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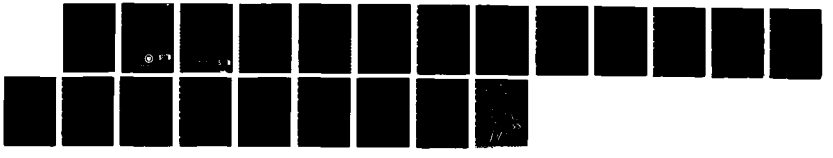

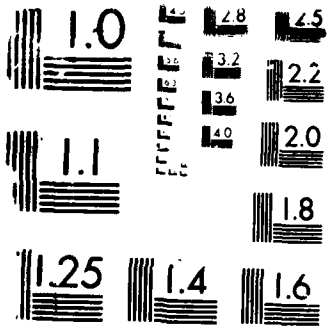

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INSTITUTE FOR COMPUTATIONAL MATHEMATICS AND APPLICATIONS

Technical Report ICMA-87-112 September 1987

ERROR QUESTIONS IN THE COMPUTATION OF SOLUTION MANIFOLDS OF PARAMETRIZED EQUATIONS

by

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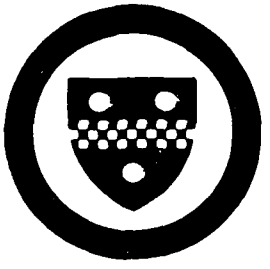

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Error Questions in the Computation of Solution Manifolds of Parametrized Equations[1]

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1.Introduction

Equilibrium problems for many physical systems are modelled by parameter dependent nonlinear equations

$$F(z,\lambda) = 0. \tag{1.1}$$

Under fairly general conditions the set of solutions (z,λ) of (1.1) forms a differentiable manifold, and, typically in applications, interest centers not so much on computing a few solutions but rather on analysing the form and special features of this manifold. In this paper we identify some of the sources of the errors which are necessarily arising in such a computational analysis.

For the presentation we adopt the same setting as in [18] or [33]. Let X and Y be real Hilbert spaces and $F: X \to Y$ a Fredholm mapping of class C^r, $r \geq 2$, and index $p \geq 1$ for which the domain contains an open set S of X. A point $x \in X$ is regular if the Jacobian DF(x) maps X onto Y. Then it is well known that the set of all regular solutions,

$$M = \{ x ; x \in S, F(x) = 0, \ x \text{ regular} \}, \tag{1.2}$$

is a p-dimensional C^r-manifold in X without boundary. By restricting consideration to this regular solution manifold we have assumed that a suitable unfolding of the problem has been chosen (see e.g. [20]). The tangent space T_xM at $x \in M$ may be identified with the kernel of DF(x); that is,

$$T_xM = \ker DF(x) = \{u; \ u \in X, DF(x)u = 0 \}, \tag{1.3}$$

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whence

(1.4) $$N_xM = (T_xM)^{\perp} = \text{rge } DF(x)^*$$

is the normal space at the point[1]. A given p-dimensional subspace T of X induces a local coordinate system of M at $x \in M$ if

(1.5) $$T \cap N_xM = \{0\}.$$

More specificallly, if (1.5) holds then there exist open neighborhoods V_1 and V_2 of the origins of T and X, respectively, as well as a unique C^{r-1} - function $w: V_1 \to T^{\perp}$, $w(0) = 0$, such that

(1.6) $$M \cap V_2 = \{ y \in X ;\ y = x + t + w(t),\ t \in V_1 \},$$

(see e.g. [33]). If (1.5) holds then x is a non-singular point with respect to the given coordinate space T, else it is a singular point or foldpoint with respect to T. Clearly, any point $x \in M$ is regular with respect to its the tangent space T_xM.

As indicated already by the form of (1.1), many applications involve a natural orthogonal splitting

(1.7) $$X = Z \oplus \Lambda\ ,\ Z = \Lambda^{\perp},$$

of the domain space X into a state space Z and a p-dimensional parameter subspace Λ. Then interest centers on determining the singular points with respect to Λ. In equilibrium problems these may be expected to be the points where a change in the stability behaviour of the physical system occurs.

The basic procedures for the computational analysis of such a manifold M are the continuation methods. When M has dimension $p > 1$, these methods require a restriction to some path on M and then produce a sequence of points along that path. Obviously, it is not easy to develop a good picture of a multi-dimensional manifold solely from information along such paths. This led

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[1] As usual, the asterisk denotes the Hilbert space adjoint.

recently to the development of methods for the computation of simplicial approximations of p-dimensional subsets of M. Two intrinsically different methods of this type have been presented in [1], [2] and [35], [36].

Besides these methods for computing certain sets of points on M, another important class of numerical procedures concerns the detection and computation of foldpoints on M with respect to a given coordinate space T, such as the natural parameter space Λ. There is a large and growing literature about such methods; further references can be found in [23],[24],[26].

This presentation will address only some aspects of these two classes of procedures. There are, of course, further related computational tasks. For example, we may wish to compute contour lines or contour surfaces of a prescribed functional on M. Alternately, many applications lead to the need for computing certain solutions of some differential equation on a manifold. This is equivalent with the solution of a differential-algebraic system of equations which, in the case of ordinary differential equations, is a topic with its own burgeoning literature.

Our interest here is not to elaborate on these various computational techniques but in identifying some of the errors arising in their connection. More specifically, in the next section we discuss the error induced by a discretization of the basic mapping F. Then, in Section 3 we turn to error questions connected with continuation methods while the final Section 4 identifies related questions in the computation of simplicial approximations of parts of M as well as of foldpoints on the manifold.

2. Discretization Errors

In practice, the mapping F often represents a differential operator involving several parameters which then, for the computation, has to be approximated by a finite-dimensional analogue. More specifically, suppose that we have a natural splitting (1.7) of the domain space X and that, as in (1.1), our problem is written in the form

$$F(z,\lambda) = 0 \quad , \quad z \in Z \quad , \lambda \in \Lambda. \tag{2.1}$$

Then only the state variable z needs to be discretized; in other words, the approximating equations will have the form

(2.2) $\qquad F_h(z_h, \lambda) = 0, \quad z \in Z_h\ ,\ \lambda \in \Lambda,$

where now F_h maps a discretized space $X_h = Z_h \oplus \Lambda$ to another such space Y_h. Since the parameter space is unchanged we may expect that the regular solutions of the discretized problems form a p-dimensional manifold M_h in X_h.

Frequently, X_h can be imbedded into X which then allows for a direct comparison of the two manifolds M and M_h. However, in order to measure the distance between these two manifolds, and hence the discretization error, we need to choose some coordinate system. More specifically, suppose that at the desired point $x \in M$ a local coordinate system has been induced by the p-dimensional subspace T of X. In other words, in a neighborhood of x the points of M are represented as $x(t) = x+t+w(t)$, $t \in T$, $w(t) \in T^{\perp}$, $w(0)=0$. If the approximation is sufficiently close, then some part of M_h should belong to the domain of validity of this local coordinate system and hence there should be a unique point x_h on M_h which has the same coordinate t=0 as x; that is, which is in $x+T^{\perp}$. We may expect also that T induces a local coordinate system at x_h on M_h, and hence that, locally near x_h, the points of M_h are representable in the form $x_h(t) = x_h+t+w_h(t)$, $t \in T$, $w_h(t) \in T^{\perp}$, $w_h(0) = 0$. Now it makes sense to measure the discretization error as the distance $||x(t)-x_h(t)||$ in X between points on the two manifolds which have the same local coordinate $t \in T$. In other words, the discretization error is a strictly local concept and depends on the choice of the particular local coordinate system.

If a natural parameter decomposition (1.7) is available and the coordinate system is induced by the choice $T = \Lambda$, then we compare points with the same λ–values and the discretization error measures the difference between the states of these points. This is often proposed as the definition of the discretization error. But, clearly, it is only a feasible choice as long as Λ induces a local coordinate system at the point $x \in M$; that is, as long as x is not foldpoint with respect to Λ. Since such foldpoints are of central importance in many applications, this is certainly not a generally acceptable approach.

The development of a rigorous theory of these discretization errors is a fairly recent undertaking. For one-dimensional solution manifolds a priori estimates were first developed in [12] and then [14]. The latter results were generalized in [16] to manifolds of arbitrary dimension. In the three parts of [12] the cases of non-singular points, limit points, and simple bifurcation points were treated separately and specific local coordinates were used at each of these points. In [14], [16] general local coordinate systems in the above sense are utilized to avoid the requirement of distinguishing between the different types of points.

All these results involve a family of approximate problems (2.2) which converge in some sense to the original problem (2.1) when the real discretization index $h > 0$ tends to zero. More specifically, the results in [14],[16] are based on projection methods; that is, a family $\{P_h\}$ of finite-rank projections is assumed to be given on the range space Y for which $\lim_{h\to 0} P_h y = y$ for each $y \in Y$. Then, with a bounded linear operator A from X to Y such that $\ker A = \Lambda$, and $A_Z = A|Z$ is an isomorphism onto Y, we can define the approximate mappings

$$F_h : X_h \to Y_h, \quad X_h = Z_h \oplus \Lambda, \; Y_h = P_h Y, \; Z_h = Q_h Z, \; Q_h = A_Z^{-1} P_h A_Z.$$

Now, if a particular stability condition holds, the estimate

$$C_0 \| (I-P_h)Ax(t) \| \leq \| x(t) - x_h(t) \| \leq C_1 \| (I-P_h)Ax(t) \|,$$

is valid for all sufficiently small $t \in T$ and $h > 0$ with constants $C_1 \geq C_0 > 0$ that are independent of h and t..

A different approach was taken in [17]. There, only a single discretized equation is considered instead of a converging family of such equations, and estimates are obtained which correspond to the local error estimates in the numerical solution of initial value problems for ordinary differential equations. These estimates have been applied to an analysis of the behavior of the socalled reduced basis techniques pioneered in structural mechanics (see [15],[28]).

These a priori estimates are of considerable theoretical interest, but for the practical application we require a posteriori estimates which measure the error of the specific computed points on the approximate solution manifold M_h. Such estimates are needed not only to judge the reliability of the computed results but also to control adaptive procedures aimed at achieving dependable results within a given range of accuracy at minimal cost.

For finite element discretizations there exists a growing literature on the computation of such a posteriori estimates; we refer only to [4] and the two proceedings [3], [6] where many other references can be found. These results concern largely linear problems, but more recently they are also being extended to nonlinear problems, see e.g., [5], [8],[32], [34]. For example, the approach in [34] supposes that -- in the notation of the a priori estimates -- the local coordinate space T belongs to the approximate domain space X_h. If the desired exact point x and the approximate computed point x_h are sufficiently close, then it can be shown that

$$(2.3) \qquad ||x - x_h|| = (1 + o(1))||y|| \quad \text{as} \quad ||x - x_h|| \rightarrow 0$$

where y is the solution of the linearized equation

$$(2.4) \qquad F(x_h) + D_W F(x_h)y = 0, \quad W = T^{\perp}.$$

The discretization of (2.4) has the exact solution $y_h = 0$ and hence $||y||$ is the discretization error of (2.4) which can be estimated by means of one of the known a posteriori estimators for linear equations.

Various computational examples for such a posteriori estimates in the case of finite-element discretizations of one-dimensional manifolds have been given in the cited articles. Corresponding estimates for two-dimensional manifolds are used in the nonlinear adaptive finite element solver NFEARS developed jointly by I.Babuska, C.K.Mesztenyi, and W.C.Rheinboldt. These results indicate that the effectivity of these error estimates corresponds to that for linear problems and that the computational cost is only a fraction of the cost of solving the nonlinear problem. In general, the errors vary considerably along a solution manifold which shows the importance of adaptive mesh-refinements.

However, there remain many open problems. In fact, it appears to be reasonable to require that such estimates (a) apply to large classes of problems, discretizations and error norms, (b) are dependable and cost-effective in the range of engineering accuracies, (c) allow for the use of most applicable local coordinate system, and (d) provide also estimates of the error of computed foldpoints. At this time we are still very far from such type of estimates, and accordingly it is well justified to characterize the computation of a posteriori estimates for nonlinear parametrized problems as being in an early stage of development.

As stressed before, all these various error estimates are local in nature and hence cannot provide information about the comparative global shapes of the exact and approximate manifolds. In particular, it turns out that the two manifold may have a different number of connected components. In other words, there may be numerical solutions which do not approximate exact solutions. Such spurious solutions have been observed in many contexts (see e.g. [9],[19],[27]).

A very simple example for such spurious solutions arises in connection with the boundary value problem

$$u'' + \lambda \sin u = 0 \quad , \quad 0 \le s \le 1, \quad u(0) = u(1) = 0 \tag{2.5}$$

which can be viewed as a model of the classical Euler rod. For $\lambda < 0$, there exists only the trivial solution $u \equiv 0$, which is physically plausible since under pure tension the rod should remain straight. Nevertheless, discretizations of (2.4) constructed either by finite differences or by finite element techniques exhibit non-zero solutions for certain negative values of λ (see e.g. [5] for some picture). These particular spurious solutions are not especially disturbing since they occur in a region of little interest and disappear to infinity when the mesh is refined.

Unfortunately, not all spurious solutions are so "harmless". For instance, the following problem

$$u'' + \alpha (1-u) \exp(-\lambda/(1+u)) = 0 \quad , 0 \le t \le 1, \quad u(0) = u(1) = 0 \tag{2.5}$$

models an exothermic chemical reaction in a slab. It can be shown that all solutions must have the symmetric property $u(t) = u(1-t)$, $t \in [0,1]$. However, a discretization, such as

$$(2.6) \quad -x_{i-1}+2x_i -x_{i+1} = h\,\alpha\,(1-x_i)\exp(-\lambda/(1+x_i)) \;,\; i=1,\ldots,n-1,\; x_0 = x_n = 0,\; h = 1/n,$$

models the same reaction only inside each one of a collection of n cells while across the interfaces there is merely mass transport. As a consequence unsymmetric solutions of (2.6) exist which branch off from the (discretized) symmetric solution at certain symmetry breaking bifurcation points. These branches tend to the exact symmetric solution when h goes to zero, but, clearly, they do not correspond to any similar feature of the original problem, (see e.g. [10], [11]).

For practical applications it is certainly of considerable interest to provide error estimators which identify spurious solutions. In [5] it was shown that, for a problem such as (2.4), the spurious solutions carry error estimators which are much larger than, say, any tolerance acceptable in engineering calculations and hence which can be rejected on that basis. There is considerable need for a more detailed study of this question.

3. Continuation Methods

As noted earlier, the basic procedures for the computational analysis of our manifold M are the continuation methods and these methods require an a priori restriction to some path on M. In other words, if M has dimension $p > 1$, then our (discretized) equations must be augmented by p-1 suitable equations which specify the desired path on M. As a consequence the continuation methods are always applied to an equation of the form

$$(3.1) \qquad F_o(x) = 0 \;,\quad F_o: R^n \rightarrow R^{n-1} \;,\; n\geq 2$$

involving an operator F_o which is of class C^r, $r \geq 2$, on some open set in R^n. We denote its regular solution manifold by $N = \{x \in R^n;\, F_o(x)=0 \;;\; \text{rank}DF_o(x)=n-1\}$. It is readily verified that, on the set of regular points of F_o, the mapping

(3.2) $\quad u: R^n \to R^n,\ DF_o(x)u(x) = 0,\ ||u(x)||_2 = 1,\ \det(DF_o(x)^T, u(x)) > 0$

defines a C^{r-1}-vector field. Let $x^o \in N$ be a given point and $y:J \to N$ the unique, maximally extended solution of the initial value problem

(3.2) $\quad y'(s) = u(y(s)),\ \forall\, s \in J,\ y(0) = x^o,$

then the trajectory y(J) is exactly the connected component N_o of N containing x^o (see, e.g., [33]). This connection between the initial value problem (3.2) and its first integral (3.1) has been used by numerous authors.

All continuation processes begin from a given point $x^o \in M$ and produce a sequence of points x^k, k=0,1,2,..., which approximate points of N. For any $k \geq 0$, the step from x^k to x^{k+1} corresponds to an implementation of the local coordinate representation (1.6). More specifically, if $T = \text{span}\{t\}$, $t \in R^n$, $t \neq 0$, is a local coordinate space of N at x^k, then, for any fixed $y \in R^n$, the Jacobian of the augmented equations

(3.3) $$\begin{pmatrix} F_o(x) \\ t^T(x-y) \end{pmatrix} = 0$$

is non-singular for all x in some neighborhood of x^k. Thus, if y approximates a point of N in that neighborhood, then it follows readily that (3.3) has a unique solution $x^{k+1} \in N$ which can be computed by means of a locally convergent iterative process applied to (3.3) and started, say, at y.

The various continuation methods differ in the choice (a) of the coordinate space T, (b) of the predicted point y, and (c) of the local iterative process for solving (3.3). In most cases a linear prediction $y = x^k + hv$ is chosen, whence (b) subdivides into the choice (b1) of the predictor-direction $v \in R^n$, and (b2) of the step-length $h > 0$. The so-called pseudo-arclength methods use for t and v the tangent vector $u(x^k)$ of N at x^k, while in the PITCON code (see [30]), only the prediction $v = u(x^k)$ is along the tangent and T is specified by a suitable natural basis vector $t = e^i$, $i = i_k$, of R^n. On the other hand, in the PLTMG code [7] both t and v are a linear combination of $u(x^k)$ and a specified vector characteristic for the problem. The local iterative process (c); that is, the corrector, usually is a chord-Newton method with the Jacobian of the mapping

(3.4) at x^k or y as the iteration matrix. Other corrector methods include, in particular, the multigrid approaches and some chord Gauss-Newton method.

In the construction of the predicted point it is highly desirable to estimate the interval of validity of the local coordinate system at x^k. This is equivalent with the requirement of estimating the distance from x^k to the nearest foldpoint of N with respect to the chosen local coordinate system. At present, there are no reliable methods for that purpose. A second critical question concerns the error $||y-x^{k+1}||$ of the prediction and many processes indeed utilize estimates of this error. For example, in PITCON such an estimate is obtained as the difference between the chosen linear predictor and some quadratic extrapolation involving in turn an approximation of the local curvature. This is then applied in the construction of the step length h.

Whenever, the corrector applied to (3.4) converges to a point where the Jacobian remains non-singular, then this limit must be a point of N. But no estimate of the prediction error by itself can guarantee that the next point x^{k+1} will again belong to N_o and not to some other component of N. An important control, which can be employed here, is the orientation of N_o given by (3.2). This is indeed incorporated in PITCON and has proved capable of identifying many of the potential "jumps" of the process between components of N. But, of course, there remain cases where jumps to components with identical orientation are possible. Clearly there is still much room for other estimates of the prediction error and for further controls that signal when the process has left the connected component N_o.

Since all solutions of (3.4) with non-singular Jacobian are points of N (although not necessarily of N_o), the quality of the approximation of N by the computed points $\{x^k\}$ is controlled by the size of the termination error of the corrector. The estimation of this termination error has been the topic of many studies, but from the convergence theory of iterative processes for nonlinear systems of equations it is well-known that exact bounds for these errors require information about the mapping in a sufficiently large neighborhood of the solution (see e.g. [13]) . Moreover, these bounds do not take into account the ill-conditioning introduced by round-off. In fact, it is well-known that the uncertainty region of the solution of a system as (3.4) can be quite large. For example, if the quartic polynomial

$$x^4 - 202\,x^3 + 1529\,x^2 - 514898\,x + 6497400 = 0, \quad x \in R^1,$$

with the roots x = 49,50,51,52 is evaluated by means of the standard Horner scheme in rounded 8-decimal digit arithmetic, then the size of the uncertainty interval $\{x;\ |x-52| < \delta\}$ of the largest root is about $\delta \approx 0.09$, (see, e.g., [31]). Clearly, the occurence of ill-conditioning of such a magnitude may destroy completely the reliability of the overall process. The control of this phenomenon appears to be one of the most promising areas for the application of interval techniques in connection with continuation methods.

4. Triangulations and Foldpoint Calculations

As observed already in the Introduction, continuation processes require us to develop a picture of the p-dimensional manifold (1.2) solely from computed information along a priori specified paths. The method introduced in [35], [36] for obtaining simplicial approximations (triangulations) of open subsets of the manifold uses almost the same tools as these continuation methods and hence has also a *similar error behavior*.

Suppose that our problem is defined by the finite dimensional mapping

(4.1) $$F: R^n \rightarrow R^m, \quad n = m+p, \quad p \geq 2$$

and that M denotes its regular solution manifold. The triangulation process then begins with the choice of a simplicial decomposition Σ of R^p, such as, for instance, the well-known Kuhn-triangulation, or, for p=2, a triangulation of R^2 by means of equilateral triangles. The aim is to transfer the knots of some part of Σ, together with their connectivity information, from R^p onto M. As in any continuation methods, a starting point x on the manifold M is assumed to be known. In its basic form the process then consists of two steps: First a suitable "patch" of the reference triangulation Σ is mapped onto the affine tangent space $x+T_xM$. using an appropriate basis of T_xM. Thereafter, a locally convergent iterative process is applied to "project" the resulting knots of the mapped simplices from $x+T_xM$ onto the manifold M. These two steps are then repeated with one of the computed points on M in place of the original point x. But, of

course, knots of Σ that have already been mapped onto M will not be used again.

In order to ensure that the images of the simplices of Σ on M form a simplicial approximation of a portion of the manifold, we need to choose bases on the tangent spaces T_xM which change smoothly from point to point. In other words, we require a moving frame on some open subset M_o of the manifold M. Recall that a moving frame of class C^s, $0<s\leq r$, associates with any $x \in M_o$ an ordered basis (frame) $\{u^1,...,u^p\}$ of T_xM such that each coordinate map u^i, $1\leq i\leq p$, from M_o into the tangent bundle TM defines a vector field of class C^s on M_o. Hence, we need an algorithm which generates for each point x of M an n x p matrix U(x) with orthonormal columns such that $DF(x)U(x) = 0$ and that the mapping $U: M_o \rightarrow R^{pxn}$ is of class C^s on M_o. Standard methods for computing tangent bases generally do not produce continuously varying matrices U(x).

A moving frame algorithm of the desired form has been introduced in [35]. It uses an n x p reference matrix T_r with orthonormal columns and assumes that some method is available for computing at any $x \in M$ an orthonormal basis matrix U(x) of T_xM which, of course, is not expected to depend continuously on x. Let M_o be the open subset of M where the subspace T of R^n spanned by the columns of T_r induces a local coordinate system. If $x \in M_o$ and we compute the singular value decomposition $A(x)^T(U(x)T_r)B(x) = D(x)$, then it was shown in [36] that the mapping $x \rightarrow U(x)A(x)B(x)^T$ is of class C^{r-1} on M_o and hence defines the desired moving frame. If the dimension p of the manifold is small in comparison with the space dimension n, then the principal cost of this algorithm derives from the computation the original basis matrix U(x).

There are various ways of implementing the computation of the tangent bases U(x) and of the local iterative process. For instance, in the cited articles the QR-factorization

$$DF(x)^T = Q\begin{pmatrix} R \\ 0 \end{pmatrix},$$

gives U(x) as the last p columns of the orthogonal n x n matrix Q, and the chord Gauss-Newton process, defined by

(i) solve $R^Tz = F(y^k)$ for $z \in R^p$, (ii) $y^{k+1} = y^k - Q(z,0)^T$, $k=0,1,2,...,$

converges locally to the unique point $y^* \in M$ with the coordinate $t = y^o - x$ in the local coordinate system induced by T_xM. On the other hand, in NFEARS the original equations are augmented, as in PITCON, by appropriate unit basis vectors of R^n, and the tangent basis is derived from a triangular factorization. Then a chord Newton method is applied as the local iterative process.

There are two controlling aspects in this process. One of them concerns the behavior of the local iterative process and hence raises analogous problems as for continuation processes. As before, three basic issues are again the estimation of the prediction error and of the termination error, as well as the control of the effects of round-off. In addition, the earlier problem about the interval of validity of the local cocordinate system becomes here a question about the numerical behavior of the moving frame algorithm. In particular, whenever we apply the algorithm at one of the already computed knots x on M, we should be able to determine whether this point x still belongs to the open subset M_o of M where the subspace T of R^n spanned by the reference matrix T_r induces a local coordinate system. This leads again to the question of estimating the distance from x to the set of foldpoints of M with respect to T. As mentioned earlier there exists no method for this. Fortunately, numerical evidence suggests that, in connection with the triangulation process, this lack is often not very critical. A related open problem concerns the quality of the computed moving frame when we come close to the boundary of M_o.

As noted in the Introduction, in many application interest centers on computing the foldpoints of M with respect to a natural parameter space Λ. But space limitations allow us only to give here a very cursory summary of some of the basic issues as they relate to our present setting. As defined earlier, a point $x \in M$ is a foldpoint with respect to Λ if the intersection $\Lambda_N = \Lambda \cap N_xM$ is non-trivial; that is, equivalently, if there is a non-zero tangent vector of x which belongs to the state space. The integer $q = \dim(\Lambda_N)$ is the first singularity index of x. With the natural splitting (1.7) we can write our equation in the form (2.1). Then a foldpoint $x = (z,\lambda) \in M$ has first singularity index q exactly if the range in Y of the partial derivative $D_ZF(x)$ of F has co-dimension q. The cut $M \cap (x + \Lambda_N^{\perp})$ of M through x orthogonal to Λ_N characterizes the type of the foldpoint (see e.g. [18]).

We mention here only a few of the numerous computational problems associated with foldpoints:

(a) Detection problem: Given a set $\{x^1,\ldots,x^k\}$ of points in X and appropriate additional information about the problem at these points, determine whether some foldpoint x^* of M is in a neighborhood of this set.
(b) Approximation error: For a given approximation $x \in X$ of a foldpoint x^* of M, estimate the distance $\| x - x^*\|$ in X between these two points.
(c) Foldpoint computation: For foldpoints x^* of M of a prescribed type design iterative processes which are locally convergent to x^* from any sufficiently close approximation $x \in X$.
(d) Discretization error: If x_h is a computed foldpoint of the discretized equations (2.2) which approximates a foldpoint x of the original problem (2.1), compute an a posteriori estimates of the distance $\|x - x_h\|$.
(e) Foldset triangulation: Compute a simplicial approximation of a set of foldpoints of M of a prescribed type.

Not only the problems(b) and (d), but also all the other problems involve error estimation questions. For example, problem (a) requires in essence an inclusion procedure for the zeros of certain nonlinear mappings. This is most easily seen in the case of a mapping (3.1) underlying a continuation method where we assume that the natural splitting (1.7) is given. Then, theoretically, the foldpoints of the regular solution manifold N are the points $x \in R^n$ which solve the constrained problem

$$(4.2) \qquad \begin{pmatrix} F_o(x) \\ \det(D_Z F_o(x)) \end{pmatrix} = 0 , \quad \operatorname{rank}(DF_o(x)) = n-1.$$

Evidently, on the basis of information at finitely many points alone we cannot expect to obtain a guaranteed inclusion result for (4.2); at least some information about F_o in a suitable neighborhood of the given set of points is needed here. This is already seen for very simple inclusion results. Suppose that $\Lambda = \operatorname{span}\{v\}$ and that x^1 and x^2 are two successive points produced by a continuation procedure. If both points belong to the same connected component of N, and $u^j = u(x^j)$, j=1,2, are the corresponding oriented tangent vectors (3.2), then $\operatorname{sgn}(v^T u^1) \neq \operatorname{sgn}(v^T u^2)$ implies that there is a limit point of odd order between the two points. Evidently, without further information about F_o we cannot verify that both points belong to the same connected component of N

and without that assumption the statement need not hold. On the other hand, suppose that we only know that $x^1, x^2 \in N$ and that we orient the tangent vectors by means of $(u^1)^T(u^2) > 0$. Now, if the determinants $\det(DF_0(x^j)^T, u^j)$, $j=1,2$, have different signs and the points are sufficiently close, then they cannot belong to the same connected component of N, and hence there must be a bifurcation point of odd order "between" them. These observations can be extended readily to the more general mappings (4.1) using points $x^j \in M$, $j=1,...,p+1$, which, for instance, form the corners of a p-simplex. But, even without entering into any details this discussion already indicates that procedures for the general problem (a) indeed require information about the behavior of the mapping on appropriate sets and, in general, also a restriction to specific types of foldpoints.

Problem (b) depends on the measure of the distance between the foldpoint x^* and its approximation. Suppose that we consider again the finite dimensional case (4.1); then the size of the smallest principal angle between the m-dimensional normal space rge(DF(x)) and the p-dimensional natural parameter space Λ gives some information about the approximation. These principal angles are readily computed, but again further information about the mapping is needed to derive from this, say, an estimate $||x-x^*||$. Except for simple special cases, there appears to exists, at present, no reliable, computable estimator for this norm difference.

As noted in the introduction, there is a large literature on local iterative methods for computing certain types of foldpoints. Many of these methods begin with a suitable augmentation of the given equation such that the Jacobian of the resulting system is square and non-singular. This allows then the application of a more or less standard iterative process for their solution. Obviously, it would lead to far to enter here into any details of the numerous augmentations that have been considered. But, clearly, in all these cases the behavior of the process is once again essentially controlled by the error of the initial approximation, the termination error of the method, and the influence of round-off on the reliability of the result. It should also be noted that for specific types of foldpoints there are other approaches which utilize the particular characterization of these points. In particular, for limit points on one-dimensional manifolds, as they arise in connection with continuation methods, there exists a wide variety of such procedures, as, for instance, the comparative study [25] shows.

As noted in Section 2, a computed foldpoint of the discretized problem (2.2) need not approximate a corresponding foldpoint of the original problem (2.1). But if it does, then it is certainly of considerable interest to estimate the distance between these two points. There appear to exist only very few results along that line. We mention here merely the a posteriori estimates given in [5] for the case of simple limit points and for a finite element discretization of a two-point boundary value problem. Further results in the important area of problem (d) are certainly very much needed.

Finally, in connection with problem (e) we mention only the methods in [22] and [29] for computing sequences of points along certain paths of limit points on two-dimensional regular solution manifolds. All these methods are closely related to the continuation procedures and hence involve essentially the same error questions. There appear to exist, at present, no methods for computing simplicial triangulations of higher dimensional sub-manifolds of foldpoints of any type.

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