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Numerical continuation methods: a perspective

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Abstract

In this historical perspective the principal numerical approaches to continuation methods are outlined in the framework of the mathematical sources that contributed to their development, notably homotopy and degree theory, simplicial complexes and mappings, submanifolds defined by submersions, and singularity and foldpoint theory. © 2000 Elsevier Science B.V. All rights reserved.

1. Introduction

The term *numerical continuation methods*, as it is typically used, covers a variety of topics which — while related — exhibit also considerable differences. This is already reflected in some of the alternate terminology that has been used, such as *imbedding methods*, *homotopy methods*, *parameter variation methods*, or *incremental methods*, just to name a few.

In order to provide an overview from a historical viewpoint, it appears that the general structure of the area is illuminated best by focusing first on the principal underlying mathematical sources that have contributed to its development. Accordingly, in the first two sections we concentrate on (i) homotopy and degree theory, (ii) simplicial complexes and mappings, (iii) submanifolds defined by submersions, and (iv) singularity and foldpoint theory. Then the subsequent sections address some of the numerical approaches growing out of this theoretical basis. Since methods based on (ii) above; that is, notably, the piecewise linear methods, are covered in another article [5] in this volume, this area will not be addressed here any further. Clearly, in a brief article as this one, only the bare outlines of the theoretical and computational topics can be sketched and many aspects had to be left out. An effort was made to give references to sources that provide not only further details but also relevant bibliographic data to the large literature in the area.

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2. Theoretical sources: homotopies

An important task in many applications is the solution of nonlinear equations defined on finite- or infinite-dimensional spaces. In order to avoid technical details we restrict here the discussion to the finite-dimensional case

$$F(y) = 0, \quad F : \mathbb{R}^m \to \mathbb{R}^m. \tag{1}$$

The computational approximation of a solution $y^* \in \mathbb{R}^m$ of (1) typically requires the application of some iterative process. However, except in rare circumstances, such a process will converge to y^* only when started from a point (or points) in a neighborhood of the desired — but, of course, unknown — point y^*. In other words, for an effective overall solution process we need tools for localizing the area of the expected solution and for constructing acceptable starting data for the iteration.

Evidently, localization requires the determination of a suitably small domain which is guaranteed to contain a solution — hopefully the one we are interested in. This represents a problem about the existence of solutions of (1). Among the many approaches for addressing it, an important one — dating back to the second half of the 19th century — is the use of homotopies.

2.1. Homotopies and Brouwer degree

Let $\Omega \in \mathbb{R}^m$ be a given open set and $C(\bar{\Omega})$ the set of all continuous mappings from the closure $\bar{\Omega}$ into $\mathbb{R}^m$. Two members $F_0, F_1 \in C(\bar{\Omega})$ are *homotopic* if there exists a continuous mapping

$$H : \bar{\Omega} \times [0,1] \to \mathbb{R}^m \tag{2}$$

such that $H(y,0) = F_0(y)$, $H(y,1) = F_1(y)$ for all $y \in \bar{\Omega}$. This introduces an equivalence relation on $C(\bar{\Omega})$. The topic of homotopy theory is the study of properties of the functions in $C(\bar{\Omega})$ that are preserved under this equivalence relation.

Among the properties of interest is, of course, the solvability of Eq. (1) defined by homotopic members of $C(\bar{\Omega})$. An important tool is here the concept of the degree of a mapping. Without entering into historical details we mention only that the concept of a local degree; that is, a degree with respect to a neighborhood of an isolated solution, was introduced by L. Kronecker in 1869. The extension of this local concept to a degree in the large was given by L. Brouwer in 1912. Then, in 1934, the seminal work of J. Leray and J. Schauder opened up the generalization to mappings on infinite-dimensional spaces. We refer, e.g., to [2,33,26] for some details and references.

The Brouwer degree is by nature a topological concept but it can also be defined analytically. We sketch only the general idea. For any C^1-map F from some open set of $\mathbb{R}^n$ into $\mathbb{R}^m$ a vector $z \in \mathbb{R}^m$ is called a *regular value* of F if $DF(y)$ has maximal rank $\min(n,m)$ for all $y \in F^{-1}(z)$. Let Ω be a bounded set and consider a mapping $F \in C(\bar{\Omega}) \cap C^1(\Omega)$ and some regular value $z \in \mathbb{R}^m$ of F. Then the cardinality of $F^{-1}(z)$ must be finite and the *degree* of F with respect to Ω and y can be defined as

$$\deg(F, \Omega, z) := \sum_{v} \operatorname{sign} \det(DF(y^v)), \tag{3}$$

where the sum is taken over all $y^v \in F^{-1}(z)$. Now, appropriately defined approximations can be used to obtain an extended definition of the degree for any $F \in C(\bar{\Omega})$ and $b \notin F(\partial\Omega)$. For the details we refer, e.g., to [33] or [26].

The following result lists some relevant properties of the Brouwer degree.

Theorem 1 (Homotopy invariance). *Let $\Omega \subset \mathbb{R}^m$ be bounded and open.*

(i) *If $deg(F,\Omega,z) \neq 0$ for $F \in C(\bar{\Omega})$ and $z \notin F(\delta\Omega)$ then $F(y) = z$ has a solution in Ω.*
(ii) *If for some mapping* (2) *the restricted mappings $H_t := H(\cdot,t)$ are in $C(\bar{\Omega})$ for each $t \in [0,1]$ and*

$$z \notin H_t(\partial\Omega), \quad \forall t \in [0,1], \tag{4}$$

then $deg(H_t,\Omega,z)$ is constant for $t \in [0,1]$.

These results show that we can deduce solvability properties for a map F_1 from corresponding known facts about another homotopic map F_0. This represents a powerful tool for the establishment of existence results and for the development of computational methods. In that connection, we note that condition (4) is indeed essential as the following example shows:

$$H : [-1,1] \times [0,1] \to \mathbb{R}^1, \quad H(y,t) := y^2 - \tfrac{1}{2} + t, \ \ z = 0. \tag{5}$$

Here $H_0(y) = 0$ has two distinct roots in $[-1,1]$ while $H_1(y) = 0$ has none. Theorem 1(ii) does not hold because $0 \in H_1(\partial\Omega)$.

2.2. Simplicial approximations

The above homotopy results constitute a theoretical source of an important subclass of continuation methods, the so-called *piecewise linear methods*. In order to see this we begin with a summary of some basic definitions.

An k-dimensional simplex (or simply k-simplex), σ^k in $\mathbb{R}^n$, $n \geqslant k \geqslant 0$, is the closed, convex hull, $\sigma^k = \mathrm{co}(u^0,\ldots,u^k)$, of $k+1$ points $u^0,\ldots,u^k \in \mathbb{R}^n$ that are not contained in any affine subspace of dimension less than k. These points form the *vertex set* $\mathrm{vert}(\sigma^k) = \{u^0,\ldots,u^k\}$ of σ^k. The *barycenter* of σ^k is the point $x = [1/(k+1)](u_0 + \cdots + u_k)$ and the *diameter* of σ^k is defined as $\mathrm{diam}(\sigma^k) = \max\{||u^j - u^i||_2 : i,j = 0,\ldots,k\}$. An ℓ-simplex $\sigma^\ell \in \mathbb{R}^n$ is an ℓ-face of σ^k if $\mathrm{vert}(\sigma^\ell) \subset \mathrm{vert}(\sigma^k)$. The unique k-face is σ^k itself and the 0-faces are the vertices.

A (finite) *simplicial complex* of dimension k is a finite set $\mathscr{S}$ of k-simplices[1] in $\mathbb{R}^n$ with the two properties

(a) If $\sigma \in \mathscr{S}$ then all its faces belong to $\mathscr{S}$ as well,
(b) for $\sigma^1, \sigma^2 \in \mathscr{S}$, $\sigma_1 \cap \sigma_2$ is either empty or a common face.

For a simplicial complex $\mathscr{S}$, the *carrier* is the set $|\mathscr{S}| = \{x \in \mathbb{R}^n : x \in \sigma \text{ for some } \sigma \in \mathscr{S}\}$, and $\mathrm{vert}(\mathscr{S}) = \{x \in \mathbb{R}^n : x \in \mathrm{vert}(\sigma) \text{ for some } \sigma \in \mathscr{S}\}$ is the *vertex set*. Since $\mathscr{S}$ is assumed to be finite, the carrier $|\mathscr{S}|$ must be a compact subset of $\mathbb{R}^n$ and the diameter $\mathrm{diam}(\mathscr{S})$ is well defined as the largest diameter of the simplices of $\mathscr{S}$.

[1] We exclude here complexes of simplices with different dimensions, usually permitted in topology.

Let $\mathscr{S}$ and $\mathscr{T}$ be two simplicial complexes of $\mathbb{R}^n$ (not necessarily of the same dimension). A mapping $K : \mathscr{S} \to \mathscr{T}$ is a *simplicial map* if it maps every simplex of $\mathscr{S}$ affinely onto a simplex of $\mathscr{T}$. Since an affine map of a simplex is fully defined by the images of its vertices, it follows that a simplicial map $K : \mathscr{S} \to \mathscr{T}$ is fully defined by specifying the image $K(x) \in \mathrm{vert}(\mathscr{T})$ of every $x \in \mathrm{vert}(\mathscr{S})$. Note that the images of different vertices of $\mathscr{S}$ need not be distinct. Clearly a simplicial map $K : \mathscr{S} \to \mathscr{T}$ induces a continuous mapping from $|\mathscr{S}|$ to $|\mathscr{T}|$.

A simplicial complex $\mathscr{T}$ is a subdivision of the simplicial complex $\mathscr{S}$ if $|\mathscr{S}| = |\mathscr{T}|$ and each simplex of $\mathscr{T}$ is contained in a simplex of $\mathscr{S}$. A subdivision of $\mathscr{S}$ is fully specified once subdivisions of each of its simplices are provided. For example, let $\mathrm{vert}(\sigma^k) = \{u^0, \ldots, u^k\}$ be the vertex set of a k-simplex σ^k and u^* its barycenter. Then, for each j, $0 \leqslant j \leqslant k$, the k-simplex $\sigma^{(k,j)}$ with the vertex set $(\mathrm{vert}(\sigma^k) \setminus u^j) \cup u^*$ is contained in σ^k and the collection of the $k+1$ simplices $\sigma^{(k,j)}$, $j = 0, \ldots, k$, forms a subdivision of σ^k, the so-called barycentric subdivision. Evidently, by repeated barycentric subdivision, complexes with arbitrarily small diameter can be generated. This holds also for various other types of subdivisions (see, e.g., [37]).

The following basic result about approximations of continuous mappings by simplicial mappings is proved, e.g., in [2]. It provides the intended connection with the results of the previous subsection.

Theorem 2. *Let $\mathscr{S}$ and $\mathscr{T}$ be simplicial complexes of $\mathbb{R}^n$ and $\mathbb{R}^m$, respectively, and suppose that $\{\mathscr{S}^r\}_{r=1}^{\infty}$ is a sequence of successive subdivisions of $\mathscr{S}$ for which the diameter tends to zero when $r \to \infty$. If $F : |\mathscr{S}| \to |\mathscr{T}|$ is a continuous mapping, then, for any $\varepsilon > 0$, there exists a sufficiently large r and a simplicial map $K_r : \mathscr{S}^r \to \mathscr{T}$ such that*

$$\max_{x \in |\mathscr{S}|} ||F(x) - K_r(x)||_2 \leqslant \varepsilon.$$

Moreover, there is a continuous homotopy $H : |\mathscr{S}| \times [0,1] \to \mathbb{R}^m$ such that $H(x,0) = K_r(x)$, $H(x,1) = F(x)$.

In other words, a continuous mapping F between the carries of the complexes $\mathscr{S}$ and $\mathscr{T}$ can be approximated arbitrarily closely by a simplicial mapping between these complexes which, at the same time, is homotopic to F. Hence, in particular, Theorem 1 can be applied here. This represents, in essence, the theoretical basis of the mentioned piecewise linear continuation methods.

3. Theoretical sources: manifolds

In applications nonlinear equations (1) typically arise as models of physical systems which almost always involve various parameters. While some of these parameters can be fixed, for others we often may know only a possible range. Then interest centers in detecting any significant changes in the behavior of the solutions when these parameters are varied, as for instance, when a mechanical structure buckles.

Problems of this type require the changeable parameters to be incorporated in the specification of the equations. In other words, in place of (1), we have to consider now equations of the form

$$F(y, \lambda) = 0, \quad F : \mathbb{R}^m \times \mathbb{R}^d \to \mathbb{R}^m, \ d > 0, \tag{6}$$

where $y \in \mathbb{R}^m$ typically represents a state vector and $\lambda \in \mathbb{R}^d$ is the parameter vector. In working with such systems, it is often desirable to combine the vectors y and λ into a single vector $x \in \mathbb{R}^n$ of dimension $n = m + d$. This means that (6) is written in the form

$$F(x) = 0, \quad F : \mathbb{R}^n \to \mathbb{R}^m \tag{7}$$

and that the *parameter splitting*

$$\mathbb{R}^n = \mathbb{R}^m \times \mathbb{R}^d, \quad x = (y, \lambda), \ \ y \in \mathbb{R}^m, \ \ \lambda \in \mathbb{R}^d \tag{8}$$

is disregarded.

For equations of form (7) (as well as (6)) it rarely makes sense to focus on the determination of a specific solution $x \in F^{-1}(0)$. Instead, as noted, interest centers on analyzing the properties of relevant parts of the solution set $\mathcal{M} = F^{-1}(0)$. In most cases, this set has the structure of a differentiable submanifold of $\mathbb{R}^n$. In the study of equilibrium problems in engineering this is often reflected by the use of the term 'equilibrium surface', although, rarely, any mathematical characterization of the manifold structure of $\mathcal{M}$ is provided.

3.1. Submanifolds of $\mathbb{R}^n$

In this section we summarize some relevant definitions and results about manifold and refer for details, e.g., to [1]. Here the dimensions n, m are assumed to be given such that $n = m + d$, $d > 0$, and ρ denotes a *positive* integer or ∞.

When $F : \mathbb{R}^n \to \mathbb{R}^m$ is of class C^ρ on a open set $\Omega \subset \mathbb{R}^n$, then F is an *immersion* or *submersion* at a point $x^0 \in \Omega$ if its first derivative $DF(x^0) \in \mathscr{L}(\mathbb{R}^n, \mathbb{R}^m)$ is a one-to-one mapping or a mapping onto $\mathbb{R}^m$, respectively. More generally, F is an immersion or submersion on a subset $\Omega_0 \subset \Omega$ if it has that property at each point of Ω_0.

We use the following characterization of submanifolds of $\mathbb{R}^n$.

Definition 3. A subset $\mathcal{M} \subset \mathbb{R}^n$ is a d-dimensional C^ρ-submanifold of $\mathbb{R}^n$ if $\mathcal{M}$ is nonempty and for every $x^0 \in \mathcal{M}$ there exists an open neighborhood $\mathcal{U}$ of x^0 in $\mathbb{R}^n$ and a submersion $F : \mathcal{U} \mapsto \mathbb{R}^m$ of class C^ρ such that $\mathcal{M} \cap \mathcal{U} = F^{-1}(0)$.

An equivalent definition utilizes the concept of a *local parametrization*:

Definition 4. Let $\mathcal{M}$ be a nonempty subset of $\mathbb{R}^n$. A local d-dimensional C^ρ parametrization of $\mathcal{M}$ is a pair $(\mathcal{U}, \phi)$ where $\mathcal{U} \subset \mathbb{R}^d$ is a nonempty open set and $\phi : \mathcal{U} \mapsto \mathbb{R}^m$ a mapping of class C^ρ such that

(i) $\phi(\mathcal{U})$ is an open subset of $\mathcal{M}$ (under the induced topology of $\mathbb{R}^n$) and ϕ is a homeomorphism of $\mathcal{U}$ onto $\phi(\mathcal{U})$,
(ii) ϕ is an immersion on $\mathcal{U}$.

If $x^0 \in \mathcal{M}$ and $(\mathcal{U}, \phi)$ is a local d-dimensional C^ρ parametrization of $\mathcal{M}$ such that $x^0 \in \phi(\mathcal{U})$, then $(\mathcal{U}, \phi)$ is called a local d-dimensional C^ρ parametrization of $\mathcal{M}$ near x^0.

Theorem 5. *A nonempty subset $\mathscr{M} \subset \mathbb{R}^n$ is a C^ρ-submanifold of $\mathbb{R}^n$ of dimension d if and only if for every $x^0 \in \mathscr{M}$ there exists a local d-dimensional C^ρ parametrization of $\mathscr{M}$ near x^0. When $\mathscr{M}$ is a d-dimensional C^ρ-submanifold of $\mathbb{R}^n$ then any local C^ρ parametrization of $\mathscr{M}$ is necessarily d-dimensional.*

The following result is central to our discussion.

Theorem 6 (Submersion Theorem)**.** *Suppose that, for the C^ρ mapping $F : \mathbb{R}^n \to \mathbb{R}^m$ on the open set Ω, the set $\mathscr{M} = F^{-1}(0)$ is not empty and F is a submersion on $\mathscr{M}$. Then $\mathscr{M}$ is a d-dimensional C^ρ-submanifold of $\mathbb{R}^n$.*

In our setting we can define tangent spaces of submanifolds of $\mathbb{R}^n$ as follows:

Definition 7. Let $\mathscr{M}$ be a d-dimensional C^ρ-submanifold of $\mathbb{R}^n$. For any $x^0 \in \mathscr{M}$ the tangent space $T_{x^0}\mathscr{M}$ of $\mathscr{M}$ at x^0 is the d-dimensional linear subspace of $\mathbb{R}^n$ defined by

$$T_{x^0}\mathscr{M} := \operatorname{rge} D\phi(\phi^{-1}(x^0)), \tag{9}$$

where $(\mathscr{U}, \phi)$ is any local C^ρ parametrization of $\mathscr{M}$ near x^0. The subset $T\mathscr{M} = \bigcup_{x\in\mathscr{M}} [\{x\} \times T_x\mathscr{M}]$ of $\mathbb{R}^n \times \mathbb{R}^n$ is the tangent bundle of $\mathscr{M}$.

This definition is independent of the choice of the local parametrization. In the setting of the Submersion Theorem 6 this follows directly from the fact that then $T_{x^0}\mathscr{M} = \ker DF(x^0)$. The following result provides a basis for the computational evaluation of local parametrizations.

Theorem 8. *Under the conditions of the submersion theorem on the mapping F let $U \in \mathscr{L}(\mathbb{R}^d, \mathbb{R}^n)$ be an isomorphism from $\mathbb{R}^d$ onto a d-dimensional linear subspace $T \subset \mathbb{R}^n$. Then the mapping*

$$K : \mathbb{R}^n \to \mathbb{R}^k \times \mathbb{R}^d, \quad K(x) := (F(x), U^{\mathrm{T}}x), \ \ \forall x \in \mathbb{R}^n, \tag{10}$$

is a local diffeomorphism on an open neighborhood of $x^c \in \mathscr{M}$ in $\mathbb{R}^n$ if and only if

$$T_{x^c}\mathscr{M} \cap T^\perp = \{0\}. \tag{11}$$

Let $j : \mathbb{R}^d \to \mathbb{R}^n \times \mathbb{R}^d$ denote the canonical injection that maps $\mathbb{R}^d$ isomorphically to $\{0\} \times \mathbb{R}^d$. If (11) holds at x^c then there exists an open set $\mathscr{U}^d$ of $\mathbb{R}^d$ such that the pair $(\mathscr{U}^d, \phi)$, defined with the mapping $\phi = K^{-1} \circ j : \mathscr{U}^d \to \mathbb{R}^n$, is a local parametrization of $\mathscr{M}$ near x^c.

We call a d-dimensional linear subspace $T \subset \mathbb{R}^n$ a *coordinate subspace* of $\mathscr{M}$ at $x^c \in \mathscr{M}$ if (11) holds. At any point $x^c \in \mathscr{M}$ an obvious choice for a coordinate subspace is $T = T_{x^c}\mathscr{M}$, the *tangential coordinate space* of $\mathscr{M}$ at that point. When we work with equations of the form (6); that, is when the parameter splitting (8) is available, then the parameter space $T = \{0\} \times \mathbb{R}^d$ is another possible choice of coordinate subspace. In that case, the point x^c where (11) fails to hold often have special significance.

A frequent approach in the study of the solution manifold $\mathscr{M} = F^{-1}(0)$ of Eq. (7) is to work with suitable paths on $\mathscr{M}$. Such a path may be specified by means of an augmented system

$$G(x) = 0, \quad G(x) := \begin{pmatrix} F(x) \\ \Gamma(x) \end{pmatrix}, \quad \Gamma : \mathbb{R}^n \to \mathbb{R}^{d-1} \tag{12}$$

of $n-1$ equations and n variables. If G is of class C^ρ on the open set Ω and a submersion on the solution set $G^{-1}(0)$, then this set is indeed a one-dimensional submanifold of $\mathscr{M}$ provided, of course, it is not empty. Thus, (12) is a problem of form (7) with $d = 1$.

Here there is certainly some similarity with the homotopy mappings (2). But the geometric meaning is very different. In fact, (2) relates the two mappings $H_0 := H(\cdot, 0)$ and $H_1 := H(\cdot, 1)$, each with their own solution set, and the t-variable does have a very specific meaning. On the other hand, (12) defines a path that connects certain points of $\mathscr{M}$; that is, solutions of (7). Moreover, unless the augmenting mapping Γ in (12) is suitably chosen, no component of x can be singled out in any way. Of course, in many cases Γ does have a special form. For instance, when the parameter splitting (8) is available then we may use, $\Gamma(y, \lambda) := (\lambda_1 - \lambda_1^0, \ldots, \lambda_{k-1} - \lambda_{k-1}^0, \lambda_{k+1} - \lambda_{k+1}^0, \ldots, \lambda_d - \lambda_d^0)^{\mathrm{T}}$, whence only the parameter component $\mu = \lambda_k$ remains variable and we may reduce (12) to an equation

$$\tilde{G}(y, \mu) = 0, \quad \tilde{G} : \mathbb{R}^m \times \mathbb{R}^1 \to \mathbb{R}^m. \tag{13}$$

3.2. Singularities

When in example (5) the subspace of the parameter t is used to define a local parametrization, then condition (11) requires that $y = 0$. In other words, the t-parametrization fails at the point $(0, \frac{1}{2})$ where the two t-parametrized solution paths $(\pm\sqrt{\frac{1}{2} - t}, t)$ meet; that is, where the number of solutions of the form $y = y(t)$ of (5) reduces to one.

This is the simplest example of a bifurcation phenomenon. Loosely speaking, in this setting, bifurcation theory concerns the study of parametrized equations with multiple solutions and, in particular, the study of changes in the number of solutions when a parameter varies. Typically, such equations arise in applications modeling the equilibrium behavior of physical systems and then bifurcations signify a critical change in the system such as the, already mentioned, collapse of a mechanical structure. Accordingly, during the past several decades, the literature on bifurcation theory and the computation of bifurcation points has grown rapidly. It is beyond the framework of this presentation to enter into any details of the wide range of results.

As shown in [17,18] an important approach to bifurcation studies is via the more general study of singularities of stable mappings. In essence, for equations of form (13) involving a scalar parameter, the theory addresses problems of the following type: (i) The identification of (usually simpler) equations that are in a certain sense equivalent to the original one with the aim of recognizing equations of a particular qualitative type, (ii) the enumeration of all qualitatively different perturbations of a given equation, in particular, in terms of a so-called *universal unfolding*, (iii) the classification of qualitatively different equations that may occur, e.g., by considering the *codimension*; that is, the number of parameters needed in the universal unfolding.

In problems involving submanifolds that are defined as the solution set $\mathscr{M} := F^{-1}(0)$ of a (smooth) submersion $F : \mathbb{R}^n \to \mathbb{R}^m$, $n = m + d$, bifurcation phenomena are closely related to the occurrence of certain foldpoints. Generally, a point $x^c \in \mathscr{M}$ is a *foldpoint* with respect to a given d-dimensional

coordinate subspace $T \subset \mathbb{R}^n$ of $\mathcal{M}$ if condition (11) fails at that point. When the parameter splitting (8) is available, the parameter space may be used as the coordinate subspace and, typically in applications, it turns out that the corresponding foldpoints are exactly the points where the solution behaviour shows drastic changes. Moreover, these points can be shown to be bifurcation points in the sense of the above-mentioned theory.

A general study and classification of foldpoints was given in [16]. This led to applications in various settings. In particular, in [27] a connection with the second fundamental tensor of the manifold was established and used for the computations of certain types of foldpoints. In [13] a different approach led to a new method for a particular subclass of foldpoints and in [19] this method was extended to problems with symmetries.

There is also a close connection between foldpoints and the general sensitivity problem for parameterized equations. If for Eq. (13) with a scalar parameter μ the solution can be written in the form $(y(\mu), \mu)$ then, traditionally, the derivative $Dy(\mu)$ is defined as a measure of the sensitivity of the solution with respect to the parameter. In [30] it was shown that this concept can be generalized to submanifolds $\mathcal{M} := F^{-1}(0)$ defined by a (smooth) submersion $F : \mathbb{R}^n \to \mathbb{R}^m$, $n = m + d$, $d \geqslant 1$. For a given local parametrization near a point $x^0 \in \mathcal{M}$ specified by the coordinate space $T \subset \mathbb{R}^n$ the sensitivity is a linear mapping Σ_T from $\mathbb{R}^d$ into $\mathbb{R}^m$. We will not give the details but note that in the above special case Σ_T reduces to $Dy(\mu)$. Moreover, as shown in [30] the Euclidean norm of Σ_T satisfies

$$||\Sigma_T||_2 = \frac{\operatorname{dist}(T, T_{x^0}\mathcal{M})}{[1 - \operatorname{dist}(T, T_{x^0}\mathcal{M})]^{1/2}}, \tag{14}$$

where, as usual, the distance $\operatorname{dist}(S_1, S_2)$ between any two, equi-dimensional linear subspaces S_1 and S_2 of $\mathbb{R}^n$ is the norm-difference $||P_1 - P_2||_2$ of the orthogonal projections P_j of $\mathbb{R}^n$ onto S_j, $j = 1, 2$. Eq. (14) shows that, in essence, the sensitivity Σ_T at $x^0 \in \mathcal{M}$ represents a measure of the distance between the local coordinate space T and the tangent space $T_{x^0}\mathcal{M}$. In other words, $||\Sigma_T||_2$ specifies how close X^0 is to the nearest foldpoint of $\mathcal{M}$ with respect to the local basis defined by T. This has been shown to be an valuable tool for identifying computationally the location of foldpoints.

4. Parametrized methods

The title of this section is intended to refer broadly to numerical methods for equations involving a *scalar* parameters. This includes the equations $H(y, t) = 0$ defined by any homotopy mapping (2) as well as those of the form (6) with a one-dimensional parameter $\lambda \in \mathbb{R}^1$. The emphasis will be on methods that do not utilize explicitly any manifold structure of the solution set even if that structure exists.

4.1. Incremental methods

For the equation $H(y, t) = 0$ defined by a continuous homotopy mapping (2), the Homotopy Invariance Theorem 1 provides information about the existence of solutions (y, t) for any given $t \in [0, 1]$ but not about, say, the continuous dependence of y upon t. For that we require additional

conditions on H. Let

$$H : \Omega \times \mathscr{J} \to \mathbb{R}^m, \quad \Omega \subset \mathbb{R}^m, \quad \mathscr{J} \subset \mathbb{R}^1, \tag{15}$$

be a C^ρ, $\rho \geqslant 2$, mapping on the product of an open set $\mathscr{D}$ and an open interval $\mathscr{J}$. Then, for any solution $(y^0, t_0) \in \Omega \times \mathscr{J}$ where $D_y H(y^0, t_0)$ is nonsingular, the implicit function theorem ensures the existence of a $C^{\rho-1}$ mapping $\eta : \mathscr{J} \to \Omega$ on some interval $\mathscr{J}_0 \subset \mathscr{J}$ containing t_0 such that $H(\eta(t), t) = 0$ for $t \in \mathscr{J}_0$. Moreover, by shrinking $\mathscr{J}_0$ if needed, $D_y H(\eta(t), t)$ will be nonsingular for t in that interval.

By repeating the process with different points in the t-intervals, we obtain ultimately a solution curve $\eta : \mathscr{J}^* \to \Omega$ on an open interval $\mathscr{J}^* \subset \mathscr{J}$ that is maximal under set-inclusion. At the endpoints of this maximal interval the process stops either because the derivative $D_y H$ becomes singular (as in the example (5)) or the curve leaves the set $\mathscr{D}$.

Various iterative processes can be used to compute any point $\eta(t)$ for given $t \in \mathscr{J}^*$ on the solution curve. For instance, Newton's method

$$u^{j+1} = u^j - [D_y H(u^j, t)]^{-1} H(u^j, t), \quad j = 0, 1, \ldots, \tag{16}$$

converges to $\eta(t)$ if only $||u^0 - \eta(t)||$ is sufficiently small. This can be guaranteed by proceeding in small t-steps along the curve. In other words, we start say from a known point (y^0, t_0) and, for $i = 1, 2, \ldots$, compute a sequence (y^i, t_i) of approximations of $(\eta(t_i), t_i)$, $t_i \in \mathscr{J}^*$, with sufficiently small t-steps $h_i = t_i - t_{i-1}$. Once (y^i, t_i) is available, (16) can be started, for instance, with $u^0 = y^i$ and $t = t_{i+1} := t_i + h_{i+1}$. Alternately, some extrapolation of the prior computed points can be generated as a starting point.

This is the basic concept of the so-called incremental methods which date back at least to the work of Lahaye [22]. Over the years numerous variations of these processes have been proposed. This includes the use of a wide variety of iterative methods besides (16) and of numerous improved algorithms for the starting points. We refer here only to the extensive literature cited, e.g., in [26,20,3,4,32].

4.2. Continuation by differentiation

Consider again a mapping (15) under the same conditions as stated there. Suppose that there exists a continuous mapping $\eta : \mathscr{J}^* \to \Omega$ which is at least C^1 on some interval $\mathscr{J}^* \subset \mathscr{J}$ and satisfies

$$H(\eta(t), t) = 0, \quad \forall t \in \mathscr{J}^*. \tag{17}$$

Then, with $y^0 = \eta(t_0)$ for given $t_0 \in \mathscr{J}^*$, it follows that $y = \eta(t)$ is a solution of the initial value problem

$$D_y H(y, t)\dot{y} + D_t H(y, t) = 0, \quad y(t_0) = y^0. \tag{18}$$

Conversely, for any solution $y = \eta(t)$ of (18) on an interval $\mathscr{J}^* \subset \mathscr{J}$ such that $t_0 \in \mathscr{J}^*$ and $H(y^0, t_0) = 0$, the integral mean value theorem implies that (17) holds.

In a lengthy list of papers during a decade starting about 1952, D. Davidenko utilized the ODE (18) for the solution of a wide variety of problems including, not only nonlinear equations, but also integral equations, matrix inversion problems, determinant evaluations, and matrix eigenvalue problems (see [26] for some references). This has led occasionally to the use of the term 'Davidenko equation' for (18).

Evidently, if $D_yH(y,t)$ is nonsingular for all $(y,t) \in \Omega \times \mathscr{J}$, then the classical theory of explicit ODEs ensures the existence of solutions of (18) through any point (y^0,t_0) in this domain for which $H(y^0,t_0)=0$. Moreover, these solutions are known to terminate only at boundary points of the set $\Omega\times\mathscr{J}$. But, if the derivative $D_yH(y,t)$ is allowed to become singular at certain points of the domain, then (18) becomes an implicit ODE and the standard ODE theory no longer applies in general. However, if we assume now that rank $DH(y,t)=m$ (whence $H^{-1}(0)$ has a manifold structure) then (18) turns out to be equivalent with an explicit ODE. Of course, its solutions can no longer be written globally as functions of t. For ease of notation, in the following result from [28] we drop the explicit t-representation and hence introduce again the combined vector $x=(y,t) \in \mathbb{R}^n$, $n=m+1$.

Theorem 9. *Suppose that $F:\mathscr{D} \to \mathbb{R}^{n-1}$ is C^1 on some open set $\mathscr{D} \subset \mathbb{R}^n$ and that* rank $DF(x) = n-1$, $\forall x \in \mathscr{D}$. *Then, for each $x \in \mathscr{D}$ there exists a unique $u_x \in \mathbb{R}^n$ such that*

$$DF(x)u_x = 0, \quad ||u_x||_2 = 1, \quad \det\begin{pmatrix} DF(x) \\ u_x^{\mathrm{T}} \end{pmatrix} > 0 \tag{19}$$

and the mapping

$$\Psi : \mathscr{D} \mapsto \mathbb{R}^n, \quad \Psi(x) = u_x, \quad \forall x \in \mathscr{D} \tag{20}$$

is locally Lipschitz on $\mathscr{D}$.

The mapping G of (20) defines the autonomous initial value problem

$$\frac{\mathrm{d}}{\mathrm{d}\tau}x = \Psi(x), \quad x(0) = x^0 \in \mathscr{D}. \tag{21}$$

By the local Lipschitz continuity of Ψ, standard ODE theory guarantees that (21) has for any $x^0 \in \mathscr{D}$ a unique C^1-solution $x : \mathscr{J} \to \mathscr{D}$ which is defined on an open interval $\mathscr{J}$ with $0 \in J$ that is maximal with respect to set inclusion. Moreover, if $s \in \partial\mathscr{J}$ is finite then $x(\tau) \to \partial\mathscr{D}$ or $||x(\tau)||_2 \to \infty$ as $\tau \to s, \tau \in \mathscr{J}$. Any solution $x = x(\tau)$ of (21) satisfies $DF(x(\tau))\dot{x}(\tau) = DF(x(\tau))\Psi(x(\tau)) = 0$ which implies, as before, that $F(x(\tau)) = F(x^0)$ for $\tau \in \mathscr{J}$.

Clearly, this is a more general result than the earlier one for (18). It can be combined with condition (4) of the homotopy invariance theorem 1 to avoid 'degeneracies' in the solution path of a given homotopy. The basis for this is the so-called Sard theorem and its generalizations covered, e.g., in some detail in [1]. The following result represents a very specified case:

Theorem 10. *Let $D_n \subset \mathbb{R}^n$ and $\mathscr{D}_k \subset \mathbb{R}^k$ be open sets and $F : \mathscr{D}_n \times \mathscr{D}_k \to \mathbb{R}^m$, $n \geqslant m$, a C^∞-map which has $z \in \mathbb{R}^m$ as regular value. Then for almost all $u \in \mathscr{D}_k$ (in the sense of Lebesgue measure) the restricted map $F_u := F(\cdot,u) : \mathscr{D}_n \to \mathbb{R}^m$ has z as regular value.*

As an application we sketch an example that follows results of Chow et al., [12]. For a bounded map $G \in C^\infty(\Omega) \cap C(\bar{\Omega})$, where $\Omega \subset \mathbb{R}^m$ is a bounded, open set, assume that $0 \in \mathbb{R}^m$ is a regular value. With $u \in \Omega$ consider the homotopy mapping

$$\hat{H} : \Omega \times \Omega \times \mathbb{R}^1 \to \mathbb{R}^m, \quad \hat{H}(y,u,t) := y - u - t(G(y) - u).$$

Then, clearly, rank $D\hat{H}(y,u,t) = m$ on the domain of $\hat{H}$; that is, $0 \in \mathbb{R}^m$ is a regular value of $\hat{H}$. Hence, for almost all $u \in \Omega$, the restricted map

$$H : \Omega \times \mathbb{R} \to \mathbb{R}^m, \quad H(y,t) := \hat{H}(y,u,t)$$

has 0 as regular value. By Theorem 9 this implies that there exists a unique solution $\tau \in \mathscr{J} \mapsto (y(\tau), t(\tau)) \in \Omega \times \mathbb{R}$ of $H(y,t) = 0$ which satisfies $(y(0), t(0)) = (u, 0)$ and is defined on some maximal open interval $\mathscr{J}$ containing the origin. We consider the solution path in the cylindrical domain $\mathscr{D} := \bar{\Omega} \times [0,1]$. From (19) it follows that at the starting point $(u,0)$ the path is not tangential to $\mathbb{R}^m \times \{0\}$ and enters $\mathscr{D}$. Hence, it can terminate only on $\partial\mathscr{D}$. Since $H(y,0) = 0$ has only the solution $(u,0)$, we see that the path cannot return to $\mathbb{R}^m \times \{0\}$ and hence must reach the set $(\bar{\Omega} \times \{1\}) \cup (\partial\Omega \times (0,1))$. Now suppose that condition (4) of the homotopy invariance theorem 1 holds. Then we obtain that the solution path must reach the set $\bar{\Omega} \times \{1\}$ at a fixed point of G in Ω.

In line with the title of [12] the concept underlying this approach has been generally called the *probability-one homotopy paradigm*. It constitutes the principal theoretical foundation of the extensive and widely used HOMPACK package which incorporates many of the solution procedures indicated here. The curve tracing algorithms of this package were described in [39] and for the latest version we refer to [40] where also other relevant references are included.

In a sense the topological degree arguments of Theorem 1 are here replaced by analytic arguments involving inverse images of points in the range of the mapping under consideration. There exists an extensive literature centered on this idea. It includes in particular, various results on numerically implementable fixed point theorems. For an overview and comprehensive bibliography we refer to [3].

5. Manifold methods

As in Section 3 let $F : \mathbb{R}^n \to \mathbb{R}^m$, $n = m + d$, be a C^ρ mapping, $\rho \geqslant 1$, on the open set $\Omega \subset \mathbb{R}^n$ and suppose that the set $\mathscr{M} = F^{-1}(0)$ is not empty and F is a submersion of $\mathscr{M}$. Hence $\mathscr{M}$ is a d-dimensional C^ρ-submanifold of $\mathbb{R}^n$.

The computational tasks involved with such an implicitly defined manifold differ considerably from those arising in connection with manifolds defined in explicit, parametric form as they occur, e.g., in computational graphics. In fact, unlike in the latter case, for implicitly defined manifolds the algorithms for determining local parametrizations and their derivatives still need to be made available. A collection of algorithms was given in [31] for performing a range of essential tasks on general, implicitly specified submanifolds of a finite-dimensional space. This includes algorithms for determining local parametrizations and their derivatives, and for evaluating quantities related to the curvature and to sensitivity measures. The methods were implemented as a FORTRAN 77 package, called MANPAK. We discuss here only briefly one of these algorithms, namely, for the computation of local parametrizations.

Theorem 8 readily becomes a computational procedure for local parametrizations by the introduction of bases. Suppose that on $\mathbb{R}^n$ and $\mathbb{R}^d$ the canonical bases are used and that the vectors $u^1, \ldots, u^d \in \mathbb{R}^n$ form an orthonormal basis of the given coordinate subspace T of $\mathscr{M}$ at x^c. Then the matrix representation of the mapping U is the $n \times d$ matrix, denoted by U_c, with the vectors $u^1, \ldots, u^d$

Table 1
Algorithm GPHI

Input: $\{y, x^c, U_c, DK(x^c),$ tolerances$\}$
$x := x^c + U_c y$;
while: 'iterates do not meet tolerances'
  evaluate $F(x)$;
  solve $DK(x^c)w = \begin{pmatrix} F(x) \\ 0 \end{pmatrix}$ for $w \in \mathbb{R}^n$;
  $x := x - w$;
  if 'divergence detected' **then return** *fail*;
endwhile
Output: $\{\phi(y) := x\}$.

as columns. It is advantageous to shift the open set $\mathscr{U}^d$ such that $\phi(0) = x^c$. Now, componentwise, the nonlinear mapping K of (10) assumes the form

$$K : \mathbb{R}^n \to \mathbb{R}^n, \quad K(x) = \begin{pmatrix} F(x) \\ U_c^{\mathrm{T}}(x - x^c) \end{pmatrix}, \quad \forall x \in \Omega \subset \mathbb{R}^n. \tag{22}$$

By definition of ϕ we have $K(\phi(y)) = jy$ for all $y \in \mathscr{U}^d$, thus, the evaluation of $x = \phi(y)$ requires finding zeroes of the nonlinear mapping $K_y(x) := K(x) - jy$. For this a chord Newton method works well in practice. With the special choice $x^0 = x^c + U_c y$, the iterates satisfy $0 = U_c^{\mathrm{T}}(x^k - x^c) - y = U_c^{\mathrm{T}}(x^k - x_0)$ which implies that the process can be applied in the form

$$x^{k+1} := x^k - DK(x^c)^{-1} \begin{pmatrix} F(x^k) \\ 0 \end{pmatrix}, \quad x^0 = x^c + U_c y, \tag{23}$$

with a y-dependence only at the starting point. By standard results, it follows that, for any y near the origin of $\mathbb{R}^d$, the algorithm of Table 1 produces the point $x = \phi(y)$ in the local parametrization $(\mathscr{U}^d, \phi)$ near x^c defined by Theorem 8. For further methods related to local parametrizations and for determining bases of suitable coordinate spaces we refer to [31].

As a special case suppose now that $d = 1$ and hence that $\mathscr{M}$ is a one-dimensional C^ρ-submanifold of $\mathbb{R}^n$. Note that $\mathscr{M}$ may well have several connected component. The continuation methods for the computation of $\mathscr{M}$ begin from a given point x^0 on $\mathscr{M}$ and then produce a sequence of points x^k, $k = 0, 1, 2, \ldots$, on or near $\mathscr{M}$. In principle, the step from x^k to x^{k+1} involves the construction of a local parametrization of $\mathscr{M}$ and the selection of a predicted point w from which a local parametrization algorithm, such as GPHI in Table 1, converges to the desired next point x^{k+1} on $\mathscr{M}$. For the local parametrization at x^k we require a nonzero vector $v^k \in \mathbb{R}^n$ such that (11) holds which here means that

$$v^k \notin \operatorname{rge} DF(x^k)^{\mathrm{T}}. \tag{24}$$

It is natural to call $T_x M^\perp = N_x M$ the normal space of $\mathscr{M}$ at x (under the natural inner product of $\mathbb{R}^n$). Thus (24) means that v^k should not be a normal vector of $\mathscr{M}$ at x^k. Once v^k is available, the

local parametrization algorithm GPHI requires the solution of the augmented system

$$\begin{pmatrix} Fx \\ (v^k)^{\mathrm{T}}(x - x^k) - y \end{pmatrix} = 0, \tag{25}$$

for given local coordinates $y \in \mathbb{R}^1$.

In summary then, three major choices are involved in the design of a continuation process of this type, namely,

(i) the coordinate direction v^k at each step,
(ii) the predicted point z^k at each step,
(iii) the corrector process for solving system (25).

In most cases a linear predictor $y = x^k + hv$ is chosen, whence (ii) subdivides into the choice (ii-a) of the predictor-direction $v_r \in \mathbb{R}^n$, and (ii-b) of the steplength h. The so-called pseudo-arclength method (see [20]) uses for u and v the (normalized) direction of the tangent of $\mathscr{M}$ at x^k while in the PITCON code (see [11]), only the prediction v is along the tangent direction while u is a suitable natural basis vector of $\mathbb{R}^n$. The local iterative process (iii); that is, the corrector, usually is a chord Newton method with the Jacobian evaluated at x^k or y as the iteration matrix. Other correctors include update methods as well as certain multigrid approaches (see e.g. the PLTMG package described in [8] and the references given there).

6. Simplicial approximations of manifolds

As before suppose that $F : \mathbb{R}^n \mapsto \mathbb{R}^m$, $n = m + d$, $d \geqslant 1$, is a C^ρ map, $\rho \geqslant 1$, and a submersion on $\mathscr{M} := F^{-1}(0)$. Then $\mathscr{M}$ is a d-dimensional C^ρ submanifold of $\mathbb{R}^n$ or the empty set, which is excluded. Obviously, for $d \geqslant 2$ we can apply continuation methods to compute paths on $\mathscr{M}$, but, it is certainly not easy to develop a good picture of a multi-dimensional manifold solely from information along some paths on it. This has led in recent years to the development of methods for a more direct approximation of implicitly defined manifolds of dimension exceeding one.

The case of implicitly defined manifolds has been addressed only fairly recently. The earliest work appears to be due to Allgower and Schmidt [6] (see also [7]) and uses a piecewise-linear continuation algorithm to construct a simplicial complex in the ambient space $\mathbb{R}^n$ that encloses the implicitly given d-dimensional manifold $\mathscr{M}$. In other words, this piecewise linear approach does not generate directly a simplicial approximation of $\mathscr{M}$ in the sense of Section 2.2. But, of course, such an approximation can be obtained from it. In fact, by using linear programming tools, points on the intersection of the n-simplices with the manifold can be computed. These points form polytopes which, in turn, can be subdivided to generate d-simplices that form the desired simplicial approximation. A disadvantage of this approach appears to be that the computational complexity is only acceptable for low ambient dimensions n. In fact, the method was mainly intended for surface and volume approximations.

A first method for the direct computation of a d-dimensional simplicial complex approximating an implicitly defined manifold $\mathscr{M}$ in a neighborhood of a given point of $\mathscr{M}$ was developed in [29]. There standardized patches of triangulations of the tangent spaces T_xM of $\mathscr{M}$ are projected onto the manifold by smoothly varying projections constructed by a moving frame algorithm. An implementation of a globalized version of the method for the case $d = 2$ is described in [32] and

Brodzik [10] extended this global algorithm to the case of dimensions larger than two. In [10] also various applications are discussed and a general survey of methods in this area is provided.

A different method was developed in [24] which does not aim at the explicit construction of a simplicial complex on the implicitly defined, two-dimensional manifold, but on tessellating it by a cell-complex. This complex is formed by nonoverlapping cells with piecewise curved boundaries that are obtained by tracing a fish-scale pattern of one-dimensional paths on the manifold. Hence this approach appears to be intrinsically restricted to two-dimensional manifolds.

7. Further topics

There are a number of topics relating to the general area of continuation methods which, in view of space limitations, could not be addressed here.

While we restricted attention to problem in finite-dimensional spaces, many of the results can be extended to an infinite-dimensional setting. But, in that case various additional questions arise. For instance, typically in applications, the nonlinear equations (1) or (6) represent parametrized boundary value problems which must be discretized before we can apply any of the computational procedures. This raises the question how to define and estimate the discretization error. For parametrized equations already the definition of such errors is nontrivial; in fact, the development of a rigorous theory of discretization errors for parametrized nonlinear boundary value problems is of fairly recent origin. The case of a scalar parameter was first studied in the three-part work [9]. There mildly nonlinear boundary value problems were considered and the three parts concerned estimates at different types of points on the solution path. In particular, Part I addressed the case when λ can be used as local variable, while in Parts II and III estimates at simple limit points and simple bifurcation points are presented, respectively. Of course, a principal aspect of the latter two cases is the development of suitable local parametrizations.

For certain discretizations of equations defined by Fredholm operators on Hilbert spaces that involve a finite-dimensional parameter vector, a general theory of discretization errors was developed in [15]. Some applications of this theory to boundary value problems of certain quasilinear partial differential equations and finite-element discretizations are given in [38].

In Sections 4 and 5 we considered only general smooth maps. For more special systems it is, of course, possible to develop further refinements of the methods. In particular, for polynomial systems an extensive literature exists on homotopy methods for computing all zeros (in principle). For references see, e.g., [25,4], as well as the discussion in [41] of a very sophisticated code for polynomial systems that exploits their structure. It may be noted that — except for some early work — these results on polynomial systems formulate the problem in the complex projective space $\mathbf{CP}^n$.

As in other areas of computational mathematics, complexity studies have also become a topic of increasing interest in connection with continuation methods. In a series of five articles Shub and Smale developed a theory on the complexity of Bezout's theorem which concerns homotopy methods for computing all solutions of a system of polynomial equations. As an introduction to the results, we cite here the survey article [35] and, for further references, the fifth part [36] of the series.

Besides our brief comments about bifurcations in Section 3.2, we had to exclude any further discussion of the numerous results on computational methods for bifurcation problems. For some introduction and references see, e.g., [21,3,4]. A survey of methods for computing the simplest type

of these points — the so-called *limit* points — was given in [23]. Methods for these and also the *simple bifurcation points* are incorporated in several of the existing packages for continuation problems, including, e.g., ALCON written by Deuflhard, Fiedler, and Kunkel [14], and BIFPACK by Seydel [34].

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