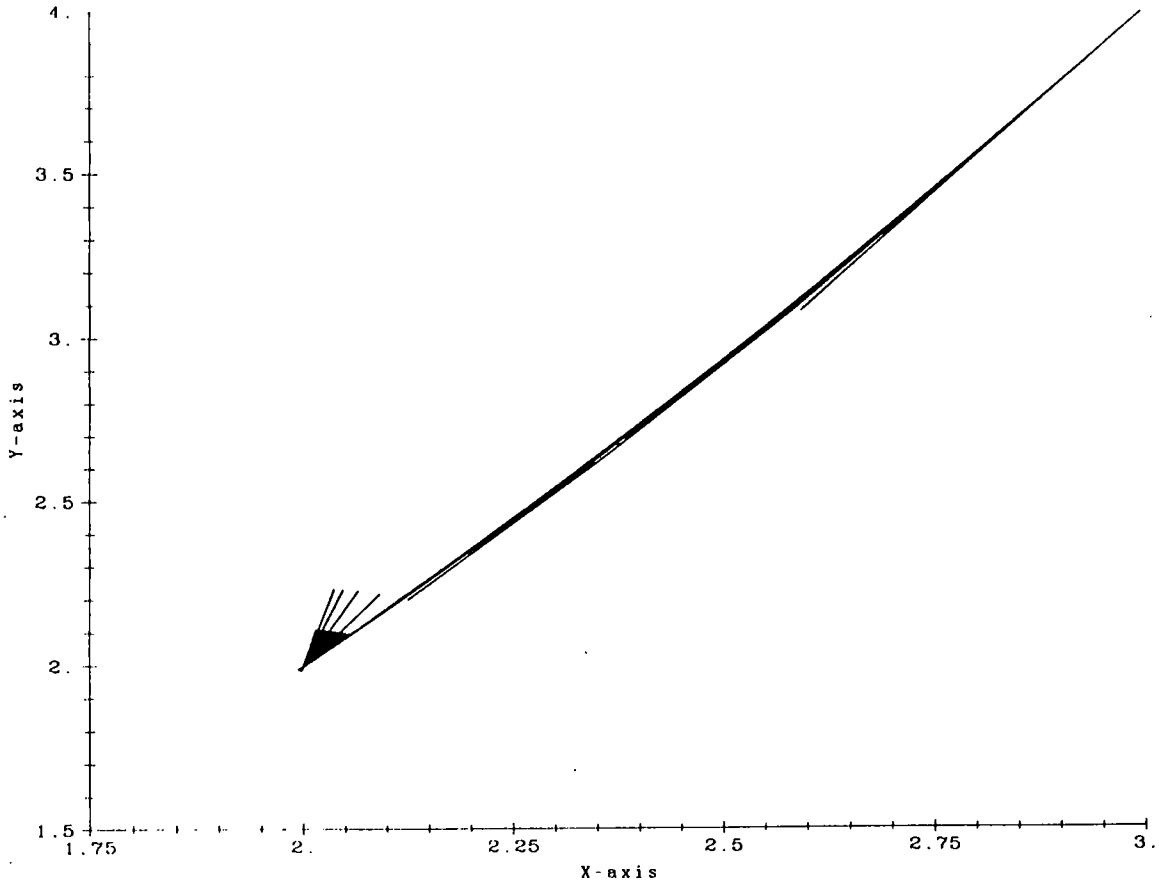

Figure 21. Several Solution Curves of the Second Problem Obtained by Algorithm A

(iii) When the starting points of these algorithms are at points where $J(x) < 0$, it should be noted that both Algorithms AA and C converge to the zero (2.0, 2.0) for $x \geq -0.9$, but they diverge for $x \leq -1.1$. On the contrary, when Algorithm B converges, it does so but to the second zero of (5.20), namely to (-1.0, -1.0). Moreover, note here that Algorithm B did not converge when the starting point lies in the rectangle $-0.4 \leq x \leq 0.4$ and $-1.5 \leq y \leq -0.6$.

(iv) Interestingly enough, when the starting points of both Algorithms AA and C are at points where $J(x) < 0$ and these algorithms converge to the zero (2.0, 2.0), the solution curves of the IVP correspond to system (5.20) must cross the line $x = 1/2$ where $J(x) = 0$, but this causes no problem for both algorithms. One can see how these solution curves jump over the line $x = 1/2$ in the case of Algorithm AA from Figure 19.

The third problem that was used in computations is the following system given by Hirsch and Smale in [29].

$$\begin{aligned} f_1(x, y) &= x^3 - 3xy^2 + 25(2x^2 + xy) + y^2 + 2x + 3y \\ f_2(x, y) &= 3x^2y - y^3 - 25(xy - y^2) + 4x^2. \end{aligned} \tag{5.21}$$

A summary of the computational results of this problem is given in Table III.

Again, one may come up with several remarks over the results of Table III:

TABLE III

SUMMARY OF THE RESULTS OF THE THIRD PROBLEM

Alg.	Initial Values	No. Iterations	Zeros and Notes
	$\epsilon = 10^{-6}$		
B	(100.0, -30.0)	6	(50.46500, -37.263)
	(1.0, 200.0)	11	(0.62774, 22.244)
	(200.0, 50.0)	9	(36.05400, 36.807)
	(-200.0, -50.0)	9	(-50.39700, -.80424)
	(-1.0, -500.0)	100	no conv.
	$\epsilon = 10^{-5}$		
C	(1.0, 200.0)	12	(.62774, 22.244)
	(200.0, 50.0)	10	(36.045, 36.807)
	(-200.0, -50.0)	10	(-50.397, -.80724)
	(-1.0, -500.0)	35	(50.465, -37.263)
	$\epsilon = 10^{-5}$, $c_1 = .8$, $c_2 = 1.2$		
AA	(200.0, -20.0)	288	(50.465, -37.263)
	(1.0, 200.0)	38	(.62774, 22.244)
	(200.0, 50.0)	202	(36.045, 36.807)
	(-200.0, -50.0)	64	(-50.397, -.80424)
	(-1.0, -500.0)	151	(.62774, 22.244)

(i) Both Algorithms B and C took almost the same number of iterations to converge to the zeros as indicated in Table III with one exception, that is, when both algorithms were started at the point (-1.0, -500.0) Algorithm B did not converge, while Algorithm C converged to the zero (50.465, -37.263). On the other hand, when Algorithm B was started at the point (100.0, -30.0), it did converge to the above zero.

(ii) Algorithm AA did converge for all cases, but was much slower than Algorithms B and C. A possible reason for this might be the stiffness of the solution curves obtained from system (5.21). Some of these solution curves are shown in Figures 22 to 24.

(iii) When Algorithm AA was started at the point (-1.0, -500.0) it converged to the zero (0.62774, 22.244), while Algorithm C when started at the same point converged to the zero (50.465, -37.263).

(iv) One should indicate here that one of the zeros of the system (5.21), namely, (36.0454, 36.8075) also was reported by Hirsch and Smale in [27], but there is a little bit of difference in the second coordinate of the zero. In fact, the answer they reported is (36.0454, 36.8056).

The fourth problem that was used in computations is the following third order system:

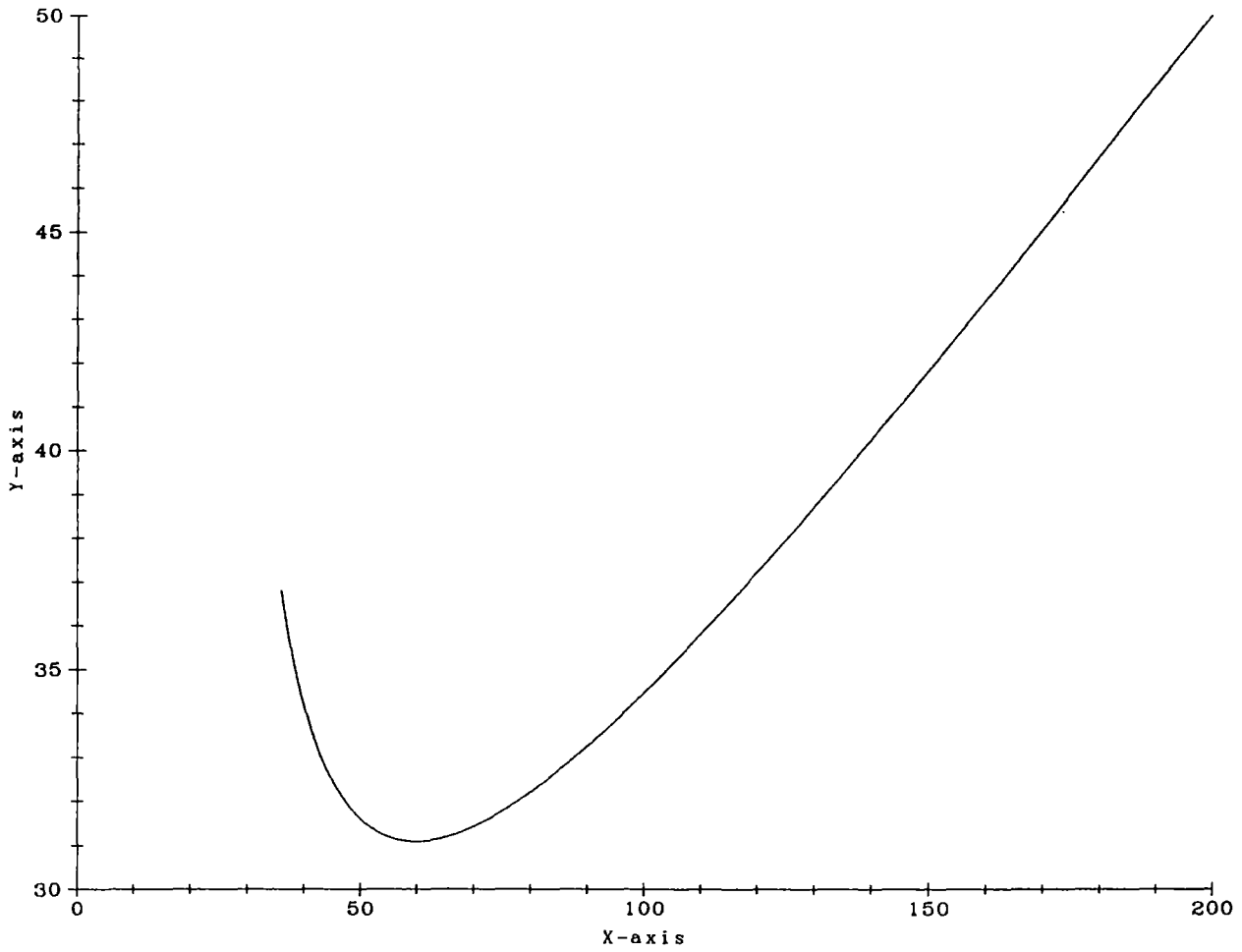

Figure 22. The Solution Curve of the Third Problem Obtained by Algorithm AA Starting at (200.,50.)

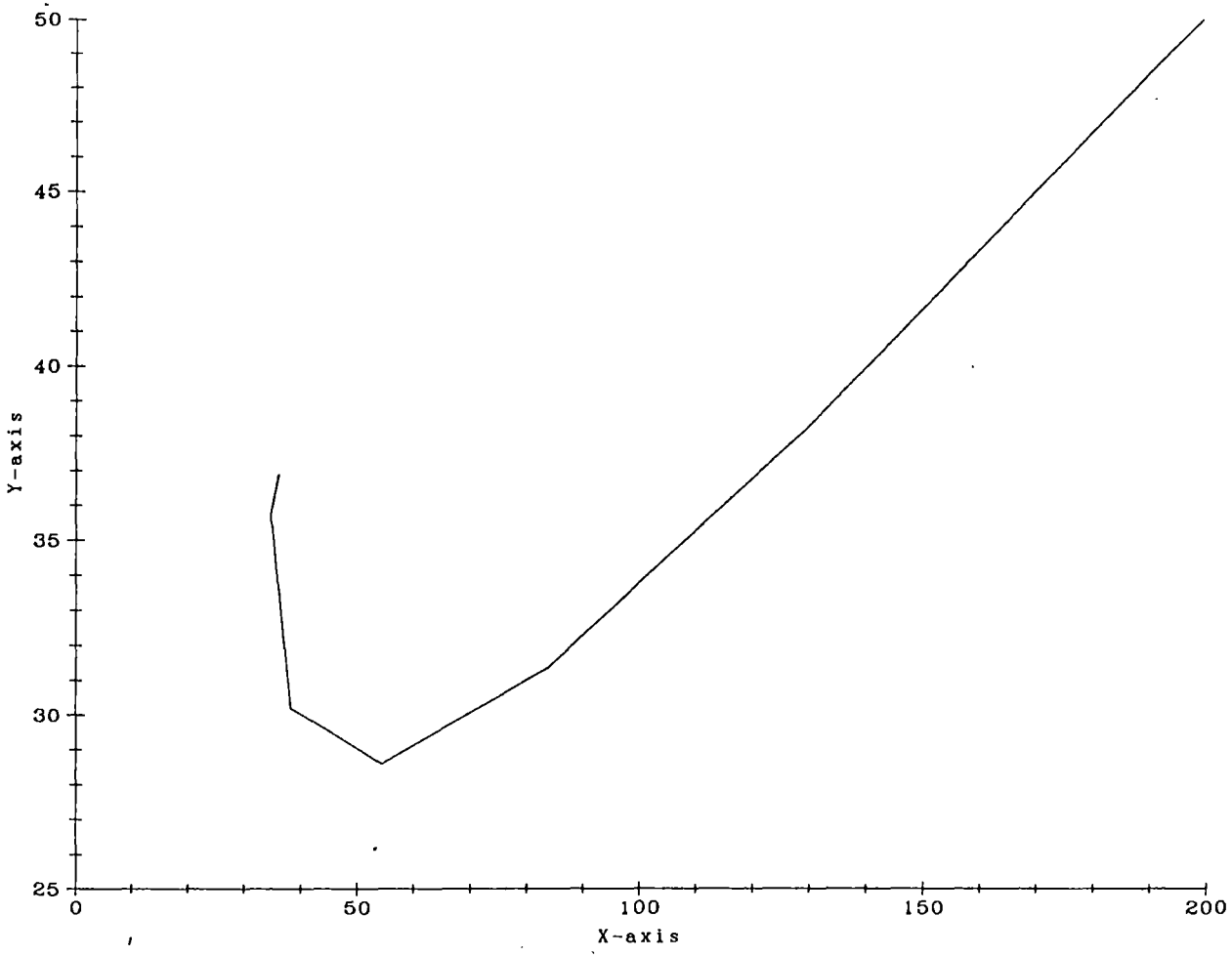

Figure 23. The Solution Curve of the Third Problem Obtained by Algorithm C Starting at (200.,50.)

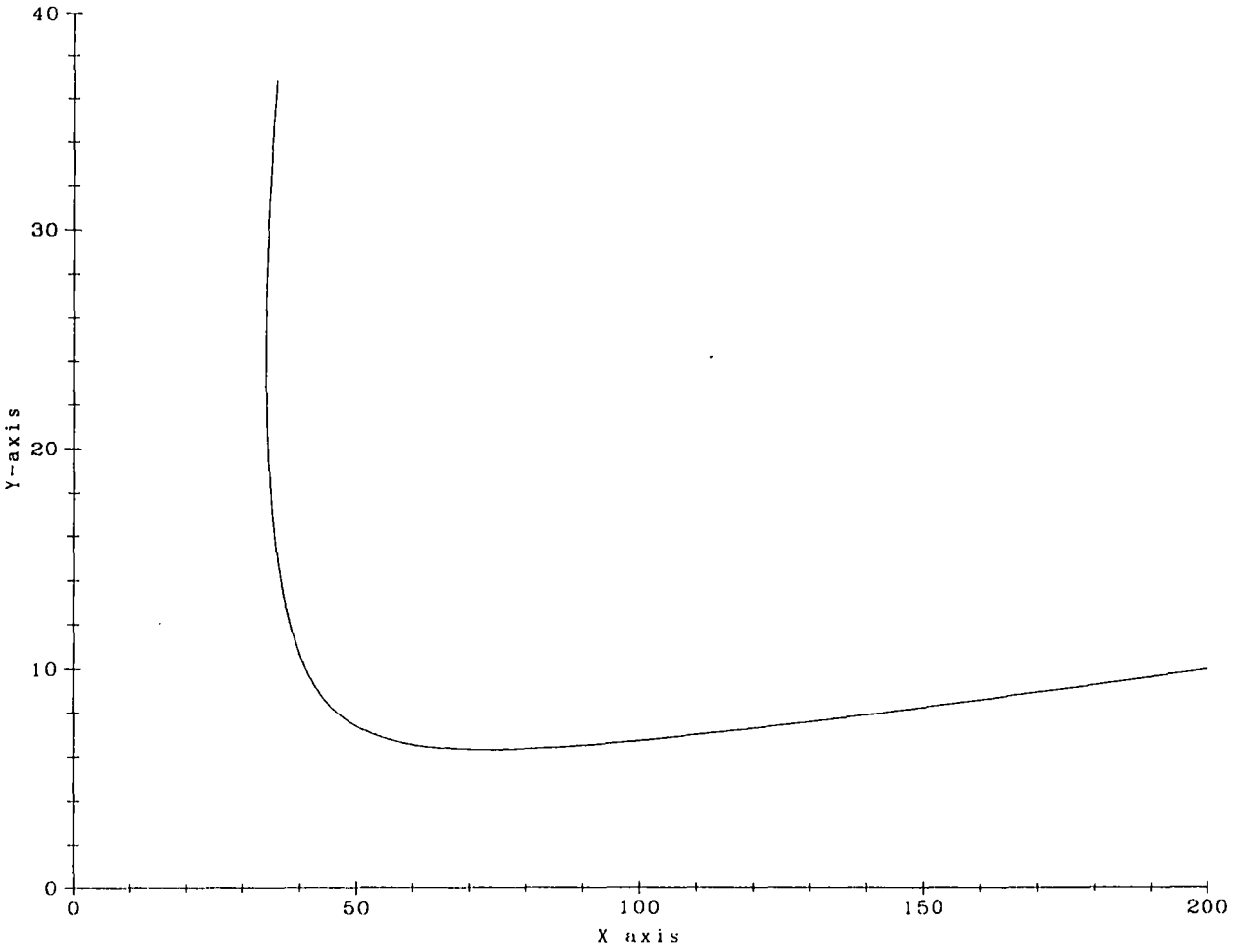

Figure 24. The Solution Curve of the Third Problem Obtained by Algorithm AA Starting at (200.,10)

$$
\begin{aligned}
f_1(x, y, z) &= x - \ln(y/z) - 1 \\
f_2(x, y, z) &= 2x^2 + y - z^2 - 0.4 \\
f_3(x, y, z) &= xy/20 - z + 2.
\end{aligned}
\tag{5.22}
$$

When Algorithm AA was started at the points (-15.0, 4.0, 5.0) and (-30.0, 4.0, 5.0) with $\epsilon = 10^{-4}$, $c_1 = .8$, $c_2 = 1.2$, it took 123 iterations to converge to the zero (-1.4453, 0.17231, 1.9875). On the contrary, Algorithm C did not converge when it was started at the above points and many others.

The last problem that was used in this computation is the following fourth order system which was reported in [15].

$$
\begin{aligned}
f_1(x_1, x_2, x_3, x_4) &= (x_1 - 0.1)^2 + x_2 - 0.1 \\
f_2(x_1, x_2, x_3, x_4) &= (x_2 - 0.1)^2 + x_3 - 0.1 \\
f_3(x_1, x_2, x_3, x_4) &= (x_3 - 0.1)^2 + x_4 - 0.1 \\
f_4(x_1, x_2, x_3, x_4) &= (x_4 - 0.1)^2 + x_1 - 0.1.
\end{aligned}
\tag{5.23}
$$

The computational results obtained from using Algorithms AA and C to solve system (5.23) are given in Table IV.

From Table IV, one may remark the following:

For the zero (-.9, -.9, -.9, -.9), even though Algorithm AA did not converge when started at the point (0.0, 0.0, 0.0, 0.0), it converged to the above zero, and so did Algorithm C when both algorithms were started at the point (-0.1, 0.0, 0.0, 0.0). On the contrary, when

TABLE IV

SUMMARY OF THE RESULTS OF THE FIFTH PROBLEM

Alg.	Initial Values	No. Iterations	Zeros and Notes
	$\epsilon = 10^{-5}$		
	(0.0, 0.0, 0.0, 0.0)	13	(-.9, -.9, -.9, -.9)
C	(-1.0, 0.0, 0.0, 0.0)	14	(-.9, -.9, -.9, -.9)
	(200., 300., 400., 100.)	0	div.
	$\epsilon = 10^{-3}$, $c_1 = .8$, $c_2 = 1.2$		
	(0.0, 0.0, 0.0, 0.0)	0	div.
	(-1.0, 0.0, 0.0, 0.0)	39	(-.9, -.9, -.9, -.9)
AA	$\epsilon = 10^{-7}$, $c_1 = .8$, $c_2 = 1.2$		
	(200., 300., 400., 100.)	298	(0.1, 0.1, 0.1, 0.1)

Algorithm C was started at the point (200.0, 300.0, 400.0, 100.0) and many other points too, it did not converge to the second zero, namely (0.1, 0.1, 0.1, 0.1). The reason might be due to the inability of Algorithm C to change its step size fast enough so that it stays close to the solution curve. This also might justify the small tolerance and many iterations used by Algorithm AA.

Computational results and the performance of Watson's and Li and Yorke's algorithms can be found in [50] and [38], respectively.

CHAPTER VI

SUMMARY AND CONCLUSIONS

The aim of this study was to explore the theory and algorithms based on the homotopy methods for solving smooth nonlinear systems of equations.

In Chapter I the precise statement of the problem at hand was stated, and at the same time the necessary background materials were given.

In Chapter II, an alternative definition to Hirsch and Smale's vector field was given. By means of this vector field an IVP was obtained. The solution curves of this IVP were used in Chapter V to find zeros of the map f.

Chapter III was devoted to homotopy methods that find certain types of fixed points of nonlinear maps.

In Chapter IV the relationship between the global Newton and the global homotopy methods was studied.

Finally, in Chapter V several algorithms based on the continuous Newton and the homotopy methods were described, and at the same time a new algorithm was given.

As it was pointed out earlier in Chapter V, there are many possibilities for modifying some of these algorithms. Also, a comparison in performance between these algorithms

and their applicability to certain types of problems are some of the points yet to be explored.

The rate of convergence of all these algorithms has not been studied. It is yet to be determined by further investigation what is the rate of convergence of each of these algorithms.

In Chapter IV it was shown how the global homotopy method may be used to determine several zeros of a nonlinear map by means of following a single solution curve of an IVP, but no algorithm based on this method was given. It would be of interest to develop and test algorithms based on this method and, at the same time, others similar to those algorithms reported in Chapter V.

The subject of using an approximation to the Jacobian matrix in Hirsch and Smale's algorithms has not been studied. It would be of interest to investigate this subject and seek a comparison in the performance of these algorithms when such an approximation takes place.

Another subject which has not been investigated is the sparsity of the Jacobian matrix in the algorithms based on the continuous Newton method in particular and the homotopy methods in general. It would be very interesting to see what is the effect of the sparsity of the Jacobian matrix on the cost of solving the linear systems which arise at each new point on the solution curves.

Finally, it would be desirable to study the performance of the algorithms based on the continuous method in very large problems.

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VITA 2

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