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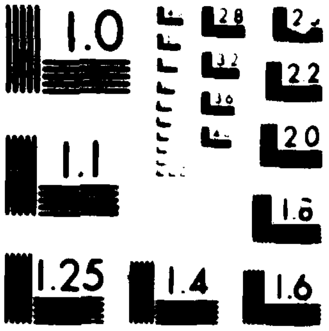
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Department of Mathematics and Statistics

University of Pittsburgh

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On a Moving-Frame Algorithm

and the Triangulation of Equilibrium Manifolds

by

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1. Introduction

Nonlinear, parametrized equations

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

represent models of equilibrium problems for many physical systems. If $F: R^n \to R^m$, $n=m+p$, $p \geq 1$, is continuously differentiable on R^n, then the regular solution manifold

$$M = \{ x \varepsilon R^n ; F(x) = 0 , \text{rank } DF(x) = m \} \tag{1.2}$$

is a p-dimensional, differentiable manifold in R^n without boundary. We shall assume always that F is at least of class C^r, $r \geq 2$.

The standard procedures for the computational analysis of such solution manifolds are the continuation methods. When the parameter dimension p exceeds unity, these methods require a restriction to some path on the manifold and then produce a sequence of points along that path. In general, it is not easy to develop a good picture of a multidimensional manifold from information along one-dimensional paths; thus there is growing interest in computational methods which generate multidimensional grids of solution points. Up to now, the only such method appears to be that of E.L. Allgower and P.H. Schmidt [1]. It utilizes a

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simplicial continuation algorithm to triangulate a p-dimensional manifold by means of p-simplices.

In [10] a new algorithm was developed for computing vertices of a triangulation (by p-simplices) of certain subsets of a p-dimensional solution manifold (1.2). It depends on an algorithm for constructing a moving frame on these subsets of M. We present here an overview of these two algorithms and illustrate their effectiveness with some numerical examples.

2. Local Coordinate Systems

At any point x of M the tangent space T_xM may be identified with the kernel of the Jacobian DF(x),

$$T_xM = \ker DF(x) = \{ u \varepsilon R^n ; DF(x)u = 0 \}, \qquad (2.i)$$

and then the corresponding normal space N_xM is specified as the orthogonal complement $N_xM = T_xM^{\perp} = \mathrm{rge}\, DF(x)^T$.

A given p-dimensional subspace $T \subset R^n$ induces a local coordinate system of M at any point $x \varepsilon M$ where

$$T \cap N_xM = \{0\} \qquad (2.2)$$

As shown, for instance, in [4] or [9], at any $x \varepsilon M$ where (2.2) holds there exist neighborhoods $V_1 \subset T$ and $V_2 \varepsilon R^n$ of the origins of T and R^n, respectively, and a unique C^{r-1} function $w: V_1 \rightarrow T^{\perp}$, $w(0) = 0$, such that

$$M \cap V_2 = \{ y \varepsilon R^n;\ y = x + t + w(t),\ t \varepsilon V_1 \} \qquad (2.3)$$

A well-known procedure for computing tangent bases is provided by the QR-decomposition

$$DF(x)^T = Q \begin{bmatrix} R \\ 0 \end{bmatrix} , \quad Q = (Q_1, Q_2) , \qquad (2.4)$$

where the $n \times n$ matrix Q is orthogonal, Q_1 has m columns, and the $m \times m$ matrix R is upper triangular and non-singular for $x \varepsilon M$. Then the p columns of Q_2 form an orthonormal basis of T_xM.

If $x \varepsilon M$ is a point where the QR-decomposition (2.4) has been computed, then with any starting-point $y = y^0$ sufficiently near x in $x+T_xM$ we may apply the chord-Gauss-Newton process:

```
For k=0,1,... until convergence
        1) solve $R^Tz = F(y)$ for $z \varepsilon R^p$                    (2.5)
        2) $y := y - Q(z,0)^T$
```

The convergence theory of these methods is well understood. In particular, a theorem of Deuflhard and Heindl [3] can be used to ensure that there exists for any $x \varepsilon M$ a neighborhood $V = V(x)$ of x in $x+TxM$ such that for any y in $V(x)$ the process (2.4) converges to some $y^* \varepsilon M$. Moreover, we can show readily that $y^*-y^0 \varepsilon N_xM$ and hence that, in the notation of (2.3), we have $y^* = x+t+w(t)$, $t=y^0-x$. In other words, the process (2.5) represents an implementation of the "corrector" mapping w of the local coordinate representation (2.3).

3. The Moving Frame Algorithm

Recall that a vector field of class C^s, $s \leq r$, on an open subset M_0 of M is a C^s function $u : M_0 \rightarrow TM$ into the tangent bundle TM such that $u(x)$ belongs to T_xM for x each M_0. A moving frame of class C^s on M_0 associates with each x of M_0 an ordered basis (frame) $\{u^1,\ldots,u^p\}$ of T_xM such that each coordinate map $u^i : M_0 \rightarrow TM$, $i=1,\ldots,p$ defines a vector field of class C^s on M_0. We shall consider only orthonormal moving frames.

In our setting, an algorithm for constructing a moving frame has to generate for each x of some open subset M_0 of M an $n \times p$ matrix $U(x)$ with orthonormal columns such that $DF(x)U(x) = 0$ and that the mapping $U : M_0 \to R^{p \times n}$ is of class C^s on M_0. As noted in [2], the QR-decomposition (2.4) does not produce continuously varying matrices $U(x)$. This observation extends to other algorithms of a similar nature. The three remedies proposed in [2] do not concern the generation of a moving frame.

For the moving frame algorithm developed in [10] we assume that some method is available for computing at the points x of M some $n \times p$ matrix $U_0(x)$ with orthonormal columns that span T_xM. Of course, $U_0(x)$ is not expected to depend continuously on x. For instance, we may use the QR-decomposition (2.4).

The algorithm is based on the selection of an $n \times p$ reference matrix T_r with orthonormal columns. Then for a point x of the manifold we proceed as follows:

(1) Compute the tangent basis matrix $U_0(x)$;
(2) form $U_0 := U_0(x)T_r$;
(3) compute the singular value decomposition (3.1)
$A^TU_0B = \Sigma$ and save A and B ;
(4) with $Q = AB^T$ form the basis matrix $U_0(x)Q$.

The following result, proved in [10], guarantees the validity of this algorithm:

Theorem: Let M_0 be the open subset of M where the subspace of R^n spanned by the columns of the reference matrix T_r induces a local coordinate system. Then the mapping $x \in M \Rightarrow U_0(x)Q \in R^{n \times p}$ given by the algorithm (3.1) is of class C^{r-1} on M_0 and defines an orthonormal moving frame on M_0.

If the QR-decomposition is used in step (1) and the dimension of the manifold is small in comparison with the space dimension, then the principal cost of (3.1) derives from the approximately $(2/3)n^3$ flops needed for the decomposition of $DF(x)^T$.

In practice, it has turned out to be advantageous to construct the reference matrix T_r in the following manner. We select a reference point x^r on M. Then the Euclidean norms

$$\tau_i = \| U_0(x^r)^T e^i \|_2 \ , \ i=1,\dots,n$$

of the rows of $U_0(x^r)$ are the cosines of the principal angles between the tangent space of M at x^r and the i-th natural basis vector e^i of R^n. The τ_i are independent of the choice of the basis matrix $U_0(x)$. Let $i_1,\dots,i_p$ be the indices of the p largest of these τ_i (with ties broken, say, lexicographically). Then we form the desired reference matrix T_r as the matrix with the columns e^i , $i=i_1,\dots,i_p$. This construction is analogous to the local parameter selection in the continuation program PITCON, [11].

4. The Triangulation Algorithm

For the triangulation of a p-dimensional manifold we begin by constructing a reference triangulation on R^p. Let Σ be the collection of simplices of this triangulation. Except for considerations of computational efficiency and simplicity, no restrictions are placed on Σ. We refer, for example, to [12] for various algorithms for triangulating R^p. For our purposes, the well-known Kuhn-triangulations have been useful, and, in the case p = 2, triangulations of R^2 by equilateral triangles have been applied as well.

Let ξ denote a given vertex of this triangulation in R^p and $h > 0$ a fixed steplength. Then for any point $x \in M$ where a basis matrix U of T_xM is known, the mapping

$$A: R^p \rightarrow x + T_xM, \quad A\eta = x + hU(\eta-\xi), \ \eta \in R^p \qquad (4.1)$$

transfers Σ from R^p onto $x + T_xM$. As before, let $V(x) \subset x + T_xM$ denote the local convergence domain of the Gauss-Newton process (2.5) . If η is a vertex of Σ for which $A\eta \in V(x)$, then (2.5) can be used to map $A\eta$ into a point $y \in M$. The set $\Gamma(\xi,x,U)$ of vertices of Σ that can be mapped onto M in this way shall be called the "patch" corresponding to ξ,x,U . (The steplength h will be held fixed throughout).

An "idealized" form of our algorithm can now be phrased as follows:

```
(1) Select a reference vertex $\xi^*$ of $\Sigma$ ;
(2) Select a reference point $x^* \in M$ and let $M_0$ be the subset
        where, by the theorem, the moving frame algorithm applies ;
(3) Set $x = x^*$,  $\xi = \xi^*$ ;
(4) Mark the vertex $\xi$ as "used" ;
(5) While x [illegible]
    (5 [illegible] $\xi$ as a "center"
    (5b) Compute the frame $U(x)$ by algorithm (3.1) ;
    (5c) Select all vertices of the patch $\Gamma(\xi,x,U(x))$
            which have not yet been marked "used" ;
    (5d) Map these vertices onto $M$ and mark them "used" ;
    (5e) Choose a "used" vertex $\xi$ of $\Sigma$ not marked a "center"
            and let x be its computed image on $M$ ;
```

The points computed on M inherit the connectivity pattern of the original simplices of Σ which, in turn, induces a simplicial approximation M_Σ of M in R^n.

The algorithm is still "idealized" because, in practice, it is impossible to check the condition $x \in M_0$ and to identify the vertices of Σ that belong to $\Gamma(\xi,x,U(x))$. Thus, special provisions have to be added in order to overcome the possible failures due to these missing checks. We shall not go into details here. The principal approach is to select a "standardized" patch of Σ which is used in step (5c) in place of $\Gamma(\xi,x,U(x))$. Then, in step (5d), appropriate alternatives are introduced for all vertices where a failure of the corrector iteration is encountered.

As noted, for two-dimensional manifolds a reference triangulation of equilateral triangles can be used. Then the "standardized" patch is the hatched, star-shaped region in the center of Figure 1. At each vertex, the second of the two integers is a counter and the first one identifies the "center" ξ that is used in mapping that vertex onto M. Thus, after the reference vertex 0, the nodes 7,...,12 become centers which serve to map the nodes 13,...,42 onto M. Then the process continues with nodes 17,18,19,23,24,28,29,33,34,38,39,42 as centers. This is no longer shown in the figure, but, in practice, we always continued through this further stage. It results in a total of 114 triangles on M and involves 19 centers and hence as many Jacobian evaluations. This indicates the efficiency of the algorithm. In fact, in terms of computed points per Jacobian evaluation, the method performes better than most continuation processes.

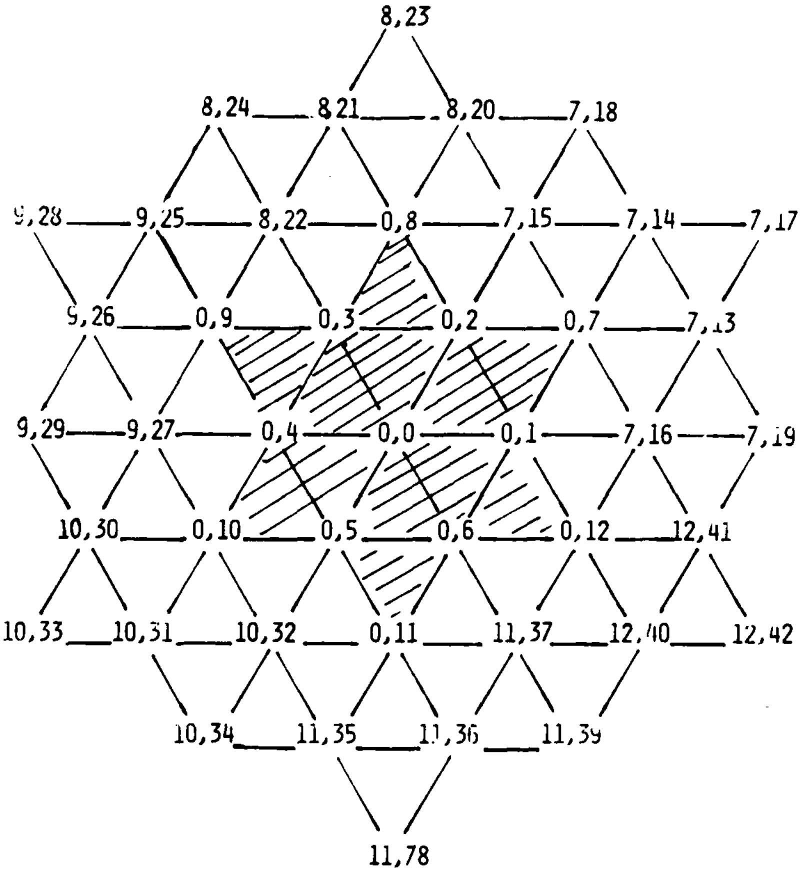

Figure 1

5. Examples

We present now a few numerical examples to indicate the performance of the methods. But space limitations force us to be brief. More extensive examples will be given elsewhere.

Our first example concerns the well-known Belousov-Zhabotinskii reaction [13]. As in [6] we write the mass balance equations in the form

$$\begin{aligned} (\mu-x_1)x_2+x_1(1-x_1)-\varepsilon_1\beta x_1 &= 0 \\ -(\mu+x_1)x_2+x_3+\varepsilon_2\beta(\alpha-x_2) &= 0 \qquad (5.1) \\ x_1-x_3(1-\beta) &= 0 \end{aligned}$$

If $\varepsilon_1 = 1/1{,}500$, $\varepsilon_2 = 1/56{,}250$, and $\mu = 8.4\times10^{-6}$, then, as discussed in [6], there is an isola point approximately at the point with the coordinates

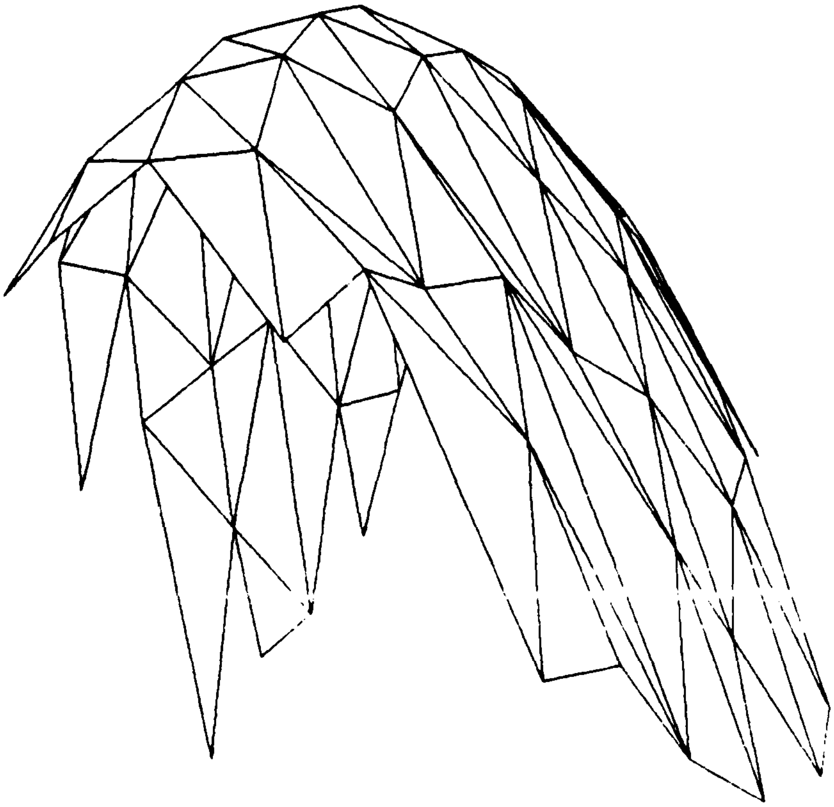

Figure 2

$x_1 = 0.249$, $x_2 = 0.750$, $x_3 = 0.125$, $\alpha = 3.508$, $\beta = 0.997$. This point was used as our reference point on M, and Figure 2 shows the computed simplicial triangulation (based on the reference triangulation of Figure 1). The printed page is the α,β-plane and x_2 is the third coordinate in the figure.

Our second example concerns the roll stability of maneuvering airplanes. Without going into details, we use the equations originally formulated in [7] and given in [8] and [5] in a simplified form $Ax+\Phi(x) = 0$, $x \in R^8$. Here A is a 5 x 8 matrix and $\Phi: R^8 \rightarrow R^5$ a quadratic function. The (dimensionless) control parameters x_6, x_7, x_8 denote the elevator, aileron, and rudder deflections, respectively. The bifurcation diagram for rudder deflections $x_8 = 0$ was given in [8] and again (with some extensions) in [5]. In the neighborhood of the origin of the x_6,x_7-plane it has the form shown in Figure 3.

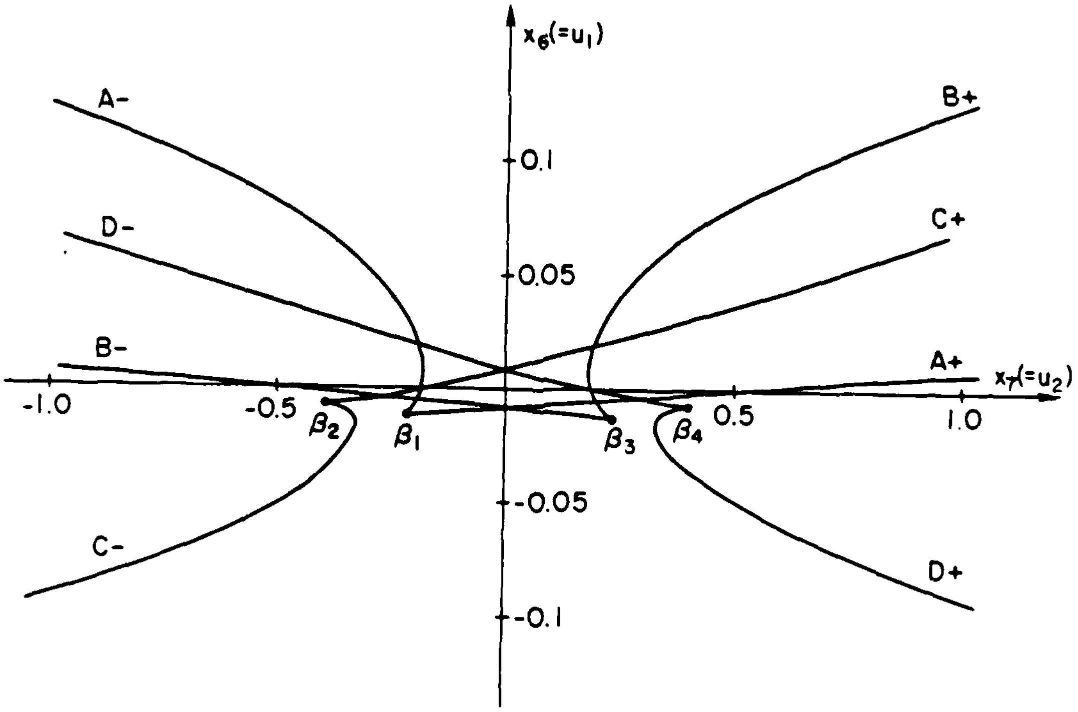

Figure 3

The process was applied with an approximate [illegible] point β_2 as center. The results are shown in Figure 4 where the [illegible] page is the x_6,x_7-plane and the third coordinate [illegible] triangulation contains also the bifurcation point [illegible] emanating from these two bifurcation points are [illegible]

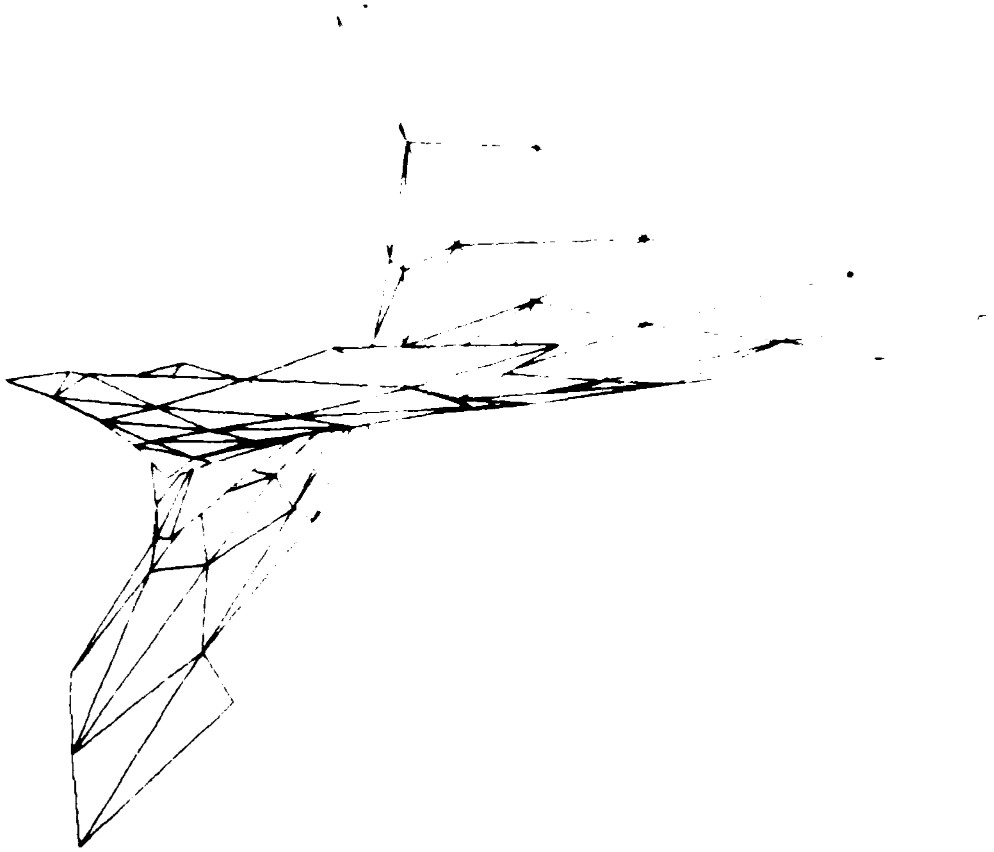

Figure 4

The examples indicate that the algorithms work very efficiently, even around singularities. Thus, as intended, they do indeed provide a new tool for deriving information about the shape and features of the manifold. Of course, besides any graphical representation, the extensive numerical output of the process contains a wealth of further information. For instance, linear interpolation between the computed points defines the earlier mentioned simplicial approximation M_Σ of M. The corrector process can be started from any point of M_Σ to produce additional points of M. In addition, for any given functional it is easy to compute a contour plot of its values on M_Σ. For instance, in some structural problems it may be of interest to determine lines of constant stress components. Similarly, the foldlines on M represent contour lines with respect to a measure of the orientation of the projection of the tangent spaces onto the parameter space. This provides for a simple method of approximating the fold-lines on M which can then be used to compute the fold points themselves by means of one of the numerous local iterative processes available for that purpose. Examples of these, and other post-processing procedures will be given elsewhere.

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