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Continuation and path following

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The main ideas of path following by predictor–corrector and piecewise-linear methods, and their application in the direction of homotopy methods and nonlinear eigenvalue problems are reviewed. Further new applications to areas such as polynomial systems of equations, linear eigenvalue problems, interior methods for linear programming, parametric programming and complex bifurcation are surveyed. Complexity issues and available software are also discussed.

CONTENTS

1. Introduction

Continuation, embedding or homotopy methods have long served as useful theoretical tools in modern mathematics. Their use can be traced back at least to such venerated works as those of Poincaré (1881–1886), Klein (1882–1883) and Bernstein (1910). Leray and Schauder (1934) refined the tool and presented it as a global result in topology, viz. the homotopy invariance of degree. The use of deformations to solve nonlinear systems of equations may be traced back at least to Lahaye (1934). The classical embedding

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methods were the first deformation methods to be numerically implemented and may be regarded as a forerunner of the predictor–corrector methods for path following which we will discuss here.

Because of their versatility and robustness, numerical continuation or path following methods have now been finding ever wider use in scientific applications. Our aim here is to present some of the recent advances in this subject regarding new adaptations, applications, and analysis of efficiency and complexity. To make the discussion relatively self-contained, we review some of the background of numerical continuation methods. Introductions into aspects of the subject may be found in the books by Garcia and Zangwill (1981), Gould and Tolle (1983), Keller (1987), Rheinboldt (1986), Seydel (1988) and Todd (1976a). The philosophy and notation of the present article will be that of our book Allgower and Georg (1990), which also contains an extensive bibliography up to 1990.

The viewpoint which will be adopted here is that numerical continuation methods are techniques for numerically approximating a solution curve c which is implicitly defined by an underdetermined system of equations. In the literature of numerical analysis, the terms *numerical continuation* and *path following* are used interchangeably.

There are various objectives for which the numerical approximation of c can be used and, depending upon the objective, the approximating technique is adapted accordingly. In fact, continuation is a unifying concept, under which various numerical methods may be subsumed which may otherwise have very little in common. For example, simplicial fixed point methods for solving problems in mathematical economics, the generation of bifurcation diagrams of nonlinear eigenvalue problems involving partial differential equations, and the recently developed interior point methods for solving linear programming problems seem to be quite unrelated. Nevertheless, there is some benefit in considering them as special cases of path following. We personally are struck by the remarkable fact that a technique which was initially developed for solving difficult nonlinear problems now turns out to be extremely useful for treating various problems which are essentially linear: e.g. linear eigenvalue problems, and linear programming and complementarity problems.

The remainder of the article is organized as follows. Section 2 contains the basic ideas of predictor–corrector path following methods. In Section 3 some technical aspects of implementing predictor–corrector methods are addressed, e.g. the numerical linear algebra involved and steplength strategies.

Section 4 deals with various applications of path following methods. We begin with a brief discussion of homotopy methods for fixed point problems and global Newton methods. Then we address the problem of finding multiple solutions. In particular, we discuss recent homotopy methods for finding all solutions of polynomial systems of equations. Next we survey some path

following aspects of nonlinear eigenvalue problems, and address the question of handling bifurcations. Finally, three new developments in path following are discussed: (1) The solution of linear eigenvalue problems via special homotopy approaches; (2) the handling of parametric programming problems by following certain branches of critical points via active set strategies; and (3) the path following aspects involved in the interior point methods for solving linear and quadratic programming problems.

Section 5 presents an introduction to the principles of piecewise linear methods. These methods view path following in a different light: instead of approximately following a smooth solution curve, they exactly follow an approximate curve (i.e. a polygonal path). Some instances where these methods are useful are discussed, e.g. linear complementarity problems or homotopy methods where predictor–corrector methods are not implementable, because of lack of smoothness. We also briefly address the related topic of approximating implicitly defined surfaces.

The issue of the computational complexity of path following is considered in Section 6. This issue is related to the Newton–Kantorovich theory and is currently of considerable interest in the context of interior point methods.

We conclude by listing some available software related to path following and indicate how the reader might access these codes. No attempt to compare or evaluate the various codes is offered. In any case, our opinion is that path following codes always need to be considerably adapted to the special purposes for which they are designed. The path following literature offers various tools for accomplishing such tasks. Although there are some general purpose codes, probably none will slay every dragon.

The extensive bibliography contains only cited items. Space considerations prohibited the addressing of some important topics, and consequently some significant recent contributions to the field are not contained in the bibliography.

2. The basics of predictor–corrector path following

The simplest (and most frequently occurring) case of an underdetermined system of nonlinear equations contains just one degree of freedom:

$$H(u) = 0 \text{ where } H : \mathbb{R}^{N+1} \to \mathbb{R}^N \text{ is a smooth map.} \tag{2.1}$$

When we say that a map is smooth we shall mean that it has as many continuous derivatives as the context of the discussion requires. For convenience, the reader may assume C^∞. In order to apply the Implicit Function Theorem, we need the following standard

Definition 2.1 We call u a *regular point* of H if the Jacobian $H'(u)$ has maximal rank. We call y a *regular value* of H if u is a regular point of

H whenever $H(u) = y$. If a point or value is not regular, then it is called *singular*.

Let $u_0 \in \mathbb{R}^{N+1}$ be a regular point of H such that $H(u_0) = 0$. It follows from the Implicit Function Theorem that the solution set $H^{-1}(0)$ can be locally parametrized about u_0 with respect to some coordinate. By a reparametrization (according to arclength), we obtain a smooth curve $c : J \to \mathbb{R}^{N+1}$ for some open interval J containing zero such that for all $s \in J$:

$$c(0) = u_0 \tag{2.2}$$

$$H'(c(s))\dot{c}(s) = 0, \tag{2.3}$$

$$\|\dot{c}(s)\| = 1, \tag{2.4}$$

$$\det \begin{pmatrix} H'(c(s)) \\ \dot{c}(s)^* \end{pmatrix} > 0. \tag{2.5}$$

These conditions uniquely determine the tangent $\dot{c}(s)$. Here and in the following, $(\,.\,)^*$ denotes the Hermitian transpose and $\|\,.\,\|$ the Euclidean norm. Condition (2.4) normalizes the parametrization to arclength. This is only for theoretical convenience, and it is not an intrinsic restriction. Condition (2.5) chooses one of the two possible orientations.

The preceding discussion motivates the following

Definition 2.2 Let A be an $(N,N+1)$-matrix with maximal rank. For the purpose of our exposition, the unique vector $t(A) \in \mathbb{R}^{N+1}$ satisfying the conditions

$$At = 0, \tag{2.6}$$

$$\|t\| = 1, \tag{2.7}$$

$$\det \begin{pmatrix} A \\ t^* \end{pmatrix} > 0, \tag{2.8}$$

will be called the *tangent vector induced by* A.

Making use of this definition, solution curve $c(s)$ is characterized as the solution of the initial value problem

$$\dot{u} = t(H'(u)), \quad u(0) = u_0 \tag{2.9}$$

which in this context is occasionally attributed to Davidenko (1953), see also Branin (1972). Note that the domain $\{u \in \mathbb{R}^{N+1} : u \text{ is a regular point}\}$ is open. This differential equation is not used in efficient path following algorithms, but it serves as a useful device in analysing the path. Two examples are:

Lemma 2.3 Let (a, b) be the maximal interval of existence for (2.9). If a

is finite, then $c(s)$ converges to a singular zero point of H as $s \to a$, $s > a$. An analogous statement holds if b is finite.

Lemma 2.4 Let zero be a regular value of H. Then the solution curve c is defined on the real line and satisfies one of the following two conditions:

1. The curve c is diffeomorphic to a circle. More precisely, there is a period $T > 0$ such that $c(s_1) = c(s_2)$ if and only if $s_1 - s_2$ is an integer multiple of T.
2. The curve c is diffeomorphic to the real line. More precisely, c is injective, and $c(s)$ has no accumulation point for $s \to \pm\infty$.

See (2.1.13) and (2.1.14) in Allgower and Georg (1990) for proofs. A more topological and global treatment of the Implicit Function Theorem can be found in the books of Hirsch (1976) or Milnor (1969).

Since the solution curve c is characterized by the initial value problem (2.9), it is evident that the numerical methods for solving initial value problems could immediately be used to numerically trace c. However, in general this is not an efficient approach, since it ignores the contractive properties which the curve c has in view of the fact that it satisfies the equation $H(u) = 0$. Instead, a typical path following method consists of a succession of two different steps:

Predictor step. An approximate step along the curve, usually in the general direction of the tangent of the curve. The initial value problem (2.9) provides motivation for generating predictor steps in the spirit of the technology of numerical solution of initial value problems.

Corrector steps. One or more iterative steps which aim to bring the predicted point back to the curve by an iterative procedure (typically of Newton or gradient type) for solving $H(u) = 0$.

It is usual to call such procedures *predictor–corrector* path following methods. However, let us note that this name should not be confused with the predictor–corrector multistep methods for initial value problems, since the latter do not converge back to the solution curve.

The following pseudocode (in **MATLAB** format) shows the basic steps of a generic predictor–corrector method.

Algorithm 2.5 u = generic_pc_method(u, h)

```
% u ∈ R^{N+1} such that H(u) ≈ 0 is an initial point, input
% h > 0 is an initial steplength, input
   WHILE a stopping criterion is not met
      % predictor step
      predict v such that H(v) ≈ 0 and ||u − v|| ≈ h
      and v − u points in the direction of traversing
```

% *corrector step*
let $w \in \mathbb{R}^{N+1}$ approximately solve ...
$\min_w \{ \|v - w\| : H(w) = 0 \}$
% *new point along* $H^{-1}(0)$
$u = w$
% *steplength adaptation*
choose a new steplength $h > 0$
END

The predictor–corrector type of algorithms for curve following seem to date to Haselgrove (1961). In contrast to the modern predictor–corrector methods, the classical embedding methods assume that the solution path is parametrized with respect to an explicit parameter which is identified with the last variable in H. Hence, we consider the equation (2.1) in the form

$$H(x, \lambda) = 0. \tag{2.10}$$

If we assume that the partial derivative $H_x(x, \lambda)$ does not vanish, then the solution curve can be parametrized in the form $(x(\lambda), \lambda)$. This assumption has the drawback that *folds* are excluded, i.e. points such that $H(x, \lambda) = 0$ and $H_x(x, \lambda) = 0$. Such points are sometimes called turning points in the literature. The assumption has, however, the advantage that the corrector steps can be more easily handled, in particular if the partial derivative of H with respect to x is sparse. In some applications it is known *a priori* that no folds are present, and then the embedding method is applicable. For purposes of illustration we present an analogous generic embedding method:

Algorithm 2.6 x = generic_embedding_method(x, λ, h)

% $(x, \lambda) \in \mathbb{R}^{N+1}$ *such that* $H(x, \lambda) \approx 0$ *is an initial point, input*
% $h > 0$ *is an initial steplength, input*
WHILE a stopping criterion is not met
let $y \in \mathbb{R}^N$ approximately solve $H(y, \lambda + h) = 0$
$(x, \lambda) = (y, \lambda + h)$
choose a new steplength $h > 0$
END

The predictor step is hidden; the predictor point would correspond to the starting point of an iterative method for solving $H(y, \lambda + h) = 0$. The most commonly used starting point is the previous point x.

It is common to blend aspects of these two algorithms. A simple example is to use a predictor tangent to the curve $(x(\lambda), \lambda)$ in the embedding algorithm. A more sophisticated example is the use of the bordering algorithm introduced in Keller (1977, 1983) in the corrector phase of the predictor–

corrector method. To avoid dealing with the arclength parameter, one can adopt a strategy of parameter switching, see, e.g., Rheinboldt (1980, 1981).

3. Aspects of implementations

Let us now turn to some of the practical aspects of implementing a predictor–corrector method.

3.1. Newton steps as corrector

A straightforward way of approximating a solution of the minimization problem in the predictor–corrector method (2.5) is given by the Newton step

$$\mathcal{N}_H(v) := v - H'(v)^+ H(v), \tag{3.1}$$

where $H'(v)^+$ denotes the Moore–Penrose inverse of $H'(v)$, see, e.g., Golub and van Loan (1989). Very commonly, an *Euler predictor*, i.e. a predictor step in the direction of the tangent to the curve is used:

$$v = u + ht(H'(u)), \tag{3.2}$$

where $h > 0$ represents the current stepsize.

The following algorithm sketches one version of the predictor–corrector method incorporating an approximate Euler predictor and one Newton-type iteration as a corrector step.

Algorithm 3.1 $u = \text{Euler\_Newton}(u, h)$

```
WHILE a stopping criterion is not met
        approximate A ≈ H'(u)
        v = u + ht(A)              % predictor step
        u = v − A⁺H(v)             % corrector step
        choose a new steplength h > 0
END
```

Discussions of Newton's method using the Moore–Penrose inverse can be found in several text books, e.g. Ortega and Rheinboldt (1970) or Ben-Israel and Greville (1974).

Let us first state a convergence result, see (5.2.1) in Allgower and Georg (1990), which ensures that this algorithm safely follows the solution curve under reasonable assumptions.

Theorem 3.2 Let $H : \mathbb{R}^{N+1} \to \mathbb{R}^N$ be a smooth map having zero as a regular value and let $H(u_0) = 0$. Denote by $c_h(s)$ the polygonal path, starting at u_0, going through all points u generated by Algorithm 3.1 with fixed steplength $h > 0$. Denote by $c(s)$ the corresponding curve in $H^{-1}(0)$ given by the initial value problem (2.9). For definiteness, we assume that

$c_h(0) = c(0) = u_0$, and that both curves are parametrized with respect to arclength. If the estimate $\|A - H'(u)\| = \mathcal{O}(h)$ holds uniformly for the approximation in the loop of the algorithm, then the following quadratic bounds hold uniformly for $0 \le s \le s_0$ and s_0 sufficiently small:

$$\|H(c_h(s))\| \le \mathcal{O}(h^2), \quad \|c_h(s) - c(s)\| \le \mathcal{O}(h^2).$$

Some major points which remain to be clarified are:

— How do we efficiently handle the numerical linear algebra involved in the calculation of $t(A)$ and $A^+H(v)$?
— How do we formulate efficient steplength strategies?

3.2. The numerical linear algebra involved

A straightforward and simple (but not the most efficient) way to handle the numerical linear algebra would be to use a QR factorization:

$$A^* = Q \begin{pmatrix} R \\ 0^* \end{pmatrix}, \tag{3.3}$$

where Q is an $(N+1, N+1)$ orthogonal matrix, and R is a nonsingular (N, N) upper triangular matrix. We assume that A is an $(N, N+1)$ matrix with maximal rank. If q denotes the last column of Q, then $t(A) = \sigma q$, where the orientation defined in (2.5) leads to the choice

$$\sigma = \operatorname{sign}\Big(\det Q \det R\Big). \tag{3.4}$$

Hence σ is easy to determine. The Moore–Penrose inverse of A can be obtained from the same decomposition in the following way:

$$A^+ = A^*(AA^*)^{-1} = Q \begin{pmatrix} (R^*)^{-1} \\ 0^* \end{pmatrix}. \tag{3.5}$$

Similar ideas apply if an LU decomposition is given:

$$PA^* = L \begin{pmatrix} U \\ 0^* \end{pmatrix}, \tag{3.6}$$

where L is a lower triangular $(N+1, N+1)$ matrix, U is an (N, N) upper triangular matrix, and P is a permutation matrix corresponding to partial pivoting which is, in general, necessary to improve the numerical stability. Let us first consider the calculation of $t(A)$. If y denotes the last column of $P^*(L^*)^{-1}$, then

$$t(A) = \sigma y/\|y\|, \quad \text{where } \sigma = \operatorname{sign}\Big(\det P \det L \det U\Big). \tag{3.7}$$

The Moore–Penrose inverse is obtained by

$$A^+ = (I - t(A)t(A)^*)P^*(L^*)^{-1} \begin{pmatrix} (U^*)^{-1} \\ 0^* \end{pmatrix}. \tag{3.8}$$

Hence, a calculation of $w = A^+ z$ amounts to essentially one forward-solving with U^*, one back-solving with L^*, and one scalar product with $t(A)$.

These methods are useful for small dense matrices A. However, in many applications of path following methods, the corresponding matrix A is large and sparse, and then this procedure is inefficient. Among such applications are the approximation of branches of nonlinear eigenvalue problems or the central path methods of linear and nonlinear programming. Let us point out some ideas which are useful in dealing with such situations.

In many applications, one encounters matrices A with the following structure:

$$A = \begin{pmatrix} L & b \end{pmatrix}, \tag{3.9}$$

where equations of the form $Lx = y$ permit a fast linear solver. If $\begin{pmatrix} c^* & d \end{pmatrix}$ denotes an additional row (typically generated via the last predictor direction), then a standard block elimination may be employed via the Schur complement.

Lemma 3.3 Let

$$s = d - c^* L^{-1} b$$

denote the Schur complement of L in the augmented matrix

$$\tilde{A} = \begin{pmatrix} L & b \\ c^* & d \end{pmatrix}.$$

Then

$$\det \tilde{A} = \det L \, \det s. \tag{3.10}$$

Furthermore, if $\tilde{A}$ is nonsingular, then

$$\tilde{A}^{-1} = \begin{pmatrix} L^{-1} + L^{-1} b s^{-1} c^* L^{-1} & -L^{-1} b s^{-1} \\ -s^{-1} c^* L^{-1} & s^{-1} \end{pmatrix}.$$

As an easy consequence, the tangent $t(A)$ is obtained via

$$t(A) = \sigma y / \|y\|, \tag{3.11}$$

where y denotes the last column of $\tilde{A}^{-1}$. The sign $\sigma \in \{\pm 1\}$ can either be obtained from an angle test with the previous predictor direction or from (3.10), since it can be shown that

$$\sigma = \operatorname{sign}\Big(\det L \, \det s \Big). \tag{3.12}$$

Note that the computational expense of determining $t(A)$ is roughly one application of the fast solver and a scalar product.

The Moore–Penrose inverse is obtained via

$$A^+ = (I - t(A) t(A)^*)(\tilde{A}^{-1})_N, \tag{3.13}$$

where $(\tilde{A}^{-1})_N$ denotes the submatrix consisting of the first N columns of $\tilde{A}^{-1}$. Hence, a calculation of $w = A^+ z$ amounts to essentially one additional call of the fast solver and two additional scalar products.

Among the fast solvers which are of importance here are direct solvers for sparse linear systems, or preconditioned iterative solvers such as conjugate-gradient or other Krylov methods, see, e.g., Freund, Golub and Nachtigal (1992).

This Schur complement construction is also valid if b, c and d are matrices (of appropriate size). This is of interest in parametric optimization, see Lundberg and Poore (1993). Watson (1986) and deSa, Irani, Ribbens, Watson and Walker (1992) discuss some numerical linear algebra aspects in the context of path following.

The popular bordering algorithm of Keller (1977), see also Chan (1984a), Keller (1983), Menzel and Schwetlick (1978, 1985), is related to these ideas. These approaches are akin to Keller's pseudo arclength method, in which the equation $H(v) = 0$ is extended by an additional parametrization condition $\mathcal{N}(u, v, h) = 0$ which is at least transversal to $H(v) = 0$ for small h, and often models an approximate arclength parametrization. This viewpoint is often convenient, in particular for structured problems.

3.3. Step length control and higher order predictors

The convergence considerations of Theorem 3.2 were carried out under the assumption that the steplength of the Algorithm 3.1 was uniformly constant throughout. This assumption is also typical for complexity studies, see Section 6. Such an approach is inefficient for any practical implementation. An efficient algorithm needs to incorporate an automatic strategy for controlling the steplength. In this respect the predictor–corrector methods are similar to the methods for numerically integrating initial value problems in ordinary differential equations. To some extent, the steplength strategy depends upon the accuracy with which it is desired to numerically trace a solution curve. Path following methods usually split into two categories:

— either the solution curve is to be approximated with some given accuracy, e.g. for plotting purposes; or
— the objective is just to safely follow the curve as fast as possible, until a certain point is reached, e.g. a zero point or critical point with respect to some additional functional defined on the curve.

We briefly sketch some ideas which are used to adjust the steplength.

Steplength control via error models. One method, due to Den Heijer and Rheinboldt (1981), is based upon an error model for the corrector iteration. For Newton corrector steps, such error models can be obtained by analysing the Newton–Kantorovich theory. The steplength is controlled by

the number of steps which are taken in the corrector iteration until a given stopping criterion is fulfilled.

We sketch a somewhat modified and simplified version of this steplength strategy. Let us assume that u is a point on the solution curve, and consider, for simplicity, an Euler predictor $v_0(h) = u + ht(H'(u))$. Let $v_0(h)$, $v_1(h)$, ..., $v_k(h)$ be an iterative corrector process for approximating the nearest point to $v_0(h)$ on the curve. Suppose a certain stopping criterion is met after k iterations. The exact nature of the criterion is not important in this context. We assume theoretical convergence to $v_\infty(h)$.

It is assumed that there exists a constant $\gamma > 0$ (which is independent of h) such that the *modified error*

$$\varepsilon_i(h) := \gamma \|v_\infty(h) - v_i(h)\|$$

satisfies inequalities of the following type

$$\varepsilon_{i+1}(h) \leq \psi(\varepsilon_i(h)),$$

where $\psi : \mathbb{R} \to \mathbb{R}$ is a known monotone function such that $\psi(0) = 0$. For example, if Newton's method is employed, Den Heijer and Rheinboldt suggest two models:

$$\psi(\varepsilon) = \frac{\varepsilon^2}{3 - 2\varepsilon}, \quad 0 \leq \varepsilon \leq 1, \tag{3.14}$$

$$\psi(\varepsilon) = \frac{\varepsilon + \sqrt{10 - \varepsilon^2}}{5 - \varepsilon^2}\varepsilon^2, \quad 0 \leq \varepsilon \leq 1. \tag{3.15}$$

We may evaluate *a posteriori* the quotient

$$\omega(h) := \frac{\|v_k(h) - v_{k-1}(h)\|}{\|v_k(h) - v_0(h)\|} \approx \frac{\|v_\infty(h) - v_{k-1}(h)\|}{\|v_\infty(h) - v_0(h)\|} = \frac{\varepsilon_{k-1}(h)}{\varepsilon_0(h)}.$$

Using the estimate $\varepsilon_{k-1}(h) \leq \psi^{k-1}(\varepsilon_0(h))$, we obtain

$$\omega(h) \leq \frac{\psi^{k-1}(\varepsilon_0(h))}{\varepsilon_0(h)}.$$

This motivates taking the solution ε of the equation

$$\omega(h) = \frac{\psi^{k-1}(\varepsilon)}{\varepsilon}$$

as an estimate for $\varepsilon_0(h)$.

We now try to choose the steplength $\tilde{h}$ so that the corrector process satisfies the stopping criterion after a chosen number (say $\tilde{k}$) of iterations. Such a steplength leads to the modified error $\varepsilon_0(\tilde{h})$. Hence, we want the modified error $\varepsilon_{\tilde{k}}(\tilde{h})$ after $\tilde{k}$ iterations to be so small that the stopping criterion is satisfied. Using the inequality $\varepsilon_{\tilde{k}}(\tilde{h}) \leq \psi^{\tilde{k}}(\varepsilon_0(\tilde{h}))$, we accept the solution ε

of the equation

$$\psi^{\tilde{k}}(\varepsilon) = \psi^k(\varepsilon_0(h))$$

as an estimate for $\varepsilon_0(\tilde{h})$. Now we use the asymptotic expansion

$$\|v_\infty(h) - v_0(h)\| = Ch^2 + \mathcal{O}(h^3)$$

to obtain the approximation

$$\left(\frac{h}{\tilde{h}}\right)^2 \approx \frac{\varepsilon_0(h)}{\varepsilon_0(\tilde{h})},$$

which can be used to determine $\tilde{h}$. This steplength $\tilde{h}$ will now be used in the next predictor step. It is usually safeguarded by some additional considerations such as limiting the steplength to some interval $h_{\min} \leq \tilde{h} \leq h_{\max}$, or limiting the factor $0.5 \leq h/\tilde{h} \leq 2$, etc.

Steplength control via asymptotic expansion. Another method, based upon asymptotic estimates in the mentality of initial value solvers, is due to Georg (1983). The basic idea in this approach is to observe the performance of the corrector procedure and then to adapt the steplength $h > 0$ accordingly. More precisely, suppose that a point u on the solution curve has been approximated. Suppose further that a steplength $h > 0$ and a predictor point are given. Then a Newton-type iterative corrector process is performed which converges to the next point $z(h)$ on the curve.

The steplength strategy is motivated by the following question: Given the performance of the corrector process, which steplength $\tilde{h}$ would have been 'best' for obtaining $z(\tilde{h})$ from u? This 'ideal' steplength $\tilde{h}$ is determined via asymptotic estimates, and it is then taken as the steplength for the next predictor step. This strategy depends primarily upon two factors: the particular predictor–corrector method being utilized, and the criteria used in deciding what performance is considered 'best'.

Let us illustrate this technique in the case of the following algorithm (cf. Algorithm 3.1):

Algorithm 3.4 $u = \text{Euler\_Newton\_it}(u, h)$

```
WHILE a stopping criterion is not met
        v = u + ht(H'(u))                    % predictor step
        A = H'(v)
        WHILE a convergence criterion is not met
                v = v − A⁺H(v)               % corrector step
        END
        u = v
        choose a new steplength h > 0
END
```

If $v(h) = u + ht(H'(u))$ denotes the predictor step depending on the steplength h, then the first corrector point is given by

$$w(h) := v(h) - H'(v(h))^+ H(v(h)).$$

Let us call the quotient of the first two successive Newton steps

$$\kappa(u,h) := \frac{\|H'(v(h))^+ H(w(h))\|}{\|H'(v(h))^+ H(v(h))\|}$$

the *contraction rate* of the corrector process. Since Newton's method is locally quadratically convergent, it is plain that $\kappa(u,h)$ will decrease (and hence Newton's method will become faster) as h decreases. The following lemma characterizes the asymptotic behaviour of $\kappa(u,h)$ with respect to h, see (6.1.2) in Allgower and Georg (1990).

Lemma 3.5 Suppose that

$$H''(u)[t(H'(u)), t(H'(u))] \neq 0$$

(i.e. the curve has nonzero curvature at u), then

$$\kappa(u,h) = \kappa_2(u)h^2 + O(h^3)$$

for some constant $\kappa_2(u) \geq 0$ which is independent of h and depends smoothly on u.

In view of this asymptotic relation, the steplength modification $h \to \tilde{h}$ is now easy to explain. Assume that an Euler–Newton step has been performed with steplength h. Then $H'(v(h))^+ H(v(h))$ and $H'(v(h))^+ H(w(h))$ will have been calculated and thus $\kappa(u,h)$ can be obtained without any significant additional cost. Now an *a posteriori* estimate

$$\kappa_2(u) = \frac{\kappa(u,h)}{h^2} + O(h)$$

is available.

In order to have a robust and efficient method we want to continually adapt the steplength h so that a nominal prescribed contraction rate $\tilde{\kappa}$ is maintained. The choice of $\tilde{\kappa}$ will generally depend upon the nature of the problem at hand, and on the desired security with which we want to traverse the curve. That is, the smaller $\tilde{\kappa}$ is chosen, the greater will be the security with which the method will follow the curve. When using the term *securely* or *safely* following the curve we mean that a safeguard prevents the method from jumping to a different part of the curve (at a significantly different arclength value) or to a different connected component of $H^{-1}(0)$. Depending on the structure of the solution manifold $H^{-1}(0)$, this may be an important issue.

Once $\tilde{\kappa}$ has been chosen, we will consider a steplength $\tilde{h}$ to be appropriate if $\kappa(u, \tilde{h}) \approx \tilde{\kappa}$. By using the above equation and neglecting higher order terms we obtain the formula

$$\tilde{h} = h \sqrt{\frac{\tilde{\kappa}}{\kappa(u, h)}}$$

as the steplength for the next predictor step.

In a similar way, other quantities which are important for the performance of the path following method can be taken into account, e.g. the angle of two successive predictor directions, the size of the first Newton step (which gives an approximation of the distance of the predictor point to the curve) or the function value $H(v(h))$. All these quantities admit asymptotic expansions in h (with varying order). For example, Algorithm 6.1.10 and Program 1 in Allgower and Georg (1990) incorporates such features in the steplength strategy.

Kearfott (1989) proposes interval arithmetic techniques to determine a first order predictor which stresses secure path following, see also Kearfott (1990).

The steplength strategies we have discussed up to now have been based upon the Euler predictor, which is only of local order two. This is very often satisfactory since it is usually used in conjunction with rapidly converging correctors such as Newton-type correctors. However, for large systems, often less rapidly convergent iterative methods such as conjugate gradient steps are used. Hence, at least in some cases, one may expect to obtain improved efficiency by using variable order predictors and formulating corresponding steplength strategies. Such strategies could be similar to the ones used in multistep methods for solving initial value problems, see, e.g., Shampine and Gordon (1975). Georg (1982), suggested such a method, see also Georg (1983). Lundberg and Poore (1991) have made an implementation using variable order Adams–Bashforth predictors. Their numerical results show that there is often a definite benefit to be derived by using higher order predictors.

Inexpensive higher order predictors are generally based on polynomial interpolation. In view of the stability of Newton's method as a corrector, it may be advantageous to use more stable predictors. Mackens (1989) has proposed such predictors which are based on Taylor's formula and which are obtained by successive numerical differentiation in a clever way, see also Schwetlick and Cleve (1987) as a predecessor. However, the gain in stability has to be paid for by additional evaluations of the map H and additional applications of the Moore–Penrose inverse of the Jacobian H' (where it may be assumed that H' has already been decomposed).

Let us sketch a general philosophy for higher order predictors which may be useful for implementations. Let u be a point on the solution curve c such

that $c(s) = u$. Consider a polynomial predictor of the form

$$c(s+h) \approx p_k(h) = u + \sum_{i=1}^{k} c_i h^i, \tag{3.16}$$

$$c_i \approx \frac{c^{(i)}}{i!}, \tag{3.17}$$

which represents an approximation of the Taylor formula. We see essentially two different ways for obtaining the coefficients c_i: (1) by divided differences or polynomial interpolation making use of previously calculated points on the curve; and (2) by successive numerical differentiation at u. The former is less expensive to calculate, but the latter is more accurate.

We sketch one possible way of determining the next steplength and the next order in the predictor. Let $\varepsilon > 0$ be a given tolerance. The term $\|c_k\|h^k$ can be viewed as a rough estimate for the truncation error of the predictor $p_{k-1}(h)$. Hence, we estimate

$$h_k = \left(\frac{\varepsilon}{\|c_k\|}\right)^{1/k}$$

as the steplength for the predictor p_{k-1} in order to remain within the given tolerance. Due to instabilities of various kinds, we anticipate that

$$h_2 < h_3 \cdots < h_q \geq h_{q+1}$$

will hold for some q. Hence, the predictor p_{q-1} with steplength h_q is our next choice.

This idea can be implemented and modified in various ways, and needs some stabilizing safeguards, such as setting a maximum increase in steplength and in the order. The strategy to be developed depends on the objective of the application at hand.

4. Applications

In this section we present a selection of applications of path following methods. Many more specific examples exist in the literature, some of them are referred to later. Our discussion of applications concentrates to a large extent on cases in which the predictor–corrector methods apply. Applications in which the dimension is relatively low and smoothness does not hold can be handled by the piecewise-linear methods discussed in Section 5.

In many applications of the numerical homotopy methods, it is possible to avoid degeneracies in the solution curve by introducing suitable parameters (perturbations). The theoretical basis of this approach lies in Sard's theorem for maps with additional parameters, see, e.g., Abraham and Robbin (1967) or Hirsch (1976). Yomdin (1990) has given a version of Sard's theorem which is adapted for numerical purposes. We consider the following general form:

Theorem 4.1. (Sard) Let A, B, C be smooth manifolds of finite dimensions with $\dim A \geq \dim C$, and let $F : A \times B \to C$ be a smooth map. Assume that $c \in C$ is a regular value of F, i.e. for $F(a,b) = c$ we have that the total derivative $F'(a,b) : T_aA \times T_bB \to T_cC$ has maximal rank. Here T_aA denotes the tangent space of A at a, etc. Then for almost all $b \in B$ (in the sense of some Lebesgue measure on B) the restricted map $F(\cdot, b) : A \to C$ has c as a regular value.

4.1. Fixed point problems

To illustrate the use of Sard's theorem, let us consider a homotopy arising from a fixed point problem. Let $f : \mathbb{R}^N \to \mathbb{R}^N$ be a smooth map which is bounded. According to the theorem of Brouwer (1912), the map f has at least one fixed point. To simplify the discussion, let us make the assumption that the map $x \mapsto x - f(x)$ has zero as a regular value. This implies that the fixed points of f are isolated, and that Newton's method converges locally. However, the global convergence of Newton's method is by no means guaranteed.

We therefore consider the homotopy

$$H(x, \lambda, p) = x - p - \lambda(f(x) - p). \tag{4.1}$$

For the *trivial level* $\lambda = 0$, we obtain the *trivial map* $H(x, 0, p) = x - p$ which has the unique zero point p, our *starting point.* On the *target level* $\lambda = 1$, we obtain the *target map* $H(x, 1, p) = x - f(x)$ whose zero points are our points of interest, i.e. the fixed points of f.

Let us illustrate by this example how Sard's theorem is typically employed: The Jacobian of H is given by

$$H'(x, \lambda, p) = (\mathrm{Id} - \lambda f'(x), p - f(x), (\lambda - 1)\mathrm{Id}).$$

The first N columns of the Jacobian are linearly independent for $H(x, \lambda, p) = 0$ and $\lambda = 1$ due to our assumptions, and clearly the last N columns are linearly independent for $\lambda \neq 1$. Consequently, by Sard's theorem we can conclude that for almost all $p \in \mathbb{R}^N$ (in the sense of N-dimensional Lebesgue measure) zero is a regular value of the restricted map $H(\cdot, \cdot, p)$.

For such a generic choice of p, the solution manifold $H(\cdot, \cdot, p)^{-1}(0)$ consists of smooth curves which are either diffeomorphic to the circle or to the real line, see Lemma 2.4. Consider the solution curve $c(s) = (x(s), \lambda(s))$ (parametrized for convenience with respect to arclength) such that $c(0) = (p, 0)$. It is easy to see that the initial tangent vector in the direction of increasing λ has the form

$$\dot{c}(0) = (1 + \|f(p) - p\|^2)^{-1/2} \begin{pmatrix} f(p) - p \\ 1 \end{pmatrix},$$

and hence the curve is transversal to the plane $\lambda = 0$.

Since the solution point $(p, 0)$ is unique for $\lambda = 0$, it follows that c is diffeomorphic to the real line. Furthermore, the boundedness of f implies that $x(s)$ is bounded for $0 \leq \lambda(s) \leq 1$. It follows that the curve c reaches the level $\lambda = 1$ after a finite arclength s_0, i.e. $c(s_0) = (x_0, 1)$, and hence x_0 is a fixed point of f which can be approximated by tracing the curve c.

Let us note that

$$(\mathrm{Id} - f'(x_0))\dot{x}(s_0) = \dot{\lambda}(s_0)(f(x_0) - p),$$

and our earlier assumption on f implies that $(\mathrm{Id} - f'(x_0))$ cannot have a nontrivial kernel, and hence $\dot{\lambda}(s_0) \neq 0$, i.e. the curve c is tranversal to the level $\lambda = 1$ at any solution.

This discussion is in the spirit of Chow, Mallet-Paret and Yorke (1978). An earlier approach based on the nonretraction principle of Hirsch (1963) was given by Kellogg, Li and Yorke (1976). General discussions concerning the correspondence between degree arguments and numerical continuation algorithms have been given in Alexander and Yorke (1978), Garcia and Zangwill (1979a, 1981) and Peitgen (1982). Since the appearance of the constructive proofs of the Brouwer fixed point theorem many other constructive existence proofs have been described. Further references may be found in Section 11.1 of Allgower and Georg (1990).

Watson and collaborators have given a great number of engineering applications where an implementation (HOMPACK) of this homotopy method has been employed. As examples, we mention Arun, Reinholtz and Watson (1990), Melville, Trajkovic, Fang and Watson (1990), Vasudevan, Lutze and Watson (1990), Watson (1981), Watson, Li and Wang (1978), Watson and Wang (1981) and Watson and Yang (1980).

4.2. Global Newton methods

Newton's method is a popular method for numerically calculating a zero point of a smooth map $G : \mathbb{R}^N \to \mathbb{R}^N$. As is well known, this method may diverge if the starting point p is not sufficiently near to a zero point $\bar{x}$ of G. Often one would like to determine whether a certain open bounded region $\Omega \subset \mathbb{R}^N$ contains a zero point $\bar{x}$ of G and furthermore, for which starting values p this solution $\bar{x}$ can be obtained by Newton's method. The so-called global Newton methods offer a possibility of answering such questions.

One may interpret Newton's method as the numerical integration of the differential equation

$$\dot{x} = -G'(x)^{-1}G(x)$$

using Euler's method with unit step size. The idea of using this flow to find zero points of G was exploited by Branin (1972). Smale (1976) gave conditions on $\partial\Omega$ under which the flow leads to a zero point of G in Ω. Such numerical methods have been referred to as *global Newton methods.*

Keller (1978) observed that this flow can also be obtained in a numerically stable way from a homotopy equation which he consequently named the *global homotopy* method. Independently, Garcia and Gould (1978, 1980) discussed this flow.

We briefly sketch Keller's approach. The global homotopy method involves tracing the curve defined by the equation $G(x) - (1 - \lambda)G(p) = 0$ *starting from* $(x, \lambda) = (p, 0) \in \partial\Omega \times \{0\}$ *inward into* $\Omega \times \mathbb{R}$. *If the level* $\Omega \times \{1\}$ is encountered, then a zero point of G has been found.

We consider Smale's assumption.

Assumption 4.2 Let the following conditions be satisfied:

1. $\Omega \subset \mathbb{R}^N$ is open and bounded and $\partial\Omega$ is a connected smooth submanifold of $\mathbb{R}^N$;
2. zero is a regular value of G;
3. $G(p) \neq 0$ for $p \in \partial\Omega$;
4. the Jacobian $G'(p)$ is nonsingular for $p \in \partial\Omega$;
5. the Newton direction $-G'(p)^{-1}G(p)$ is not tangent to $\partial\Omega$ at p.

The *global homotopy* $H : \mathbb{R}^N \times \mathbb{R} \times \partial\Omega \longrightarrow \mathbb{R}^N$ is defined by

$$H(x, \lambda, p) := G(x) - (1 - \lambda)G(p).$$

Since p varies over the $(N-1)$-dimensional surface $\partial\Omega$, it is somewhat difficult to apply Sard's theorem. This task was achieved by Percell (1980). Hence, for almost all $p \in \partial\Omega$ the global homotopy has 0 as a regular value.

Let p be such a generic choice. We consider again the solution curve $c(s) = (x(s), \lambda(s))$ in $H(\cdot\,, \cdot\,, p)^{-1}(0)$ such that $c(0) = (p, 0)$ and $\dot{x}(0)$ points into Ω. Keller (1978) showed that the curve hits the target level $\Omega \times \{1\}$ in an odd number of points. This possibility of obtaining more than one solution was first observed by Branin and Hoo (1972).

Given the conditions 1 and 2 of assumption 4.2, the boundary conditions 3–5 can be shown to hold for a sufficiently small ball Ω around a zero point of G. Thus, in a certain sense the global homotopy extends the well known Newton–Kantorovich-type theorems concerning the local convergence of Newton's method, see, e.g., Ortega and Rheinboldt (1970).

4.3. Multiple solutions

In the previous section it was observed that the global homotopy method might actually yield more than one zero point of the map G in a bounded region Ω. This raises the question as to whether one might be able to compute more zero points of G in Ω in addition to those which lie on the global homotopy path. To be more precise, let us suppose that $\Omega \subset \mathbb{R}^N$ is an open bounded region, and that $G : \mathbb{R}^N \to \mathbb{R}^N$ is a smooth map having a zero point $z_0 \in \Omega$. The task is now to find additional zero points of G in Ω,

provided they exist. One method which has often been used for handling this problem is deflation, see, e.g., Brown and Gearhart (1971). In this method *a deflated map* $G_1 : \mathbb{R}^N \setminus \{z_0\} \to \mathbb{R}^N$ is defined by $G_1(x) = G(x)/\|x - z_0\|$. One then applies an iterative method to try to find a zero point of G_1. Numerical experience with deflation has shown that it is often a matter of seeming chance whether one obtains an additional solution and if one is obtained, it is very often not the one which is nearest to z_0.

By utilizing homotopy-type methods we can give some conditions which will guarantee the existence of an additional solution and yield insights into the behaviour of deflation. This additional solution will lie on a homotopy path. We illustrate this approach with a discussion of the *d-homotopy*. Let us consider the homotopy map $H_d : \mathbb{R}^N \times \mathbb{R} \to \mathbb{R}$ defined by

$$H_d(x, \lambda) := G(x) - \lambda d$$

where $d \in \mathbb{R}^N$ is some fixed vector with $d \neq 0$. Since we assume that a zero point z_0 is already given, we have $H_d(z_0, 0) = 0$. Let us further assume zero is a regular value of G. Then it follows from Sard's theorem that zero is also a regular value of H_d for almost all $d \in \mathbb{R}^N$. In order to ensure that the solution curve c in $H_d^{-1}(0)$ which contains $(z_0, 0)$ again reaches the level $\lambda = 0$, we need to impose a boundary condition. The following proposition uses a boundary condition which is motivated by a simple degree consideration.

Proposition 4.3 Let the following hypotheses hold:

1. $G : \mathbb{R}^N \to \mathbb{R}^N$ is a smooth map with zero as a regular value;
2. $d \in \mathbb{R}^N \setminus \{0\}$ is a point such that the homotopy H_d also has zero as a regular value;
3. $\Omega \subset \mathbb{R}^N$ is a bounded open set which contains a (known) initial zero point z_0 of G;
4. the *boundary condition* $H_d(x, \lambda) = G(x) - \lambda d \neq 0$ holds for all $x \in \partial\Omega$, $\lambda \in \mathbb{R}$;

Then the curve c in $H_d^{-1}(0)$ which contains $(z_0, 0)$ intersects the level $\Omega \times \{0\}$ an even number of times at points $(z_i, 0)$, $i = 0, \ldots, n$, at which $G(z_i) = 0$.

See (11.5.3) in Allgower and Georg (1990) for a proof. Any two zero points of G which are consecutively obtained by traversing the curve c have opposite index. Allgower and Georg (1983b) have shown that this d-homotopy can be viewed as a continuous version of the deflation technique of Brown and Gearhart.

4.4. Polynomial systems

In the preceding section we considered the task of computing multiple zero points of general smooth maps. In the case of complex polynomial systems

it is actually possible to compute (at least in principle) all of the zero points by means of homotopy methods. This subject has received considerable attention in recent years. The book of Morgan (1987) deals exclusively with this topic, using the path following approach. It also contains a number of interesting applications to robotics and other fields.

We consider a system of complex polynomials $P : \mathbb{C}^n \to \mathbb{C}^n$. The task is to find *all* solutions of the equation $P(z) = 0$. If a term of the kth component P_k of P has the form

$$az_1^{r_1} z_2^{r_2} \cdots z_n^{r_n},$$

then its degree is $r_1 + r_2 + \ldots + r_n$. The degree d_k of P_k is the maximum of the degrees of its terms. The *homogeneous part* $\hat{P}$ of P is obtained by deleting in each component P_k all terms having degree less than d_k. The *homogenization* $\tilde{P}$ of P is obtained by multiplying each term of each component P_k with an appropriate power z_0^r such that its degree is d_k. Note that the homogenization $\tilde{P} : \mathbb{C}^{n+1} \to \mathbb{C}^n$ involves one more variable z_0. If

$$(w_0, \ldots, w_n) \neq 0$$

is a zero point of $\tilde{P}$, then the entire ray

$$[w_0 : \cdots : w_n] := \{(\xi w_0, \ldots, \xi w_n) \mid \xi \in \mathbb{C}\}$$

consists of zero points of $\tilde{P}$. Usually, $[w_0 : \cdots : w_n]$ is regarded as a point in the complex projective space $\mathbb{CP}^n$. There are two cases to consider:

1 The solution $[w_0 : \cdots : w_n]$ intersects the hyperplane $z_0 = 0$ transversely, i.e. without loss of generality, $w_0 = 1$. This corresponds to a zero point $(w_1, \ldots, w_n)$ of P. Conversely, each zero point $(w_1, \ldots, w_n)$ of P corresponds to a solution $[1 : w_1 : \cdots : w_n]$ of $\tilde{P}$.

2 The solution $[w_0 : \cdots : w_n]$ lies in the hyperplane $z_0 = 0$, i.e. $w_0 = 0$. This corresponds to a *nontrivial* solution $[w_1 : \cdots : w_n]$ of the homogeneous part $\hat{P}$, and such solutions are called *zero points of P at infinity.*

As in the case of one variable, it is possible to define the multiplicity of a solution. The higher dimensional analogue of the fundamental theorem of algebra is Bezout's theorem, which states that the number of zero points of P (counting their multiplicities and zeros at infinity) equals the product $d = d_1 d_2 \cdots d_n$, provided all solutions are isolated.

Garcia and Zangwill (1979b) and Chow, Mallet-Paret and Yorke (1979) introduced homotopy methods in $\mathbb{C}^n \times \mathbb{R}$ for finding all solutions of the equation $P = 0$. Wright (1985) realized that their approaches could be simplified by going into the complex projective space $\mathbb{CP}^n$. We use his approach to illustrate the homotopy idea for polynomial systems.

Define a homotopy $H = (H_1, \ldots, H_n)$ by involving the homogenization $\tilde{P}$

of P via

$$H_k(z_0, \ldots, z_n, \lambda) = (1 - \lambda)(a_k z_k^{d_k} - b_k z_0^{d_k}) + \lambda \tilde{P}_k(z_0, \ldots, z_n).$$

Wright shows by Sard-type arguments that for almost all coefficients $a_k, b_k \in \mathbb{C}$ the restricted homotopies $H^{(j)}$ which are obtained from H by fixing $z_j = 1$ for $j = 0, \ldots, n$ have zero as a regular value for $\lambda < 1$. He concludes that for $\lambda < 1$, the homogeneous system of polynomials H has exactly d simple zero point curves $c_i(\lambda) \in \mathbb{CP}^n$, $i = 1, \ldots, d$, in complex projective n-space. On the trivial level $\lambda = 0$, the d solutions are obvious, and it is possible to trace the d curves emanating from these solutions into the direction of increasing λ. The solution curves are monotone in λ, and hence all have to reach the target level $\lambda = 1$ on the compact manifold $\mathbb{CP}^n$. Thus, in this approach solutions at infinity are treated no differently than finite solutions. The solution curves are traced in the projective space $\mathbb{CP}^n$, and from the numerical point of view we have the slight drawback that occasionally a chart in $\mathbb{CP}^n$ has to be switched.

Recently, attention has been given to the task of trying to formulate homotopies which eliminate the sometimes wasteful effort involved in tracing paths which go to solutions of $P(z_1, \ldots, z_n) = 0$ at infinity. Work in this direction has been done in Morgan (1986), Li, Sauer and Yorke (1987, 1989) and Li and Wang (1992a,b). Morgan and Sommese (1987) describe the easily implemented 'projective transformation' which allows the user to avoid the drawback of changing coordinate charts on $\mathbb{CP}^n$. Morgan and Sommese (1989) show how to exploit relations among the system coefficients, via 'coefficient parameter continuation'. Such relations occur commonly in engineering problems, as described in Wampler and Morgan (1991), Wampler, Morgan and Sommese (1990, 1992). The papers (Morgan, Sommese and Wampler, 1991–1992) combine a homotopy method with contour integrals to calculate singular solutions to polynomial and nonlinear analytic systems. Morgan, Sommese and Watson (1989) documented that `HOMPACK`, see Watson, Billups and Morgan (1987), in the case of polynomial systems has some stability issues that `CONSOL8`, see Morgan (1987), does not have. The path following approach to systems of polynomial equations is particularly suited for parallel processing, see Allison, Harimoto and Watson (1989).

4.5. Nonlinear eigenvalue problems, bifurcation

Path following methods are frequently applied in numerical studies of bifurcation problems. Up to this point we have assumed that zero is a regular value of the smooth mapping $H : \mathbb{R}^{N+1} \to \mathbb{R}^N$. However, bifurcation points are singular points on $H^{-1}(0)$ and hence, if path following algorithms are applied, some special adaptations are required. Generally, bifurcation points are defined in a Banach space context, see for example the book by Chow

and Hale (1982). In the case that H represents a mapping arising from a discretization of an operator of the form $\mathcal{H} : E_1 \times \mathbb{R} \to E_2$ where E_1 and E_2 represent appropriate Banach spaces, it is usually of interest to approximate bifurcation points of the operator equation $\mathcal{H} = 0$. Often one can make the discretization H in such a way that the resulting discretized equation $H = 0$ also has a corresponding bifurcation point. Under reasonable assumptions of nondegeneracy it is possible to obtain error estimates for the bifurcation point of the original problem $\mathcal{H} = 0$. Such studies are presented in the papers by Brezzi, Rappaz and Raviart (1980a,b, 1981), Crouzeix and Rappaz (1990), Fink and Rheinboldt (1983, 1984, 1985) and Liu and Rheinboldt (1991).

Since we are primarily concerned with bifurcation in the numerical curve following context, we confine our discussion to the case of the finite dimensional (discretized) equation $H = 0$. However, we note that the theoretical discussion later will essentially extend to the Banach space context if we assume that H is a Fredholm operator of index one. We will discuss how certain types of bifurcation points along a solution curve c can be detected, and having detected a bifurcation point, how one can numerically switch from c onto a bifurcating branch.

Some of the fundamental results on the numerical solution of bifurcation problems are due to Keller (1970), see also Keener and Keller (1974) and Keller (1977). The recent literature on the numerical treatment of bifurcation is very extensive. For an introduction into the field we suggest the lecture notes of Keller (1987). See also the two articles by Doedel, Keller and Kernévez (1991a,b) which discuss the use of the software package AUTO. For surveys and bibliography we suggest the recent book by Seydel (1988) and the recent proceedings (Mittelman and Roose, 1989; Roose, de Dier and Spence, 1990; Seydel, Schneider, Küpper and Troger, 1991). Most authors study bifurcation problems in the context of a nonlinear eigenvalue problem

$$H(x, \lambda) = 0,$$

where λ is the eigenvalue parameter which usually has some physical significance. Conventionally, the solution branches are parametrized according to λ. We have taken the viewpoint that the solution branches c_i are parametrized with respect to the arclength. There is only one essential difference, namely that the former approach also considers folds with respect to λ as singularities.

Such folds are frequently of intrinsic interest, and there are special algorithms for detecting and calculating them. We omit this subject here for reasons of space limitations, and refer the interested reader to, e.g., Bolstad and Keller (1986), Chan (1984b), Fink and Rheinboldt (1986, 1987), Melhem and Rheinboldt (1982), Pönisch and Schwetlick (1981), Schwetlick (1984ab) and Ushida and Chua (1984).

A standard approach to the determination of bifurcation or other singular points is to directly characterize such points by adjoining additional equations to $H = 0$ and handling the resulting new set of equations by some special iterative method. In this context, continuation methods often are used to obtain starting points for these direct methods, see, e.g., Griewank (1985), Moore and Spence (1980) and Yang and Keller (1986). A hybrid method for handling unstable branches has been developed by Shroff and Keller (1991).

Mittelmann and collaborators have made extensive applications of path following and bifurcation methods in the context of minimal surfaces, free boundary problems, obstacle problems and variational inequalities, see, e.g., Hornung and Mittelmann (1991), Maurer and Mittelmann (1991), Miersemann and Mittelmann (1989–1992) and Mittelmann (1990).

In view of the extensive literature we can only touch upon the problem here, and we will confine our discussion to the task of detecting a simple bifurcation point along a solution curve c and effecting a branch switching numerically. We will see that the detection of simple bifurcation points requires only minor modifications of predictor–corrector algorithms. A more detailed discussion along these lines can be found in Chapter 8 of Allgower and Georg (1990). Let us begin by defining a bifurcation point.

Definition 4.4 Suppose that $c : J \to \mathbb{R}^{N+1}$ is a smooth curve, defined on an open interval J containing zero, and parametrized (for reasons of simplicity) with respect to arc length such that $H(c(s)) = 0$ for $s \in J$. The point $c(0)$ is called a *bifurcation point* of the equation $H = 0$ if there exists an $\varepsilon > 0$ such that every neighbourhood of $c(0)$ contains zero points z of H which are not on $c(-\varepsilon, \varepsilon)$.

An immediate consequence of this definition is that a bifurcation point of $H = 0$ must be a singular point of H. Hence the Jacobian $H'(c(0))$ must have a kernel of dimension at least two. We consider the simplest case:

Definition 4.5 A point $\bar{u} \in \mathbb{R}^{N+1}$ is called a *simple bifurcation point* of the equation $H = 0$ if the following conditions hold:

1. $H(\bar{u}) = 0$;
2. $\dim \ker H'(\bar{u}) = 2$;
3. $e^* H''(\bar{u})\big|_{(\ker H'(\bar{u}))^2}$ has one positive and one negative eigenvalue. where e spans $\ker H'(\bar{u})^*$.

Using the well known Liapunov–Schmidt reduction, the following theorem can be shown, which is essentially a restatement of a famous result from Crandall and Rabinowitz (1971).

Theorem 4.6 Let $\bar{u} \in \mathbb{R}^{N+1}$ be a simple bifurcation point of the equation $H = 0$. Then there exist two smooth curves $c_1(s), c_2(s) \in \mathbb{R}^{N+1}$,

parametrized with respect to arclength s, defined for $s \in (-\varepsilon, \varepsilon)$ and ε sufficiently small, such that the following holds:

1. $H(c_i(s)) = 0$, $i \in \{1,2\}$, $s \in (-\varepsilon, \varepsilon)$,;
2. $c_i(0) = \bar{u}$, $i \in \{1,2\}$,;
3. $\dot{c}_1(0)$, $\dot{c}_2(0)$ are linearly independent;
4. $H^{-1}(0)$ coincides locally with range $(c_1) \cup$ range (c_2), more precisely: $\bar{u}$ is not in the closure of $H^{-1}(0) \setminus (\text{range}(c_1) \cup \text{range}(c_2))$.

By differentiating the equation $e^* H(c_i(s)) = 0$ twice and evaluating the result at $s = 0$, we obtain the following

Lemma 4.7 Let $\bar{u} \in \mathbb{R}^{N+1}$ be a simple bifurcation point of the equation $H = 0$. Then

1. $\ker H'(\bar{u}) = \text{span}\{\dot{c}_1(0), \dot{c}_2(0)\}$,
2. $e^* H''(\bar{u})[\dot{c}_i(0), \dot{c}_i(0)] = 0$ for $i \in \{1,2\}$.

The following theorem reflects the well known fact, see Krasnosel'skiĭ (1964) or Rabinowitz (1971), that simple bifurcation points cause a switch of orientation along the solution branches. This furnishes a numerically implementable criterion for detecting a simple bifurcation point when traversing one of the curves c_i. For a proof, see, e.g., Theorem (8.1.14) in Allgower and Georg (1990).

Theorem 4.8 Let $\bar{u} \in \mathbb{R}^{N+1}$ be a simple bifurcation point of the equation $H = 0$. Then the determinant of the following augmented Jacobian

$$\det \begin{pmatrix} H'(c_i(s)) \\ \dot{c}_i(s)^* \end{pmatrix}$$

changes sign at $s = 0$ for $i \in \{1,2\}$.

This theorem implies that when traversing a solution curve c, a simple bifurcation point is detected by a change in orientation. Depending upon the method used to perform the decomposition of the Jacobian during path following, this orientation can often be calculated at very small additional cost. A predictor–corrector algorithm generally has no difficulty in *jumping over*, i.e. proceeding beyond the bifurcation point $\bar{u}$. That is, Keller (1977) has shown that for sufficiently small steplength h, the predictor point will fall into the 'cone of attraction' of the Newton corrector. See Jepson and Decker (1986) for further studies.

Conversely, suppose that a smooth c in $H^{-1}(0)$ is traversed and that $c(0)$ is an isolated singular point of H such that the determinant changes sign at $s = 0$, then using a standard argument in degree theory, see Krasnosel'skiĭ (1964) or Rabinowitz (1971), it can be shown that $c(0)$ is a bifurcation point of $H = 0$. However, $c(0)$ is not necessarily a simple bifurcation point.

Multiple bifurcations often arise from symmetries with respect to certain group actions, i.e. H satisfies an equivariance condition

$$H(\gamma x, \lambda) = \gamma H(x, \lambda)$$

for γ in a group Γ. See the books by Golubitsky and Schaeffer (1985), Golubitsky, Stewart and Schaeffer (1988) and Vanderbauwhede (1982). These symmetries can also be exploited numerically, see, e.g., , Allgower, Böhmer and Mei (1991a,b), Allgower, Böhmer, Georg and Miranda (1992b), Cliffe and Winters (1986), Dellnitz and Werner (1989), Georg and Miranda (1990, 1992), Jepson, Spence and Cliffe (1991), Healey (1988–1989), Healey and Treacy (1991) and Hong (1991); see also the proceedings (Allgower, Böhmer and Golubitsky, 1992a). As this partial list suggests, there is currently very much interest in this topic. However, constraints on our available space prohibits a detailed discussion.

The determinant in Theorem 4.8 is only the simplest example of a so-called *test function.* Such test functions are real functions defined on a neighbourhood of the curve c and are monitored during path following to reveal certain types of singular points by a change of sign. In the case of Hopf bifurcation, the determinant is not an adequate test function. Recently, several authors have proposed and studied classes of test functions for various types of singular points, see, e.g., Dai and Rheinboldt (1990), Garratt, Moore and Spence (1991), Griewank and Reddien (1984), Seydel (1991b) and Werner (1992). A different approach for the prediction of singular points along the path c has been given by Huitfieldt and Ruhe (1990).

Switching branches via perturbation. In the previous section we have seen that it is possible to detect and jump over simple bifurcation points while numerically tracing a solution curve c via a predictor–corrector method. The more difficult task is to numerically branch off onto the second solution curve at the detected bifurcation point $\bar{u}$. The simplest device for branching off numerically rests upon Sard's theorem (4.1). If a small perturbation vector $d \in \mathbb{R}^N$ is chosen at random, then the probability that d is a regular value of H is unity. Of course, in this case $H^{-1}(d)$ has no bifurcation point. Since $d \in \mathbb{R}^N$ is chosen so that $\|d\|$ is small, the solution sets $H^{-1}(0)$ and $H^{-1}(d)$ are close together. On $H^{-1}(d)$, no change of orientation can occur. Therefore, corresponding solution curves in $H^{-1}(d)$ must branch off near the bifurcation point $\bar{u}$. It is easy to implement this idea, see, e.g., Allgower and Chien (1986), Allgower, Chien, Georg and Wang (1991c), Chien (1989), Georg (1981) and Glowinski, Keller and Reinhart (1985).

Recently, an interesting variation on this idea has been proposed by Huitfieldt (1991). He introduces an additional parameter on the perturbation and an additional constraint equation to obtain the *branch connecting equa-*

tion

$$\mathcal{B}(u,\tau) := \begin{pmatrix} H(u) + \tau d \\ \|u - \hat{u}\|^2 + \tau^2 - \varepsilon^2 \end{pmatrix} = 0, \tag{4.2}$$

where $\hat{u}$ is an approximation to the bifurcation point $\bar{u}$. Such approximations are easily obtained via path following together with test function monitoring as described earlier. Note the relationship between this homotopy and the d-homotopy discussed in Section 4.3 in connection with finding multiple solutions.

It is not difficult to see that for almost all d and $\varepsilon > 0$, zero is a regular value of $\mathcal{B}$, provided that $\bar{u}$ is an isolated singular point of H in $H^{-1}(0)$. Let us assume that such a generic choice of d and ε has been made.

Then the solution manifold $\mathcal{B}^{-1}(0)$ splits into one or more simple closed curves of the form $(b(s), \tau(s))$. For $\tau(s) = 0$ we obtain $H(b(s)) = 0$. Hence the curves connect points in the intersection of $H^{-1}(0)$ with the sphere $\|u-\hat{u}\|^2 = \varepsilon^2$. Starting points for a path following of $(b(s), \tau(s))$ are available from the tracing of the current solution curve c of $H = 0$. Let $b_i = b(s_i)$, $i = 0, 1, \ldots$, be successively obtained points such that $\tau(s_i) = 0$. It remains to be demonstrated that b_i and b_{i+1} are on different solution branches of the equation $H = 0$.

Since this seems to have been omitted in the paper of Huitfieldt (1991), we sketch a proof. It is easily seen that the determinant of the matrix

$$\begin{pmatrix} H'(b(s)) & d \\ (b(s) - \hat{u})^* & \tau(s) \\ \dot{b}(s)^* & \dot{\tau}(s) \end{pmatrix}$$

never changes sign since it never becomes singular. By multiplying this matrix on the right with

$$\begin{pmatrix} \mathrm{Id} & \dot{b}(s) \\ 0^* & \dot{\tau}(s) \end{pmatrix}$$

we obtain

$$\begin{pmatrix} H'(b(s)) & 0 \\ (b(s) - \hat{u})^* & 0 \\ \dot{b}(s)^* & 1 \end{pmatrix}.$$

Since $\dot{\tau}(s_i)$ changes sign for successive i, we obtain that the determinant of

$$\begin{pmatrix} H'(b_i) \\ (b_i - \hat{u})^* \end{pmatrix}$$

changes sign for successive i. Under reasonable assumptions this implies that $t(H'(b_{i+1}))$ points out of the sphere $\|u - \hat{u}\|^2 = \varepsilon^2$ if $t(H'(b_i))$ points into it. For a simple bifurcation point (or more generally for a bifurcation point

hich is detected by a change of determinant in the sense of Theorem 4.8), iis means that b_i and b_{i+1} cannot lie on the same solution branch.

Huitfeldt reports very successful numerical tests on some interesting probms of applied mathematics: the Taylor problem, and the von Karman plate juations. In his experiments he succeeded in obtaining all of the bifurcating ranches at several multiple bifurcation points, i.e. the 1-manifold $\mathcal{B}^{-1}(0)$ as connected in all cases he considered. However, it does not seem that iis should always be the case. Advantages of this approach are that no *a riori* information concerning the multiplicity of the bifurcation is needed, nd that it enjoys better numerical stability properties than ordinary perirbation. It should, however, be emphasized that any existing symmetries ading to higher multiplicities ought to be taken into account initially, i.e. y using group actions in the formulation of the problem, see Golubitsky *et l.* (1988) and other references cited earlier.

Branching off via the bifurcation equation. Although the branching ff via perturbation techniques works effectively, this approach can have ome shortcommings. In general, it cannot be decided in advance which f the two possible directions along the bifurcating branch will be taken. 'urthermore, if the perturbation vector d is not chosen correctly (and it is ot always clear how this is to be done), one may still have some difficulty a tracing the resulting path. The solution set $H^{-1}(0)$ can be approximated ear the bifurcation point $\bar{u}$ only after an additional bifurcating branch has een approximated.

To obtain an approximation of $H^{-1}(0)$ near a simple bifurcation point $\bar{u}$, he alternative is a direct approach. This may consist of two steps, see, e.g., ection 8.3 of Allgower and Georg (1990):

.. Approximation of the bifurcation point $\bar{u}$ by adjoining additional equations to $H = 0$ and handling the resulting new set of equations by some special iterative method.

2. Construct a numerical model for the so-called bifurcation equation in order to approximate all tangents of the bifurcating branches in $\bar{u}$. Lemma 4.7 describes such an equation for the case of a simple bifurcation point. The approaches in Keller (1977, 1987) and Rheinboldt (1978) deal with this idea.

4.6. *Complex bifurcation*

It has been observed by Allgower (1984) and Allgower and Georg (1983a) hat folds in the λ coordinate of solution curves of $H(x, \lambda) = 0$ lead to bifurcation points in a setting of complex extension, see also Section 11.8 of Allgower and Georg (1990). This observation can be used to connect separated real components of $H^{-1}(0)$, and hence may serve as a tool to

find additional solutions of the equation $H = 0$. Henderson (1985) and Henderson and Keller (1990) study complex bifurcation in a general Banach space setting. Let us briefly summarize one of their main results.

Let $\mathbf{B}$ be a real Banach space which can be complexified into $\mathbf{B} \oplus \mathrm{i}\mathbf{B}$. We use the notation $z = x + \mathrm{i}y$ for $z \in \mathbf{B} \oplus \mathrm{i}\mathbf{B}$ and $x, y \in \mathbf{B}$. We consider B to be naturally embedded into $\mathbf{B} \oplus \mathrm{i}\mathbf{B}$ via $x \mapsto x + \mathrm{i}0$. In most cases which occur in applications, e.g. function spaces, the precise meaning of this setting is obvious.

Consider a smooth nonlinear problem of the form

$$H(z, \lambda) = H(x + \mathrm{i}y, \lambda) = 0, \quad H : \mathbf{B} \oplus \mathrm{i}\mathbf{B} \times \mathbb{R} \to \mathbf{B} \oplus \mathrm{i}\mathbf{B}, \tag{4.3}$$

where H is analytic in the complex variable $z = x + \mathrm{i}y$. Furthermore, we assume that H is real for real arguments, and denote the restriction to real arguments by $H_{\mathbf{R}}$, i.e. $H_{\mathbf{R}} : \mathbf{B} \times \mathbb{R} \to \mathbf{B}$.

Let $c(s) = (x(s), \lambda(s))$ be a solution curve of (the real) equation $H_{\mathbf{R}} = 0$ consisting of regular points. We assume that $c(0)$ is a *simple fold*, i.e.

$$\dot{\lambda}(0) = 0, \quad \ddot{\lambda}(0) \neq 0. \tag{4.4}$$

Then $c(0)$ is a simple bifurcation point of (the complex) equation $H = 0$.

In fact, it can be seen that for the bifurcating curve

$$c_1(s) = (x_1(s) + \mathrm{i}y_1(s), \lambda_1(s))$$

the following characterization holds at $s = 0$, see Proposition (11.8.16) of Allgower and Georg (1990):

$$\dot{x}_1(0) = 0, \quad \dot{y}_1(0) = \pm\dot{x}(0), \quad \dot{\lambda}_1(0) = 0, \quad \ddot{\lambda}_1(0) = -\ddot{\lambda}(0).$$

Proposition 2.1 in Li and Wang (1992b) generalizes this result to complex folds.

4.7. Linear eigenvalue problems

In recent years many of the classical problems of numerical linear algebra have been re-examined in the context of homotopies and path following. One of the earliest contributors has been Chu (1984–1991). In these papers iterative processes and matrix factorizations have been studied in the context of flows satisfying various differential equations. A typical example is the Toda flow which has been studied as a continuous analogue of the QR algorithm. A survey of these ideas has been given by Watkins (1984). According to Watkins, although it seems that the Toda flow and related flows yield insight into the workings of algorithms, they do not necessarily directly offer algorithms which are competitive with standard library algorithms that have been developed and polished over numerous years.

Surprisingly, Li and Li (1992), Li and Rhee (1989), Li, Zeng and Cong

(1992) and Li, Zhang and Sun (1991) have been able to construct special implementations of homotopy methods which are now at least competitive with the library routines of EISPACK and IMSL for linear eigenvalue problems.

The versatility of homotopy methods also permits their application to generalized eigenvalue problems, see Chu, Li and Sauer (1988) and non-symmetric matrices, see Li and Zeng (1992) and Li *et al.* (1992). In this case complex eigenvalues are likely to arise, and it is necessary to invoke the idea of complex bifurcation, see Section 4.6.

As an example, let us briefly discuss the homotopy approach given by Li *et al.* (1991). Consider a real symmetric tridiagonal matrix A. We assume that A is irreducible, since otherwise one off-diagonal element $A[i+1,i] = A[i,i+1]$ would vanish and the matrix A would split into two blocks which can be treated independently. We consider a homotopy $H : \mathbb{R}^N \times \mathbb{R} \times [0,1] \to \mathbb{R}^N \times \mathbb{R}$ defined by

$$H(x,\lambda,s) = \begin{pmatrix} \lambda x - [(1-s)D + sA]x \\ x^*x - 1 \end{pmatrix}.$$

Here D is a real symmetric reducible tridiagonal matrix which is generated from A by setting some of the off-diagonal entries of A to zero. The simplest example for D would be to set all off-diagonal entries to zero. However, it is advantageous to only reduce D to tridiagonal block structure with relatively small blocks, e.g. of size < 50. This technique is referred to as *divide and conquer.*

Since $A(s) := (1-s)D + sA$ is irreducible for all $s > 0$, the solution set of $H = 0$ consists of $2n$ disjoint smooth curves c (*eigenpaths*) which can be parametrized with respect to s. Note that s is not the arclength, but the homotopy parameter. Hence

$$c(s) = (\pm x(s), \lambda(s)) \quad \text{for } 0 \le s \le 1.$$

The curves obviously occur in pairs, and only one of each pair needs to be traced. At the level $s = 0$, initial values on the curves can be obtained by approximating all eigenvectors and eigenvalues of all small blocks in D. If D is diagonal, this is trivial, and otherwise a QR routine has to be employed.

Let us sketch a typical step of the predictor-corrector method. We note first that it follows from differentiation of $H(c(s)) = 0$ with respect to s that

$$\dot{\lambda}(s) = x(s)^*(A - D)x(s). \tag{4.5}$$

Assume that $(x(s), \lambda(s))$ is (approximately) known. After having decided on a stepsize h (we are not going to discuss this feature), a predicted eigenvalue $\tilde{\lambda}(s+h)$ is obtained from this differential equation by a two-step ODE method. Now a predicted eigenvector $\tilde{x}(s+h)$ is obtained by one step of

the inverse power method with shift, i.e. solve

$$(A(s+h) - \tilde{\lambda}(s+h)\mathrm{Id})y = x(s) \quad \text{for } y$$

and set $\tilde{x}(s+h) = y/\|y\|$. Then a Rayleigh quotient iteration is performed as a corrector to approximate $(x(s+h), \lambda(s+h))$.

There are some stability problems for the case that different eigenvalues become close. Sturm sequences are computed to stabilize the procedure.

Let us finally note that this homotopy method has an order-preserving property, i.e. different λ-paths can never cross. Hence the jth eigenvalue of A can be calculated without calculating any other eigenvalues. This is very often an advantageous feature for applications. On the other hand, the homotopy method lends itself conveniently to parallelization, since each solution path can be traced independently of the others and hence also simultaneously.

4.8. Parametric programming problems

Parametric programming problems and sensitivity analysis can also be studied in the context of continuation methods. Consider the problem

$$\min\{f(x,\alpha) : c_i(x,\alpha) = 0,\ i \in E,\ c_i(x,\alpha) \leq 0,\ i \in I\}, \tag{4.6}$$

where $f, c_i : \mathbb{R}^{n+1} \to \mathbb{R}$ are smooth functions. Here

$$E = \{1, \ldots, q\} \quad \text{and} \quad I = \{q+1, \ldots, q+p\}$$

denote the index sets for the equality and inequality constraints, respectively. The local sensitivity of such systems has been analysed, e.g., in Fiacco (1983, 1984) and Robinson (1987). Many authors have used bifurcation and singularity theory to investigate the local behaviour and persistence of minima at the singular points of this system, see, e.g., Bank, Guddat, Klatte, Kummer and Tammer (1983), Gfrerer, Guddat and Wacker (1983), Gfrerer, Guddat, Wacker and Zulehner (1985), Guddat, Guerra Vasquez and Jongen (1990), Guddat, Jongen, Kummer and Nožička (1987), Jongen, Jonker and Twilt (1983, 1986), Jongen and Weber (1990), Kojima and Hirabayashi (1984) and Poore and Tiahrt (1987, 1990). Rakowska, Haftka and Watson (1991) discuss algorithms for tracking paths of optimal solutions. Lundberg and Poore (1993) report on a numerical implementation of a path following method for this problem. Our discussion is motivated by their exposition.

The Fritz John first-order necessary conditions for (4.6) imply the existence of $(\lambda, \nu) \in \mathbb{R}^{p+q} \times \mathbb{R}$ such that

$$\mathcal{L}_x(x, \lambda, \nu, \alpha) = 0, \tag{4.7}$$

$$c_i(x,\alpha) = 0, \quad i \in E, \tag{4.8}$$

$$\lambda_i c_i(x,\alpha) = 0, \quad i \in I, \tag{4.9}$$

$$\nu \geq 0,\ c_i(x,\alpha) \leq 0, \quad \lambda_i \geq 0,\ i \in I, \tag{4.10}$$

where $\mathcal{L}(x, \lambda, \nu, \alpha) = \nu f(x, \alpha) + \sum \lambda_i c_i(x, \alpha)$ is the Lagrangian.

Now an active set strategy is implemented by using the following homotopy equation for a path following algorithm:

$$H(x, \{\lambda_i\}_{i \in \mathcal{A}}, \nu, \alpha) = \begin{pmatrix} \mathcal{L}_x(x, \{\lambda_i\}_{i \in \mathcal{A}}, \nu, \alpha) \\ c_i(x, \alpha), \ i \in \mathcal{A} \\ \nu^2 + \sum \lambda_i^2 - 1 \end{pmatrix} = 0, \tag{4.11}$$

where $\mathcal{A}$ is the set of active constraints. Hence $\mathcal{A}$ includes all of the indices E and some of the indices I. During the path following procedure, this active set is adapted in such a way that the inequalities (4.10) are respected.

There are various technical difficulties (such as handling singularities or efficiently adapting the active set) which have to be overcome in order to create a successful implementation.

4.9. Linear and quadratic programming

Khachiyan (1979) started a new class of polynomial time algorithms for solving the linear programming problem. Karmarkar (1984) subsequently gave a much noted polynomial time algorithm based upon projective rescaling. Gill, Murray, Saunders, Tomlin and Wright (1986) noted that Karmarkar's algorithm is equivalent to a projected Newton barrier method which in turn is closely related to a recent class of polynomial time methods involving a continuation method, namely the tracing of the 'central path'. This last technique can be extended to quadratic programming problems, and both linear and nonlinear complementarity problems. Typically, algorithms of this nature are now referred to as *interior point* methods.

The presentation of a continuous trajectory (central path) of the iterative Karmarkar method was extensively studied by Bayer and Lagarias (1989), see also Sonnevend (1985). Megiddo (1988) related this path to the classical barrier path of nonlinear optimization (Fiacco and McCormick, 1968). Several authors have proposed algorithms that generally follow the central path to a solution, see, e.g., Renegar (1988a), Gonzaga (1988), Vaidya (1990), Kojima, Mizuno and Yoshise (1988, 1989) and Monteiro and Adler (1989).

To make the algorithms more efficient, variable steplength and/or higher order predictor algorithms have been proposed in Adler, Resende, Veiga and Karmarkar (1989), Mizuno, Todd and Ye (1992) and Sonnevend, Stoer and Zhao (1989, 1991). The algorithm of Mizuno *et al.* (1992) has subsequently been shown by Ye, Güler, Tapia and Zhang (1991) to have both polynomial time complexity and quadratic convergence. Kojima, Megiddo and Mizuno (1991a) think that there still remain differences between the theoretical primal-dual algorithms which enjoy global and/or polynomial-time convergence and the efficient implementations of primal-dual algorithms, see, e.g., Marsten, Subramanian, Saltzman, Lustig and Shanno (1990) and McShane, Monma and Shanno (1989).

Adler et al. (1989) report extensive computational experiments for an interior point implementation with solution times being in most cases less than those required by a state-of-the-art simplex method MINOS, see Murtagh and Saunders (1987). Karmarkar and Ramakrishnan (1991) report computational experience on large scale problems which are representative of large classes of applications of current interest. Their interior point implementation incorporates a preconditioned conjugate gradient method as a corrector step and is consistently faster than MINOS by orders of magnitude. Further computational experience comparing an interior point method OB1 and a simplex method CPLEX is reported in technical reports Bixby, Gregory, Lustig, Marsten and Shanno (1991), Carpenter and Shanno (1991) and Lustig, Marsten and Shanno (1991). Polak, Higgins and Mayne (1992) have given an algorithm for solving semi-infinite minimax problems which bears a resemblance to the interior penalty function methods. They report numerical results which show that the algorithm is extremely robust and its performance is at least comparable to that of current first-order minimax algorithms.

There is currently immense activity in studying and developing implementations of interior point algorithms. It is to be expected that our brief account will be outdated in a few years. For further details and literature, we refer to the recent surveys of Gonzaga (1992), Kojima, Megiddo, Noma and Yoshise (1991c), Todd (1989), Wright (1992), and the proceedings edited by Roos and Vial (1991). As an example, we outline the central path approach for a primal-dual linear programming problem, following the introductory parts of Monteiro and Adler (1989) and Mizuno *et al.* (1992).

Consider the following linear programming problem and its corresponding dual form:

Problem 4.9

$$\min_x \{c^* x : Ax = b,\ x \geq 0\}, \tag{4.12}$$

$$\max_y \{b^* y : A^* y + z = c,\ z \geq 0\}, \tag{4.13}$$

We make the following standard assumption.

Assumption 4.10 The rank of A equals the number of its rows, and the interior feasible set of the primal-dual problem

$$\mathcal{F}^o := \{(x, z) : x, z > 0,\ Ax = b,\ A^* y + z = c \text{ for some } y\}$$

is not empty.

It is well established that the linear programming problem has a unique

solution under these assumptions. The logarithmic barrier function method associated with Problem 4.9 is

$$\min_x \left\{ c^*x - \mu \sum_j \ln x_j : Ax = b,\ x > 0 \right\}, \tag{4.14}$$

where $\mu > 0$ is the barrier penalty parameter. Under Assumption 4.10, the logarithmic barrier function is strictly convex and has a unique minimal point $x(\mu)$ for all $\mu > 0$. Moreover, $x(\mu)$ tends to the unique solution of Problem 4.9 as μ tends to zero.

The Karush–Kuhn–Tucker optimality condition which characterizes the solution $x(\mu)$ can be expressed in the following way: $(x(\mu), z)$ must belong to the set

$$\mathcal{C} := \{(x, z) \in \mathcal{F}^o : \operatorname{diag}(x)z = \mu e\}, \tag{4.15}$$

where e denotes the column of ones. In fact, $\mathcal{C}$ is parametrized by μ and is commonly called the *central path* of the problem. It turns out that μ is related to the so-called *duality gap*: $c^*x - b^*y = x^*z$ via

$$\mu = \frac{x^*z}{n} \tag{4.16}$$

for $(x, z) \in \mathcal{C}$, where n is the number of columns of A.

From these remarks, it is clear that the objective now is to follow the central path $\mathcal{C}$ as μ tends to zero. In fact, most interior point methods can be viewed, one way or another, as a special path following method along these lines. The methods differ in the choice of predictor step, corrector procedure (usually one or several Newton type iterations) and predictor steplength control. Many papers discussing such methods or introducing new methods also contain a sophisticated complexity analysis, see, for example, Section 6.

These interior point algorithms typically require a phase I in which a feasible starting point is generated. A somewhat different approach is taken by Freund (1991) who introduces a shifted barrier function approach so that the need for phase I is obviated.

Finally, this technique is quite general and can be extended to quadratic programming problems and linear and nonlinear complementarity problems, see, e.g., Kojima, Megiddo and Ye (1992). The literature on interior methods is rapidly increasing, and the subject has become one of the major topics of mathematical programming. In our opinion, it is only a question of time until the venerable simplex methods will be superceded by interior point implementations.

5. Piecewise-linear methods

Up to now we have assumed that the map $H : \mathbb{R}^{n+1} \to \mathbf{R}^n$ was smooth. Next we will discuss piecewise-linear methods which can again be viewed as curve tracing methods, but which can be applied to nonsmooth situations. The piecewise-linear methods trace a polygonal path which is obtained by successively stepping through certain 'transversal' cells of a piecewise-linear manifold. The first and most prominent example of a piecewise-linear algorithm was designed by Lemke and Howson (1964) and Lemke (1965) to calculate a solution of the linear complementarity problem, see Section 5.2. This algorithm played a crucial role in the development of subsequent piecewise-linear algorithms. Scarf (1967) gave a numerically implementable proof of the Brouwer fixed point theorem, based upon Lemke's algorithm. Eaves (1972) observed that a related class of algorithms can be obtained by considering piecewise-linear approximations of homotopy maps. Thus the piecewise-linear continuation methods began to emerge as a parallel to the classical embedding or predictor–corrector methods.

The piecewise-linear methods require no smoothness of the underlying equations and hence have, at least in theory, a more general range of applicability than classical embedding methods. In fact, they can be used to calculate fixed points of set-valued maps. They are more combinatorial in nature and are closely related to the topological degree, see Peitgen and Siegberg (1981). Piecewise-linear continuation methods are usually considered to be less efficient than the predictor–corrector methods when the latter are applicable, especially in higher dimensions. The reasons for this lie in the fact that steplength adaptation and exploitation of special structure are more difficult to implement for piecewise-linear methods.

Eaves (1976) has given a very elegant geometric approach to general piecewise-linear methods, see also Eaves and Scarf (1976). We adopt this point of view and cast the notion of piecewise-linear algorithms into the general setting of subdivided manifolds which we will call *piecewise-linear manifolds*. Our exposition follows the introduction of Georg (1990) to some extent.

Let $\mathbf{E}$ denote some ~~am~~bient finite dimensional Euclidean space which contains all points arising in the sequel. A *half-space* η and the corresponding *hyperplane* $\partial\eta$ are defined by $\eta = \{y \in \mathbf{E} : x^*y \leq \alpha\}$ and $\partial\eta = \{y \in \mathbf{E} : x^*y = \alpha\}$, respectively, for some $x \in \mathbf{E}$ with $x \neq 0$ and some $\alpha \in \mathbb{R}$. A finite intersection of half-spaces is called a *cell*. If σ is a cell and ξ a half-space such that $\sigma \subset \xi$ and $\tau := \sigma \cap \partial\xi \neq \emptyset$, then the cell τ is called a *face* of σ. For reasons of notation we consider σ also to be a face of itself, and all other faces are *proper* faces of σ. The *dimension* of a cell is the dimension of its affine hull. In particular, the dimension of a singleton is 0 and the dimension of the empty set is -1. If the singleton $\{v\}$

is a face of σ, then v is called a *vertex* of σ. If τ is a face of σ such that $\dim \tau = \dim \sigma - 1$, then τ is called a *facet* of σ.

Definition 5.1 A *piecewise-linear manifold* of dimension n is a system $\mathcal{M} \neq \emptyset$ of cells of dimension n such that the following conditions hold:

1. If $\sigma_1, \sigma_2 \in \mathcal{M}$, then $\sigma_1 \cap \sigma_2$ is a common face of σ_1 and σ_2.
2. A cell τ of dimension $n-1$ can be a facet of at most two cells in $\mathcal{M}$.
3. The family $\mathcal{M}$ is locally finite, i.e. any relatively compact subset of

$$|\mathcal{M}| := \bigcup_{\sigma \in \mathcal{M}} \sigma \tag{5.1}$$

meets only finitely many cells $\sigma \in \mathcal{M}$.

The simplest example of a piecewise-linear manifold is $\mathbb{R}^n$ subdivided into unit cubes with integer vertices.

We introduce the *boundary* $\Delta\mathcal{M}$ of $\mathcal{M}$ as the system of facets which are common to exactly one cell of $\mathcal{M}$. Generally, we cannot expect $\Delta\mathcal{M}$ to again be a piecewise-linear manifold. However, this is true for the case that $|\mathcal{M}|$ is convex. Two cells which have a common facet τ are called *adjacent.* We say that one cell is *pivoted* into the other cell across the facet τ. We will see that piecewise-linear algorithms perform pivoting steps.

Typical for piecewise-linear path following is that only one current cell is stored in the computer, along with some additional data, and the pivoting step is performed by calling a subroutine which makes use of the data to determine an adjacent cell which then becomes the new current cell.

A cell of particular interest is a *simplex* $\sigma = [v_1, v_2, \ldots, v_{n+1}]$ of dimension n which is defined as the convex hull of $n+1$ affinely independent points $v_1, v_2, \ldots, v_{n+1} \in \mathbf{E}$. These points are the vertices of σ. If a piecewise-linear manifold $\mathcal{M}$ of dimension n consists only of simplices, then $\mathcal{M}$ is called a *pseudo manifold* of dimension n. Such manifolds are of special importance, see, e.g., Gould and Tolle (1983) and Todd (1976a). If a pseudo manifold $\mathcal{T}$ subdivides a set $|\mathcal{T}|$, then we also say that $\mathcal{T}$ *triangulates* $|\mathcal{T}|$. Some triangulations of $\mathbb{R}^n$ of practical importance had been previously considered by Coxeter (1934) and Freudenthal (1942), see also Todd (1976a). Eaves (1984) gave an overview of standard triangulations.

A simple triangulation can be generated by the following pivoting rule, see Allgower and Georg (1979) or Coxeter (1973): if

$$\sigma = [v_1, v_2, \ldots, v_i \ldots, v_{n+1}]$$

is a simplex in $\mathbf{R}^n$, and τ is the facet opposite a vertex v_i, then σ is pivoted across τ into $\tilde{\sigma} = [v_1, v_2, \ldots, \tilde{v}_i \ldots, v_{n+1}]$ by setting

$$\tilde{v}_i = \begin{cases} v_{i+1} + v_{i-1} - v_i & \text{for } 1 < i < n+1, \\ v_2 + v_{n+1} - v_1 & \text{for } i = 1, \\ v_n + v_1 - v_{n+1} & \text{for } i = n+1. \end{cases}$$

In fact, a minimal (nonempty) system of n-simplices in $\mathbb{R}^n$ which is closed under this pivoting rule is a triangulation of $\mathbb{R}^n$.

Let $\mathcal{M}$ be a piecewise-linear manifold of dimension $n+1$. We call $H : |\mathcal{M}| \to \mathbb{R}^n$ a *piecewise-linear map* if the restriction $H_\sigma : \sigma \to \mathbb{R}^n$ of H to σ is an affine map for all $\sigma \in \mathcal{M}$. In this case, H_σ can be uniquely extended to an affine map on the affine space spanned by σ. The Jacobian H'_σ has the property $H'_\sigma(x-y) = H_\sigma(x) - H_\sigma(y)$ for x, y in this affine space. Note that under an appropriate choice of basis H'_σ corresponds to an $(n, n+1)$-matrix which has a one-dimensional kernel in case of nondegeneracy, i.e. if its rank is maximal.

A piecewise-linear algorithm is a method for following a polygonal path in $H^{-1}(0)$. To avoid degeneracies, we introduce a concept of regularity, see Eaves (1976). A point $x \in |\mathcal{M}|$ is called a *regular point* of H if x is not contained in any face of dimension $< n$, and if H'_τ has maximal rank n for all facets τ. A value $y \in \mathbb{R}^n$ is a *regular value* of H if all points in $H^{-1}(y)$ are regular. By definition, y is vacuously a regular value if it is not contained in the range of H. If a point or value is not regular it is called *singular*. An analogue of Sard's theorem 4.1 holds, see, e.g., Eaves (1976) or Peitgen and Siegberg (1981) for details. This enables us to confine ourselves to regular values. We note that degeneracies could be handled via the concept of lexicographical ordering, see Dantzig (1963) and Todd (1976a).

Hence, for reasons of simplicity, we assume that all piecewise-linear maps under consideration here have zero as a regular value. This implies that $H^{-1}(0)$ consists of polygonal paths whose vertices are always in the interior of some facet. If σ is a cell, then $\sigma \cap H^{-1}(0)$ is a segment (two endpoints), a ray (one endpoint) or a line (no endpoint). The latter case is not of interest for piecewise-linear path following. A step of the method consists of following the ray or segment from one cell into a uniquely determined adjacent cell. The method is typically started at a point of the boundary or on a ray (coming from infinity), and it is typically terminated at a point of the boundary or in a ray (going to infinity). The numerical linear algebra required to perform one step of the method is typical for linear programming and usually involves n^2 operations for dense matrices (at least in the case that the cells are simplices).

Nearly all piecewise-linear manifolds $\mathcal{M}$ which are of importance for practical implementations, are orientable. If $\mathcal{M}$ is orientable and of dimension $n+1$, and if $H : \mathcal{M} \to \mathbb{R}^n$ is a piecewise-linear map, then it is possible to introduce an index for the piecewise-linear solution manifold $H^{-1}(0)$ which has important invariance properties and occasionally yields some useful information, see Eaves (1976), Eaves and Scarf (1976), Lemke and Grotzinger (1976), Shapley (1974) and Todd (1976c). It should be noted that this index is closely related, see, e.g., Peitgen (1982), to the topological index which

is a standard tool in topology and nonlinear analysis. Occasionally, index arguments are used to ensure a certain behaviour of the solution path.

We now give some examples of how the piecewise-linear path following methods are used.

5.1. Piecewise-linear homotopy algorithms

Let us first show how these ideas can be used to approximate a fixed point of a continuous bounded map $f : \mathbb{R}^n \to \mathbb{R}^n$ by applying piecewise-linear path following to an appropriate piecewise-linear homotopy map. Eaves (1972) presented the first such method. A restart method based on somewhat similar ideas was developed by Merrill (1972). A number of authors have studied the efficiency and complexity of piecewise-linear homotopy algorithms, see, e.g., Alexander (1987), Eaves and Yorke (1984), Saigal (1977, 1984), Saigal and Todd (1978), Saupe (1982), Todd (1982) and Todd (1986).

As an example of a piecewise-linear homotopy algorithm, let us sketch the algorithm of Eaves and Saigal (1972). We consider a triangulation $\mathcal{T}$ of $\mathbb{R}^n \times (0, 1]$ into $(n+1)$-simplices σ such that every simplex is contained in some slab $\mathbb{R}^n \times [2^{-k}, 2^{-k-1}]$ for $k = 0, 1, \ldots$. Let us call the maximum of the last coordinates of all vertices of σ the *level* of σ. We call $\mathcal{T}$ a *refining* triangulation if for $\sigma \in \mathcal{T}$, the diameter of σ tends to zero as the level of σ tends to zero. The first such triangulation was proposed by Eaves (1972). Todd (1976a) gave a triangulation with refining factor 1/2. Subsequently, many triangulations with arbitrary refining factors were developed, see Eaves (1984).

Consider the homotopy

$$\tilde{H}(x, \lambda) = x - \lambda x_0 - (1 - \lambda) f(x).$$

The idea is to follow a solution path from $(x_0, 1)$ to $(\bar{x}, 0)$ where x_0 is the starting point of the method and $\bar{x}$ is a fixed point of f we wish to approximate. However, there are no smoothness assumptions on f, and therefore a more subtle path following approach involving piecewise-linear approximations is required.

We denote by H the piecewise-linear map which interpolates $\tilde{H}$ on the vertices of the given refining triangulation $\mathcal{T}$. Then it is possible to follow the polygonal solution path $c(s) = (x(s), \lambda(s))$ in $H^{-1}(0)$ starting at $c(0) = (x_0, 1)$. For convenience we regard c to be parametrized by arclength $0 \leq s < s_0 \leq \infty$. From the boundedness of the map f it follows that $\lambda(s)$ tends to zero as s tends to s_0. Furthermore,

$$\lim_{s \to s_0} \|x(s) - f(x(s))\| = 0.$$

Since $x(s)$ remains bounded as s tends to s_0, this implies that every accumulation point of $x(s)$ is a fixed point of f.

These ideas can be extended to set-valued maps.

5.2. Lemke's algorithm

The first and most prominent example of a piecewise-linear algorithm was designed by Lemke (1965) and Lemke and Howson (1964) in order to calculate a solution of the linear complementarity problem. Subsequently, several authors have studied complementarity problems from the standpoint of piecewise-linear homotopy methods, see, e.g., Kojima (1974, 1979), Kojima, Nishino and Sekine (1976), Saigal (1971, 1976) and Todd (1976b). Complementarity problems can also be considered from an interior point algorithm viewpoint, see Section 4.9, hence by following a smooth path, see, e.g., Kojima, Mizuno and Noma (1990b), Kojima, Mizuno and Yoshise (1991d), Kojima, Megiddo and Noma (1991b), Kojima, Megiddo and Mizuno (1990a) and Mizuno (1992).

We present the Lemke algorithm as an example of a piecewise-linear algorithm since it played a crucial role in the development of subsequent piecewise-linear algorithms. Let us consider the following *linear complementarity problem*: Given an affine map $g : \mathbb{R}^n \to \mathbb{R}^n$, find an $x \in \mathbb{R}^n$ such that

$$x \in \mathbb{R}^n_+; \quad g(x) \in \mathbb{R}^n_+; \quad x^* g(x) = 0.$$

Here $\mathbb{R}_+$ denotes the set of nonnegative real numbers, and in the sequel we also denote the set of positive real numbers by $\mathbb{R}_{++}$. If $g(0) \in \mathbb{R}^n_+$, then $x = 0$ is a trivial solution to the problem. Hence this trivial case is always excluded and the additional assumption

$$g(0) \notin \mathbb{R}^n_+$$

is made. Linear complementarity problems arise in quadratic programming, bimatrix games, variational inequalities and economic equilibria problems, and numerical methods for their solution have been of considerable interest, see, e.g., Cottle (1974), Cottle and Dantzig (1968), Cottle, Golub and Sacher (1978) and Lemke (1980). See also the proceedings (Cottle, Gianessi and Lions, 1980) for further references.

For $x \in \mathbb{R}^n$ we introduce the positive part $x_+ \in \mathbb{R}^n_+$ by setting $e_i^* x_+ := \max\{e_i^* x, 0\}$, $i = 1, \ldots, n$ and the negative part $x_- \in \mathbb{R}^n_+$ by $x_- := (-x)_+$. The following formulae are then obvious: $x = x_+ - x_-$, $(x_+)^*(x_-) = 0$.

It is not difficult to show the following: Define $f : \mathbb{R}^n \to \mathbb{R}^n$ by $f(z) := g(z_+) - z_-$. If x is a solution of the linear complementarity problem, then $z := x - g(x)$ is a zero point of f. Conversely, if z is a zero point of f, then $x := z_+$ solves the linear complementarity problem.

The advantage which f provides is that it is obviously a piecewise-linear map if we subdivide $\mathbb{R}^n$ into orthants. This is the basis for our description of Lemke's algorithm. For a fixed $d \in \mathbb{R}^n_{++}$ we define the homotopy H :

$\mathbb{R}^n \times [0,\infty) \to \mathbb{R}^n$ by

$$H(x,\lambda) := f(x) + \lambda d.$$

For a given subset $I \subset \{1,2,\ldots,n\}$ an orthant can be written in the form

$$\sigma_I := \{\,(x,\lambda) : \lambda \geq 0,\ e_i^* x \geq 0 \text{ for } i \in I,\ e_i^* x \leq 0 \text{ for } i \notin I\,\}.$$

The collection of all such orthants forms a piecewise-linear manifold $\mathcal{M}$ (of dimension $n+1$) which subdivides $\mathbb{R}^n \times [0,\infty)$. Furthermore it is clear that $H : \mathcal{M} \to \mathbb{R}^n$ is a piecewise-linear map since $x \mapsto x_+$ switches its linearity character only at the coordinate hyperplanes.

Let us assume for simplicity (as usual) that zero is a regular value of H. Lemke's algorithm is started on a ray: if $\lambda > 0$ is sufficiently large, then

$$(-g(0) - \lambda d)_+ = 0 \quad \text{and} \quad (-g(0) - \lambda d)_- = g(0) + \lambda d \in \mathbb{R}^n_{++},$$

and consequently

$$H(-g(0) - \lambda d,\ \lambda) = 0.$$

Hence, the ray defined by

$$\lambda \in [\lambda_0,\infty) \longmapsto -g(0) - \lambda d \in \sigma_\emptyset \tag{5.2}$$

$$\text{for} \qquad \lambda_0 := \max_{i=1,\ldots,N} \frac{-g(0)[i]}{d[i]} \tag{5.3}$$

is used (for decreasing λ-values) to start the path following. Since the piecewise-linear manifold $\mathcal{M}$ consists of the orthants of $\mathbb{R}^n \times [0,\infty)$, it is finite, and there are only two possibilities:

1. The algorithm terminates on the boundary $|\partial\mathcal{M}| = \mathbb{R}^n \times \{0\}$ at a point $(z,0)$. Then z is a zero point of f, and hence z_+ solves the linear complementarity problem.
2. The algorithm terminates on a secondary ray. Then it can be shown, see Cottle (1974), that the linear complementarity problem has no solution, at least if the Jacobian g' belongs to a certain class of matrices.

5.3. Variable dimension algorithms

In recent years, a new class of piecewise-linear algorithms has attracted considerable attention. They are called *variable dimension algorithms* since they all start from a single point, a zero-dimensional simplex, and successively generate simplices of varying dimension, until a so-called completely labelled simplex is found. Numerical results from Kojima and Yamamoto (1984) indicate that these algorithms improve the computational efficiency of piecewise-linear homotopy methods. The first variable dimension algorithm is due to Kuhn (1969). However, this algorithm had the disadvantage that it could only be started from a vertex of a large triangulated standard simplex S, and therefore piecewise-linear homotopy algorithms were preferred.

By increasing the sophistication of Kuhn's algorithm considerably, van der Laan and Talman (1979) developed an algorithm which could start from any point inside S. It soon became clear, see Todd (1978), that this algorithm could be interpreted as a homotopy algorithm. Numerous other variable dimension algorithms were developed. Some of the latest are due to Dai, Sekitani and Yamamoto (1992), Dai and Yamamoto (1989), Kamiya and Talman (1990), Talman and Yamamoto (1989). Two unifying approaches have been given, one due to Kojima and Yamamoto (1982), the other due to Freund (1984a,b). A variable dimension algorithm which is easy to comprehend and may serve the reader as a gateway is the octrahedral algorithm of Wright (1981).

5.4. Approximating manifolds

The emphasis of this survey is on path following methods. We should note, however, that the ideas of predictor–corrector and piecewise-linear curve tracing can be extended to the approximation of implicitly defined manifolds $H^{-1}(0)$ where $H : \mathbb{R}^{N+K} \to \mathbb{R}^N$. Limitations of space preclude a detailed discussion.

There are two basic types of algorithms: one is the moving frame algorithm of Rheinboldt (1987), see also Rheinboldt (1988b), which is a higher dimensional analogue of the predictor–corrector method, the other is a piecewise-linear algorithm which has been developed in Allgower and Gnutzmann (1987), Allgower and Schmidt (1985), Gnutzmann (1989), Widmann (1990a,b), see also Chapter 15 of Allgower and Georg (1990).

The moving frame algorithm involves predictors that arise from a local triangulation of the tangent space at a current point. The corrector consists of a Newton-like method for projecting the generated mesh back to the manifold. This method is well-suited for smooth manifolds in which the dimension N is large, such as in multiple parameter nonlinear eigenvalue problems, see, e.g., Rheinboldt (1988b, 1992a). It has been applied to the calculation of fold curves and to differential-algebraic equations, see Dai and Rheinboldt (1990) and Rheinboldt (1986, 1991, 1992b).

So far, it has not been possible to make the moving frame algorithm global in the sense that a compact manifold is approximated (without holes or overlaps) by a piecewise-linear compact manifold. The latter task can be accomplished by the application of piecewise-linear algorithms. However, these algorithms become extremely costly for large N. The piecewise-linear algorithms have been applied to the visualization of body surfaces, see Allgower and Gnutzmann (1991), and to the approximation of surface and body integrals, see Allgower, Georg and Widmann (1991d). They can also be used as automatic mesh generators for boundary element methods, see Georg (1991).

6. Complexity

In modern complexity investigations of continuation-type methods the so-called α-theory of Smale (1986) is a convenient tool. This theory is closely related to the classical Kantorovich estimates for Newton iterations, see, e.g., Ortega and Rheinboldt (1970) and Deuflhard and Heindl (1979). In contrast to the Kantorovich estimates, Smale's estimates are based on information at only one point, involving however all derivatives. The maps under consideration have to be analytic.

On the other hand, an analytic map is characterized by all its derivatives at one point. In fact, Rheinboldt (1988a) showed that Smale's estimates can be derived from the Kantorovich estimates. However, for complexity considerations, it is more convenient to have all the relevant information situated at only one point. Let us briefly present Smale's estimates and show how they are used for complexity discussions. Our presentation is based on the introductory parts of the papers of Shub and Smale (1991) and Renegar and Shub (1992).

Let E, F be complex Banach spaces and $f : E \to F$ an analytic map. It would be possible to assume that f is given only on some open domain, but for reasons of simplicity of exposition we assume f to be defined on all of E. Then for each point $x \in E$ such that $Df(x) : E \to F$ is an isomorphism the following quantities are defined:

$$\beta(f,x) = \|Df(x)^{-1}f(x)\|, \tag{6.1}$$

$$\gamma(f,x) = \sup_{k>1} \frac{1}{k!}\|Df(x)^{-1}D^k f(x)\|^{1/(k-1)}, \tag{6.2}$$

$$\alpha(f,x) = \beta(f,x)\gamma(f,x), \tag{6.3}$$

$$\mathcal{N}_f(x) = x - Df(x)^{-1}f(x). \tag{6.4}$$

Note that $\mathcal{N}_f(x)$ is the Newton iterate of x. It it also convenient to introduce the notation

$$\mathcal{N}_f^\infty(x) = \lim_{i\to\infty} \mathcal{N}_f^i(x) \tag{6.5}$$

provided Newton's method started at x is convergent.

A related one-dimensional 'control' Newton method is occasionally generated from the following family of functions

$$h_{\beta,\gamma}(t) = \beta - t + \frac{\gamma t^2}{1-\gamma t}. \tag{6.6}$$

For $0 < \alpha < 3 - 2\sqrt{2} \approx 0.1716$, the function $h_{\beta,\gamma}$ has two real positive roots,

the smaller one being

$$\frac{\tau(\alpha)}{\gamma} = \frac{(\alpha+1) - \sqrt{(\alpha+1)^2 - 8\alpha}}{4\gamma}. \tag{6.7}$$

Moreover, $h''_{\beta,\gamma} > 0$ on the interval $(0, 1/\gamma)$. Thus, Newton's method starting at zero generates a strictly increasing sequence $t_i(\beta,\gamma) = \mathcal{N}^i_{h_{\beta,\gamma}}(0)$ converging to this root.

Occasionally, a slightly smaller upper bound for α is used, namely $\alpha_0 = \frac{1}{4}(13 - 3\sqrt{17}) \approx 0.1577$.

The following is a modification of Smale's α-theorem.

Theorem 6.1 Let $x_0 \in E$, $\alpha = \alpha(f, x_0)$, $\gamma = \gamma(f, x_0)$. If $\alpha \leq \alpha_0 \approx 0.1577$, then the iterates $x_{i+1} = \mathcal{N}_f(x_i)$ are defined and converge to a zero point $x_\infty = \mathcal{N}_f^\infty(x_0) \in E$ with the rate

$$\|x_{i+1} - x_i\| \leq \left(\tfrac{1}{2}\right)^{2^i - 1} \|x_1 - x_0\|.$$

Moreover, the following estimates hold:

$$\|x_\infty - x_0\| \leq \frac{\tau(\alpha)}{\gamma}, \quad \|x_\infty - x_1\| \leq \frac{\tau(\alpha) - \alpha}{\gamma}.$$

An easy consequence is

Corollary 6.2 $\|x_\infty - x_i\| \leq \varepsilon$ for $i \geq 1 + \log|\log \tau(\alpha)/\varepsilon\gamma|$.

Furthermore, by using the control Newton iterates $t_i = t_i(\beta,\gamma)$, a stricter estimate can be obtained under the same hypotheses:

Theorem 6.3 $\|x_i - x_{i-1}\| \leq t_i - t_{i-1}$.

Another property which is important for complexity discussions is the fact that α is upper semi-continuous, more precisely:

Proposition 6.4 Let $\psi(u) := 2u^2 - 4u + 1$ and $u := \gamma(f, x_0)\|x_0 - x\|$. Then

$$\alpha(f, x) \leq \frac{\alpha(f, x_0)(1-u) + u}{\psi(u)^2}.$$

From the previous proposition it is possible to obtain a uniform estimate for Newton steps:

Theorem 6.5 There are universal constants $\bar{\alpha} \approx 0.0802$ and $\bar{u} \approx 0.0221$ with the following property: Let $\bar{\gamma} > 0$ and $x, \zeta \in E$. If $\beta(f,\zeta) \leq \bar{\alpha}/\bar{\gamma}$ and $\|x - \zeta\| \leq \bar{u}/\bar{\gamma}$, then $\|\mathcal{N}_f(x) - \mathcal{N}_f^\infty(\zeta)\| \leq \bar{u}/\bar{\gamma}$.

This theorem is used to investigate the complexity of path following in the following way: Let $H : [0,1] \times E \to F$ be a continuous (homotopy) map which is analytic in the second argument. We further assume that a

continuous solution path $\zeta : [0,1] \to E$ exists, i.e. $H(t, \zeta(t)) = 0$ for $t \in [0,1]$, such that the derivative $H_\zeta(t, \zeta(t))$ is an isomorphism. The following crude path-following method can be designed: choose a subdivision $0 = t_0 < t_1 < \cdots < t_k = 1$ and define

$$x_i := \mathcal{N}_{H(t_i,.)}(x_{i-1}) \quad \text{for } i = 1, \ldots, k. \tag{6.8}$$

It is clear that this method follows the solution curve if $\|x_0 - \zeta(0)\|$ and $|t_i - t_{i-1}|$ are small enough. Of course, the crucial number for complexity considerations is the number k of Newton steps involved in this embedding method. If it is wished to obtain some points of the solution curve with high accuracy, then the complexity described in Corollary 6.2 has to be added.

The preceding analysis immediately furnishes a tool to determine the estimates necessary for a successful tracing of the solution curve:

Theorem 6.6 Let $\|x_0 - \zeta(0)\| \leq \bar{u}/\bar{\gamma}$, and let the mesh t_i be so fine that $\beta(H(t_i, .), \zeta(t_{i-1})) \leq \bar{\alpha}/\bar{\gamma}$ and $\gamma(H(t_i, .), \zeta(t_{i-1})) \leq \bar{\gamma}$. Then the embedding method (6.8) follows the solution path ζ. In fact, $\|x_i - \zeta(t_i)\| \leq \bar{u}/\bar{\gamma}$.

To summarize, we have outlined a program for approaching complexity investigations when Newton steps are the primary tool of path following methods. As can be seen from the last theorem, the success of the approach depends heavily on the availability of estimates $\beta(H(t, .), \zeta(s)) \leq C_1|t - s|$ and $\gamma(H(t, .), \zeta(s)) \leq C_2|t - s|$ with explicit constants C_1 and C_2.

This program was carried out by Shub and Smale (1991) for the case of a homotopy method for calculating all solutions of a system of polynomial equations (Bezout's theorem). A previous effort along similar lines was described by Renegar (1987).

Recently, this approach has also been used by Renegar and Shub (1992) for a unified complexity analysis of various interior methods designed for solving linear and convex quadratic programming problems. They obtain and rederive various 'polynomial time' estimates. The linear programming barrier method was first analysed by Gonzaga (1988). The quadratic programming barrier method was analysed by Goldfarb and Liu (1991). A primal-dual linear programming algorithm was investigated by Kojima *et al.* (1988) and Monteiro and Adler (1989). The algorithm has roots in Megiddo (1988). Primal-dual linear complementarity and quadratic programming algorithms were discussed by Kojima *et al.* (1989) and Monteiro and Adler (1989). All of these algorithms follow the *central trajectory* studied by Bayer and Lagarias (1989) and Megiddo and Shub (1989). For the case of the linear complementarity problem, Mizuno, Yoshise and Kikuchi (1989) present several implementations and report computational experience which confirms the polynomial complexity.

This discussion involved path following methods of Newton type. Renegar

(1985), see also Renegar (1988b), has made complexity investigations for piecewise-linear path following methods.

7. Available software

We conclude the paper by listing some available software related to path following and indicate how the reader might access these codes. No attempt to compare or evaluate the various codes is offered. In any case, our opinion is that path following codes always need to be considerably adapted to the special purposes for which they are designed. The path following literature offers various tools for accomplishing such tasks. Although there are some general purpose codes, probably none will slay every dragon.

Rheinboldt, Roose and Seydel (1990) present a list of features and options that appear to be necessary or desirable for continuation codes. This should be viewed as a guideline for people who want to create a new code.

Several of the codes can be accessed via *netlib*: The best way to obtain them is to ftp into `netlib@research.att.com`, login as netlib, password = your e-mail address. It is also possible to e-mail to netlib by writing *send index*. Information on how to proceed will then be e-mailed back to you.

7.1. ALCON

This sofware package has been written by Deuflhard, Fiedler and Kunkel (1987). `ALCON` is a continuation method for algebraic equations $f(x,\tau) = 0$, based on QR factorization as a solver for the arising equations in the Gauss–Newton iteration of the corrector step. Turning points and simple bifurcations can be computed on demand. It can be found in the electronic library of the Konrad Zuse Zentrum für Informationstechnik in Berlin. The reader may telnet or ftp to sc.ZIB-Berlin.de (130.73.108.11) and login under the user identification elib, no password is required. The sources can be found in the directory /pub/ELIB/codelib either in unpacked form or as a tar.Z file.

7.2. AUTO

This is a software package written by E. Doedel. It is mainly intended to investigate bifurcation phenomena. There is a charge of $175 for the software, a manual by Doedel and Kernévez (1986) is also available, contact: S. K. Shull, Applied Mathematics, 217-50, California Institute of Technology, Pasadena, CA 91125, USA. Telephone: (818) 356-4560.

7.3. BIFPACK

This package has been written by Seydel (1991a). It is meant primarily for bifurcation analysis of ODEs. This is not a public domain software.

However, as a research tool, it is freely distributed for *noncommercial* use, except for a $20 contribution for handling. Indicate whether you prefer `BIFPACK` on 5.25 in or on 3.5 in diskette (1.4 MB, DOS double-density). Contact: Professor Rüdiger Seydel, Abt. Mathematik VI, Universität Ulm, Postfach 4066, W - 7900 Ulm, Germany.

e-mail: `seydel@rz.uni-ulm.dbp.de`

7.4. CONKUB

This is an interactive program for continuation and bifurcation of large systems of nonlinear equations written by Mejia (1986), see also Mejia (1990). It is currently available from him via e-mail:

`ray@helix.nih.gov`.

7.5. DERPAR

This package was written by Kubíček (1976), and Holodniok and Kubíček (1984). This is a Fortran subprogram for the evaluation of the dependence of the solution of a nonlinear system on a parameter. The modified method of Davidenko, which applies the Implicit Function Theorem, is used in combination with Newton's method and Adam's integration formulae. The program can be accessed via netlib, see number 502 in the directory *toms*.

7.6. HOMPACK

This is a suite of FORTRAN 77 subroutines for solving nonlinear systems of equations by homotopy methods, written by L. T. Watson, see Watson *et al.* (1987). There are subroutines for fixed point, zero finding, and general homotopy curve tracking problems, utilizing both dense and sparse Jacobian matrices, and implementing three different algorithms: ODE-based, normal flow and augmented Jacobian. The program can be accessed via netlib under the directory *hompack*. See also number 652 in the directory *toms*.

7.7. LOCBIF

A. Khibnik and collaborators in Moscow have developed several codes for path following and bifurcation analysis. `CYCLE` is a one-parameter continuation program for limit cycles. `LINLBF` has been designed for multi-parameter bifircation analysis of equilibrium points, limit cycles, fixed points of maps, respectively. `LOCBIF` is an interactive program built originally on the top of `LINLBF`. People interested in trying this software should contact A. Khibnik via e-mail:

`na.khibnik@na-net.ornl.gov`.

7.8. OB1

This interior point method has been written by I. J. Lustig, R. E. Marsten and D. F. Shanno. The version of `OB1` that implements a primal-dual algorithm for linear programming is available in source code form to academics from Roy Marsten at Georgia Tech. This is the December 1989 version, also known as the WRIP (Workshop on Research in Programming) version. The current version of `OB1` is commercial. It implements a primal-dual predictor–corrector algorithm for linear programming and is available from XMP Software at prices ranging from $15,000 to $100,000: XMP Software, Suite 279, Bldg 802, 930 Tahoe Blvd, Incline Village, NV 89451, phone: (702) 831- 4XMP, e-mail:

`tlowe@mcimail.com`

7.9. PATH

This software package for dynamical systems was originally coded in FORTRAN 77 by Kaas-Petersen (1989), and is currently modified to include a graphical interface. According to the workers at the Technical University of Denmark, it seems to be able to handle much larger systems of ODE's than `AUTO`. For more details and availability, readers may contact Michael Rose via e-mail:

`lamfmr@lamf.dth.dk.`

7.10. PITCON

This is a Fortran subprogram for continuation and limit points, written by Rheinboldt and Burkardt (1983b), see also Rheinboldt and Burkardt (1983a). It is used for computing solutions of a nonlinear system of equations containing a parameter. The location of target points where a given variable has a specified value can be located. Limit points are also identified. It uses a local parameterization based on curvature estimates to control the choice of parameter value. The program can be accessed via netlib under the directory *contin*. See also number 596 in the directory *toms*.

7.11. PLALGO

This is a software for piecewise-linear homotopy methods developed by Todd (1981). It can be obtained from him via e-mail:

`miketodd@orie.cornell.edu.`

No support is available, and he says that on-line documentation is weak, although he can send a hard copy.

7.12. pla_s_k

This is a C program, written by Widmann (1990a), for triangulating surfaces in $\mathbb{R}^3$ which are implicitly defined, see Section 5.4. It incorporates mesh smoothing and some other features. It is particularly suited for mesh generation (e.g. for boundary element methods) and for visualization purposes. The program can be obtained via e-mail:

`Georg@Math.ColoState.Edu.`

7.13. PLTMG

This package has been written by R. E. Bank, see also Bank and Chan (1986). It solves elliptic partial differential equations in general regions of the plane. It features adaptive local mesh refinement, multigrid iteration, and a pseudo-arclength continuation option for parameter dependencies. The package includes an initial mesh generator and several graphics packages. Full documentation can be obtained in the PLTMG User's Guide by R. E. Bank, available from SIAM publications via e-mail:

`SIAMPUBS@wharton.upenn.edu.`

The program can be accessed via netlib under the directory *pltmg*.

7.14. Last and least

The book Allgower and Georg (1990) contains several Fortran codes for path following which are to be regarded primarily as illustrations. The intention was to encourage the readers to experiment and be led to make improvements and adaptations suited to their particular applications. We emphasize that these programs should not be regarded as programs of library quality. They can be obtained via e-mail:

`Georg@Math.ColoState.Edu.`

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