HOMOTOPY METHODS AND GLOBAL CONVERGENCE

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PREFACE

This Proceedings presents refereed versions of most of the papers presented at the NATO Advanced Research Institute on Homotopy Methods and Global Convergence held in Porto Cervo, Sardinia, June 3-6, 1981. This represents the fourth recent occurrence of an international conference addressing the common theme of fixed point computation. The first such conference, titled "Computing Fixed Points with Applications," was held in the Department of Mathematical Sciences at Clemson University, Clemson, South Carolina, June 26-28, 1974 and was sponsored by the Office of Naval Research and the Office of the Army Research Center. The second conference, "Symposium on Analysis and Computation of Fixed Points," was held at the University of Wisconsin, Madison, May 7-8, 1979, under the sponsorship of the National Science Foundation, the U.S. Army, and the Mathematics Research Center of the University of Wisconsin, Madison. The third conference, titled "Symposium on Fixed Point Algorithms and Complementarity," was held at the University of Southampton, Southampton, UK, July 3-5, 1979 and was sponsored by U.N.E.S.C.O., European Research Office (London), Department of Mathematics (University of Southampton), I.B.M. U.K., Ltd., Lloyds Bank, Ltd., and the Office of Naval Research (London).

The Advanced Research Institute held in Sardinia was devoted to the theory and application of modern homotopy methods. The following topics were stressed: Path-Following Techniques; Bottom-Line Applications; Global vs. Classical Methods; and State-of-the-Art, Perspectives and Potential. The papers presented were selected so as to devote more or less uniform attention to these four areas. In addition, workshop sessions were held on different days in each of these four subject areas. While the papers reproduced herein will serve to memorialize the formal presentations, the informal presentations and interactions during the workshops, in spite of their value, and in spite of the efforts of several members of the organizing committee to edit transcriptions, will not be documented. The stimulation provided by these interactions will hopefully be a source of future motivation for the participants and thus, indirectly, will be captured in their work.

A final and somewhat unique feature of this volume is a list of some computer codes currently in use for implementing the homotopy method. Descriptions of these codes have been provided by the originators. Researchers in the field who wish to profit from the existence of any of these codes may directly contact the author of the code.

I am indebted to the Systems Science Programme of the Scientific Affairs Division of NATO for their generous support of this Institute, to Professor Jean Abadie for his initial encouragement, to Professor Donald Clough for his many suggestions and thoughtful guidance, to the Organizing Committee, consisting of Professors Michael J. Todd, James Yorke, Heinz-Otto Peitgen, and Herbert E. Scarf, to all of the participants for their lively contributions, and finally to Ms. Maggie Newman for her grudging devotion and her many and varied contributions to the success of the Institute as well as the production of this Proceedings.

F. J. Gould, Director
Chicago, Illinois

CONTENTS

Piecewise Smooth Homotopies 1
J. C. Alexander, T.-Y. Li, and J. A. Yorke

Global Convergence Rates of Piecewise-Linear Continuation Methods: A Probabilistic Approach 15
J. C. Alexander and E. V. Slud

Relationships between Deflation and Global Methods in the Problem of Approximating Additional Zeros of a System of Nonlinear Equations 31
E. L. Allgower and K. Georg

Smooth Homotopies for Finding Zeros of Entire Functions 43
Jack Carr and John Mallet-Paret

Where Solving for Stationary Points by LCPs Is Mixing Newton Iterates 63
B. Curtis Eaves

On the Equivalence of the Linear Complementarity Problem and a System of Piecewise Linear Equations: Part II 79
B. C. Eaves and C. E. Lemke

Relations between PL Maps, Complementary Cones, and Degree in Linear Complementarity Problems 91
C. B. Garcia, F. J. Gould, and T. R. Turnbull

A Note on Stepsize Control for Numerical Curve Following 145
K. Georg

On a Class of Linear Complementarity Problems of Variable Degree 155
Roger Howe

Linear Complementarity and the Degree of Mappings 179
Roger Howe and Richard Stone

Sub- and Supersolutions for Nonlinear Operators: Problems of Monotone Type 225
Michael Prüfer

An Efficient Procedure for Traversing Large Pieces in Fixed Point Algorithms 239
R. Saigal

The Application of Fixed Point Methods to Economics 249
John B. Shoven

On a Theory of Cost for Equation Solving 263
Mike Shub and Steven Smale

Algorithms for the Linear Complementarity Problem Which Allow an Arbitrary Starting Point 267
Dolf Talman and Ludo Van der Heyden

Engineering Applications of the Chow-Yorke Algorithm 287
Layne T. Watson

Availability of Computer Codes for Piecewise-Linear and Differentiable Homotopy Methods 309

Index 317

PIECEWISE SMOOTH HOMOTOPIES

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1. INTRODUCTION

In [1, 2, 3, 7, 14, 16] there is developed a class of continuation methods for solving nonlinear systems of equations which have the feature that, under broad topological assumptions which guarantee the existence of solutions of the system, the methods are guaranteed with probability one to generate a curve which approaches arbitrarily close to a solution of the system. In the above papers it is assumed that the nonlinear system is defined by smooth functions. Piecewise linear techniques are similarly used; see for

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example [5]. The purpose of this paper is to develop path following methods for a class of problems including both piecewise linear and smooth systems of equations. We formulate the method for "piecewise smooth functions" on a "piecewise smooth domain," and we give similar guaranteed convergence results.

The concepts of piecewise smooth manifolds and functions can be defined in a variety of ways, to fit the problem at hand. In [1, Appendix 1], we announced preliminary results for the simplest useful version of these definitions. We adopt that version here.

As an illustration of the kinds of problems we want to be able to handle, we let B be the ball in R^n and let $f : B \to B$ be piecewise smooth in the sense defined in the next section. (In particular we assume f is continuous.) Following the homotopy approach formally we choose $z \in B$ and write the homotopy

$$F_z(x,t) = (1-t)z + tf(x) - x$$

where $t \in [0,1]$. The zeroes of $F_z(1,x)$ are the fixed points of f while z is the unique zero of $F_z(0,x)$. When f is smooth (C^2), it is shown in [3] that for almost every $z \in B$ a smooth path in $B \times [0,1]$ leads from $(0,z)$ to at least one zero at $t = 1$. The objective of this paper is to develop a corresponding theory which permits f to be piecewise smooth and to show there is a piecewise smooth path of zeroes of F_z that leads to a fixed point (or possibly to a larger set of fixed points) of f. The facts about the paths for F_z follow from the general theory we develop here, and we develop only enough theory for us to handle applications. We give applications to show how the piecewise smooth formulation can be used, and these are discussed in more detail. First we consider the nonlinear complementarity problem. We put it in our context and prove an existence result. The continuation method we develop is a nonlinear form of Lemke's algorithm. Second we consider nonlinear constrained optimization.

2. THE PIECEWISE SMOOTH FORMULATION

We set some notation. Let $\langle x,y\rangle$ denote the inner product in n-dimensional Euclidean space R^n. For $U \subset R^n$ an open set, we speak of smooth mappings $F : U \to R^m$ where "smooth" means C^k for k large ($k \geq 2$ is usually sufficient). If F is smooth, let $DF(x)$, for $x \in U$, denote the $m \times n$ matrix of first partial derivatives of F. Let $y \in R^p$, $z \in R^q$, $p + q = n$. We denote by F_z the map from a domain of R^p to R^m defined by holding z fixed in (y,z). We let $D_yF = DF_z$ be the derivative of F with respect to the y variables. Let $I = [0,1]$.

For convenience we recall the development in [1]. Let M be an n-dimensional topological manifold. Let $U_1,\ldots,U_I$ be a finite open cover of M. Each is to have a smooth structure compatible with its structure as an open topological submanifold of M (a <u>local smoothing</u> of M). Suppose for each $i \in \{1,\ldots,I\}$ there are defined smooth functions

$$\psi_{i,1},\ldots,\psi_{i,J} : U_i \to R$$

where $J = J(i)$, which satisfy the following transversality conditions:

i) 0 is a regular value of each $\psi_{i,j} : U_i \to R$, i.e., rank $(D\psi_{i,j}(x)) = 1$ if $\psi_{i,j}(x) = 0$;

ii) 0 is a regular value of each $\psi_{i,j} \times \psi_{i,k} : U_i \to R \times R$ if $j \neq k$; i.e., $\operatorname{rank}\begin{pmatrix} D\psi_{i,j}(x) \\ D\psi_{i,k}(x) \end{pmatrix} = 2$ if $\psi_{i,j}(x) = \psi_{i,k}(x) = 0$.

Thus the $\psi_{i,j}^{-1}(0)$ are codimension 1 submanifolds of M which meet pairwise transversally. For each i, let

$$V_i = \{x \in M : \psi_{i,j}(x) > 0 \quad \text{for} \quad j = 1,\ldots,J(i)\}.$$

We require that $V_i \cap V_{i'} = \phi$ if $i \neq i'$, that each $\overline{V}_i \subset U_i$ and that $M = \cup\overline{V}_i$. Such a collection of data we call a <u>piecewise smooth decomposition</u> of M. The V_i are to be pieces on which things are smooth. The edges of M_i consist of those x such that some $\psi_{i,j}(x) = 0$. The corners of M_i are those sets where for some i

$$\psi_{i,j}(x) = \psi_{i,k}(x) = 0$$

for some $j \neq k$. The V_i themselves are the regions or faces of the decomposition. Note that an edge point that is not a corner is either on the boundary of M or is an edge point for precisely two faces.

A continuous map $f : M \to R^n$ is called piecewise smooth if there is a collection of smooth functions $f_i : U_i \to R^n$ for $i = 1,\ldots,I$ such that $f|V_i = f_i$. Intuitively, f is smooth on each face V_i but can have sharp turns at the edges. Let $\pi : M \times I \to M$ be the projection. We define a piecewise smooth decomposition of $M \times I$ by letting $\tilde{U}_i = \pi^{-1}U_i$, $\tilde{\psi}_{i,j} = \psi_{i,j}\pi$. Thus $M \times I$ is decomposed by cylinders $V_i \times I$. Let A (the parameter manifold) be a smooth manifold. Now suppose $\phi : A \times M \to R^n$ is a smooth function and let $f_\alpha(x) = \phi(\alpha, x)$ for each $\alpha \in A$. Let $F_\alpha : M \times I \to R^n$ be defined by

$$F_\alpha(x,t) = (1-t)f_\alpha(x) + tf(x).$$

Similarly define $F_{i,\alpha} : U_i \times I \to R^n$ by

$$F_{i,\alpha}(x,t) = (1-t)f_\alpha(x) + tf_i(x).$$

We say $F_\alpha^{-1}(0)$ is transverse to the decomposition of $M \times I$ if for $t < 1$

t-0) 0 is a regular value of each $F_{i,\alpha} : U_i \times I \to R^n$

t-i) 0 is a regular value of each

$$F_{i,\alpha} \times \tilde{\psi}_{i,j} : U_i \times I \to R^n \times R$$

t-ii) 0 is a regular value of each

$$F_{i,\alpha} \times \tilde{\psi}_{i,j} \times \tilde{\psi}_{i,k} : U_i \times I \to R^n \times R \times R \quad \text{for} \quad j \neq k.$$

Condition t-0) implies that each $F^{-1}_{i,\alpha}(0)$ is a smooth curve and thus $F^{-1}_{\alpha}(0)$ is a piecewise smooth curve. Condition t-i) implies that each $F^{-1}_{i,\alpha}(0)$ intersects each edge transversally. Condition t-ii) implies $F^{-1}_{i,\alpha}(0)$ contains no corner points.

Recall that $\phi : A \times M \to R^n$ is <u>sufficient</u> if rank $D_{\alpha}\phi(\alpha,x) = n$ for all (α,x). The following is the main result. A proof is sketched in [1]. It is standard, except that extra care has to be taken at the edges and corners.

<u>Theorem 1</u>. <u>If $\phi : A \times M \to R^n$ is sufficient, the set $F^{-1}_{\alpha}(0)$ is transverse to the decomposition with probability 1 in α (i.e., for a full residual set of α).</u>

Thus with probability 1, $C = C_{\alpha} = F^{-1}_{\alpha}(0)$ is a piecewise smooth curve intersecting edges transversally and corners not at all. In applications, one follows C from the $t = 0$ level to a solution of $f(x) = 0$ at $t = 1$.

3. EXAMPLES

Since most applications concern maps $f : R^n \to R^n$, the basic manifold M is R^n. We present the orthant piecewise smooth decomposition. It is an easy one to visualize and is used in the application of the next section.

Let i range over the 2^n subsets of the integers $1,\ldots,n$. For each i, let $U_i = R^n$. Let each $J(i) = n$. Let

$$\psi_{i,j}(x_1,x_2,\ldots,x_n) = \begin{cases} x_j & j \in i, \\ -x_j & j \notin i. \end{cases}$$

Note that

$$D\psi_{i,j}(x_1,\ldots,x_n) = (0,\ldots,0,\pm1,\ldots,0)$$

(here the ±1 is in the jth position) and

$$D(\psi_{i,j} \times \psi_{i,k})(x_1,\ldots,x_n) = \begin{pmatrix} 0,\ldots,0,\pm 1,0,\ldots,0,0,0,\ldots,0 \\ 0,\ldots,0,0,0,\ldots,0,\pm 1,0,\ldots,0 \end{pmatrix}$$

(here the ± 1 are in the <u>jth</u> <u>kth</u> columns).

Thus conditions (i), (ii) are satisfied and we have defined a piecewise smooth decomposition of R^n, the <u>orthant</u> decomposition. Note

$$V_i = \{(x_1,\ldots,x_n) : x_j > 0 \text{ if } j \in i \text{ and } x_j < 0 \text{ if } j \notin i\}.$$

The edges are the coordinate hyperplanes and the corners are where two or more coordinate hyperplanes intersect. If a curve C is transverse to the orthant decomposition (or its product with I), at each edge exactly one coordinate of the position vector of C changes sign.

The orthant decomposition is of course actually piecewise linear, and it could be hoped a simpler theory could be used. However, we are considering functions that are not piecewise linear, and it seems the full concept of piecewise smooth manifolds is needed. Of course, an actual implementation might benefit from the simplicity of the orthant decomposition.

The definition is flexible enough to accommodate manifolds with "sharp bends". For example, the surface of a cube in three-dimensional space is topologically equivalent to the surface of a sphere, however, the surface of the cube has a different piecewise differentiable structure.

To illustrate in more detail, we consider the simplest case. Suppose M is the union of the non-negative parts of the two-dimensional space:

$$M = \{(x,y) : x \geq 0 \text{ or } y \geq 0\}.$$

We put the natural piecewise differentiable structure on M. Let $U_1 = U_2 = M$. Both U_i are to be smoothly like R^1 via the homeomorphism $h : U_i \to R^1$:

$$h(x,0) = x,$$

$$h(0,y) = -y.$$

Then the functions $\psi_1 : U_1 \to R^1$, $\psi_2 : U_2 \to R^1$:

$$\psi_1(x,0) = x, \qquad \psi_2(x,o) = -x,$$

$$\psi_1(0,y) = -y, \qquad \psi_2(0,y) = y$$

are smooth. The required conditions on the ψ_i are satisfied. The faces V_1, V_2 are respectively the positive x- and y-axes. The sole edge is the origin.

A function on M defines a piecewise smooth function if it is smooth on each axis (using one-sided derivatives at the origin). Each of the two pieces of the function—one on each axis—can be extended smoothly to all of the U_i. Note that the U_i are technical artifacts. For manifolds with sharp bends, the key requirement for piecewise smooth functions is that good one-sided derivatives exist at the edges. The example we present of constrained optimization is a more complicated case in point.

4. NONLINEAR COMPLEMENTARITY

Let $g : R^n \to R^n$ be smooth. The complementarity problem is to find an $x \in R^n$ such that

$$x \geq 0, \qquad g(x) \geq 0, \qquad \langle x,g(x)\rangle = 0.$$

If $s \in R$, let $s^+ = \max(0,s)$, $s^- = \min(0,s)$ and if $x = (x_1,\ldots,x_n) \in R^n$, let $x^\pm = (x_1^\pm,\ldots,x_n^\pm)$. We write $x < y$ if each $x_i < y_i$, $i = 1,\ldots,n$. Let $R^n_\pm = \{x : x^\pm = x\}$. Consider the map $f : R^n \to R^n$ defined by

$$f(x) = x^- + g(x^+).$$

If $f(x_0) = 0$ for some $x_0 \in R^n$, then x_0^+ is a solution of the complementarity problem associated with f. For $f(x_0) = 0$ implies

$$0 = \langle x_0^+, f(x_0)\rangle = \langle x_0^+, x_0^-\rangle + \langle x_0^+, g(x_0^+)\rangle = \langle x_0^+, g(x_0^+)\rangle$$

and $g(x_0^+) = -x_0^- \geq 0$.

Moreover, note that $f(x)$ is piecewise smooth with respect to the orthant subdivision of R^n. So we set $\phi : R^n \times R^n \to R^n$ as $\phi(z,x) = x^- - z$. Thus the homotopy

$$F_z(x,t) = tg(x^+) + x^- - (1-t)z.$$

Since $-D_z\phi$ is the identity matrix, ϕ is sufficient. Thus for almost all z, $F_z^{-1}(0)$ is a piecewise smooth curve transverse to the decomposition. Let $C = C_z$ be the component continuing $(z,0)$. To ensure the curve converges to a solution, we use a variation of a condition of Eaves [4]. Related conditions are in [5, 8, 11, 12, 17].

Eaves' condition is: for a non-empty open set Ω of $z > 0$, there is a bounded set $U(z)$ which intersects any closed unbounded connected set in R_+^n which contains 0 (i.e., $U(z)$ <u>separates</u> 0 from ∞ in R_+^n), and such that for each $x \in U(z)$ there is $w \in R_+^n$ such that

$$\langle x-w, z\rangle > 0 \text{ and } \langle x-w, g(x)\rangle \geq 0.$$

Let $-\Omega = \{z \in R_-^n : -z \in \Omega\}$.

<u>Theorem 2</u>. <u>Suppose Eaves' condition holds. For almost all</u> $z \in -\Omega$, <u>the curve</u> $C = C_z$ <u>is a piecewise smooth curve containing</u> $(z,0) \in R^n \times I$ <u>and eventually remaining arbitrarily close to the (non-empty) set</u> $\{(f^{-1}(0),1)\} \subset R^n \times I$.

<u>Proof</u>. We need only prove the last statement. First note that if $(x,0) \in C$, then $x = z$. This is because $x^- = z$, thus all components of x^- are non-zero and $x^+ = 0$. Thus C cannot return to the $t = 0$ level. Next we show C is bounded. If not, there exist (x,t) on C with either $|x^+| \to \infty$ or $|x^-| \to \infty$. Suppose

$|x^+|$ remains bounded. Then $x^- = -tg(x^+) + (1-t)z$ also remains bounded. Thus $|x^+| \to \infty$. Consider the set $U(-z)$ from Eaves' condition. It is bounded, say it is contained in the ball of radius $\frac{1}{2}P$. The set

$$C^+ = \{x^+ : (x,t) \in C\}$$

is unbounded and connected in R^n_+ and contains 0. There is some $t_0 < 1$ such that $(x_0,t_0) \in C$ with $|x_0^+| > P$. Consider the set

$$C_0^+ = \{x^+ : (x,t) \in C,\ t \le t_0\} \cup \{x^+ \in R^n_+ : |x^+| \ge P\}.$$

It is a closed, unbounded, connected set in R^n_+ which contains 0. By Eaves' condition, the set $U(-z)$ intersects C_0^+. So, there is $(x,t) \in C$ such that $x^+ \in U(-z)$. Let $w \ge 0$ be as in Eaves' condition. Then

$$\begin{aligned} 0 = \langle F_z(x,t), x^+-w\rangle &= t\langle g(x^+), x^+-w\rangle + \langle x^-, x^+-w\rangle - (1-t)\langle z, x^+-w\rangle \\ &= t\langle g(x^+), x^+-w\rangle - \langle x^-, w\rangle - (1-t)\langle z, x^+-w\rangle \\ &> 0 \end{aligned}$$

since $t < 1$. Thus C must remain bounded. The rest of the argument is standard (e.g. [7], Theorem 2.2).

5. CONSTRAINED OPTIMIZATION

Let $f(x)$ and $g_i(x)$, $1 \le i \le m$ be smooth real valued functions on R^n. We consider the nonlinear programming problem:

$$\underline{\text{minimize}}\ f(x)\ \underline{\text{with}}\ g_i(x) \le 0.$$

As is well known [10] if x^* is a solution of this problem, there exist numbers λ_j, $1 \le j \le m$ (Lagrange multipliers) such that

$$\text{(5.1)}\quad \begin{aligned} &Df(x^*) + \sum_1^m \lambda_j Dg_j(x^*) = 0 \\ &g_j(x^*) \le 0, \quad \lambda_j \ge 0, \quad \lambda_j g_j(x^*) = 0, \quad 1 \le j \le m. \end{aligned}$$

This formulation is the one actually solved. To show x^* is actually a minimum usually requires further checking. Homotopy methods for solving such non-linear problems have been developed in [9, 13, 15].

Equations (5.1) look something like a complementarity problem. That observation leads to the following homotopy method. Consider the mapping $G : R^{n+m} \to R^{n+m}$ defined by

$$G(x,\lambda) = \begin{pmatrix} Df(x) + \sum_1^m \lambda_j^+ Dg_j(x) \\ \\ \lambda_i^- - g_i(x) \end{pmatrix}_{1 \le i \le m}.$$

Then (5.1) holds if $G(x,\lambda) = 0$. Moreover, G is piecewise smooth with respect to the orthant decomposition of R^{n+m}. Let

$$\Omega = \{x \in R^n : g_i(x) < 0 \quad i = 1,\dots,m\}.$$

Assume $\Omega \neq \phi$. Consider the homotopy $F : \bar{\Omega} \times R^{n+m} \times I \to R^{n+m}$ defined by

$$F(z,x,\lambda,t) = \begin{pmatrix} t[Df(x) + \sum_1^m \lambda_j^+ Dg_j(x)] + (1-t)(x-z) \\ \\ \lambda_i^- - g_i(x) \end{pmatrix}_{1 \le i \le m}.$$

This would seem to give a reasonable homotopy algorithm. However, as is, it cannot be proved to be by the general theory. The reason is that DF_z never has full rank; the last m rows are always zero. Indeed z ranges over an n-dimensional set and the range is $(m+n)$-dimensional. The problem is that the constraints $\lambda_i^- - g_i(x) = 0$ are independent of z. For certain innocuous g_i (e.g., some $g_i(x) = x_i$), there are families of curve with segments totally contained within edges of the orthant decomposition.

We overcome this problem by reinterpreting the homotopy problem on an n-dimensional manifold, although an implementation can use the above F directly.

We need a standard condition on the g_i. For any $x \in \bar{\Omega}$, let $I(x) = \{i : g_i(x) = 0\}$. We assume: for any x, the vectors $(Dg_i(x))_{i \in I(x)}$ are linearly independent.

Let

$$M = \{(x,\lambda) : g_i(x) \le 0, \quad \lambda_i \ge 0, \quad \lambda_i g_i(x) = 0, \quad 1 \le i \le m\}.$$

It is straightforward, using the above condition, to put a piecewise smooth structure on M so that the following sets V_I are the regions. Let $I \subset \{1,\ldots,m\}$ be an arbitrary subset (possibly empty). Then

$$V_I = \{(x,\lambda) : g_i(x) = 0 \text{ for } i \in I, \quad \lambda_j = 0 \text{ for } j \notin I\}.$$

Thus the manifold M incorporates the constraints $g_i(x) \le 0$ in its definition. The homotopy F on M becomes

$$F(z,x,\lambda,t) = t[Df(x) + \sum_1^m \lambda_i Dg_i(x)] + (1-t)(x-z).$$

This homotopy has the standard form with $\phi(x,z) = x - z$. It is trivial that ϕ is sufficient; thus for almost all $z \in \Omega$, the set $F_z^{-1}(0)$ is a piecewise smooth curve. It is precisely the curve obtained from the earlier homotopy; we now know for almost all z it is well-behaved at edges and misses corners.

To get a convergence result, we impose rather standard conditions. Assume $\bar{\Omega}$ is convex. Assume there is a compact set $A \subset R^n$ such that for $x \notin A$,

$$\langle x, Df(x)\rangle > 0, \quad \langle x, Dg_i(x)\rangle > 0, \qquad i = 1,\ldots,m.$$

Theorem 3. Under these assumptions and the assumption on the $Dg_i(x)$, for almost all $z \in \Omega$, the set $C = F_z^{-1}(0)$ is a piecewise