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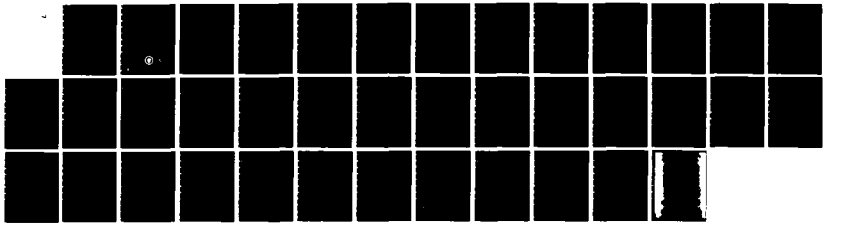

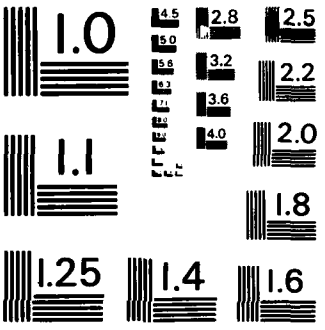

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INSTITUTE FOR COMPUTATIONAL MATHEMATICS AND APPLICATIONS

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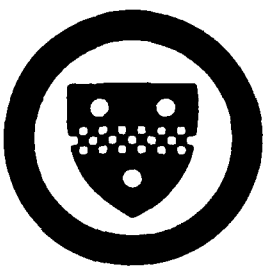

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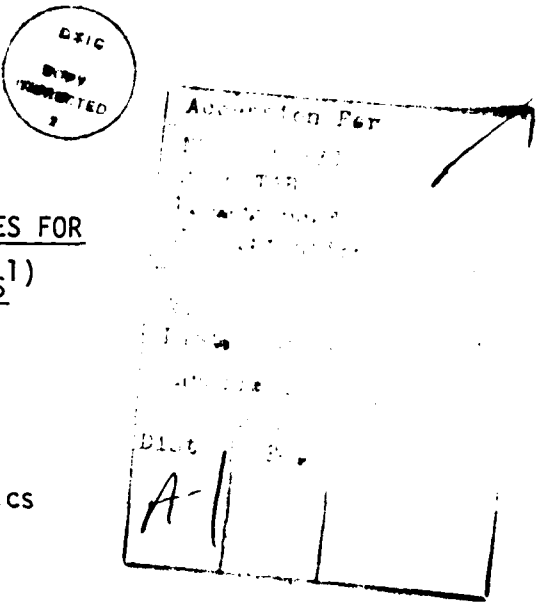

ERROR ESTIMATIONS AND ADAPTIVE TECHNIQUES FOR NONLINEARIZED PARAMETRIZED EQUATIONS[1)]

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1. INTRODUCTION

Many problems in science and engineering concern the determination of steady-state equilibrium solutions of nonlinear equations. In general, for such problems, interest centers not so much of the computation of a few specific equilibria rather than on an assessment of the response of the system to the action of various external or internal influence quantities. In other words, we are interested in the effect of changes of the values of certain parameters upon the computed equilibria. Thus, other than in the typical linear case, for nonlinear problems we usually have to consider equations of the form

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

which depend nonlinearly not only on the state variable z but also on a parameter vector λ. Typically, z varies in some infinite-dimensional space Z while λ belongs to a space Λ with some finite dimension $m \geq 1$.

In line with the indicated objectives it is not enough to find solutions z of (1.1) for a few a priori specified parameter vectors λ. Instead, we have to look at the solutions of (1.1) as points (z,λ) in the product

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1) This paper was in part supported by the Office of Naval Research under Contract N0014-80-C-0455 and the National Science Foundation under Grant MCS-83-09926.

$X = Z \times \Lambda$ of the state and parameter space. Under fairly general conditions, the set of all solutions (z,λ) of (1.1) in X forms a smooth surface -- or more precisely an m-dimensional differentiable manifold -- in that space. When (1.1) represents the equilibrium equation of a mechanical system, this manifold has been called the equilibrium surface of the system (see e.g. [31]).

Broadly speaking, our task then is the computational analysis of this solution manifold of (1.1). The specific aims of that analysis depend on the problem at hand. For example, practical needs often demand the explicit computation of a sufficient number of points in a selected portion of the manifold which may be used, for instance, as the basis of certain post-processing calculations. Another need may concern the determination of the stability properties of the system. In terms of the manifold this leads typically to the study of structural stability as defined by modern bifurcation theory. In essence, an equilibrium point on the manifold is structurally stable if in some neighborhood all points on the manifold have the same qualitative behavior and the task is to determine the points where structural stability is lost and what behavior may be expected there. (See e.g. [33] for some interesting applications in mechanical engineering.)

These are only two of the many different aspects of an analysis of the solution manifold of a parametrized equation (1.1). In this presentation, we consider some of the questions relating to a computational determination of parts of the manifold. As with all engineering computations, the aim here is to obtain solutions which are sufficiently accurate and reliable to allow for a decision about the system under study. For this it has become widely accepted that the computational procedures should include, at least,

(i) facilities for the efficient and reliable estimation of the errors of the computed results; and

(ii) adaptive controls of the computation to achieve the desired error tolerances with minimal cost.

For the solution of certain classes of linear problems by finite element techniques algorithms for these and other desirable features are now beginning to be well understood (see e.g. [1], [10]). But in the nonlinear case much still needs to be done before satisfactory procedures of this type are available. The aim of this paper is to survey some recent results in the area and to point to various open questions.

It turns out that a central aspect of any computational study of a manifold is the availability of simple, but effective local coordinate systems. Some approach to this is sketched in Section 2 below. Then in Section 3 we turn to the question of estimating the discretization errors between the original manifold and that of a corresponding discretized equation. It is important to note that these errors also depend on the choice of the local coordinate system. Section 4 then presents a new approach to the calculation of a posteriori estimates of the discretization errors and shows their efficiency in the case of a two-dimensional nonlinear boundary value problem. In Section 5 we discuss the basic form of a continuation method for approximating one-dimensional manifolds and relate it to a general form of feedback process. This in turn opens up questions about measuring the performance of the method. Finally, in Section 6 we outline an algorithm for the adaptive control of the discretization errors during the course of the continuation procedure and show its performance in the case of a model problem.

2. LOCAL COORDINATES

As noted before, under certain conditions the solution manifold of equation (1.1) is a finite-dimensional, differentiable manifold. In practical applications (1.1) is usually a boundary value problem. Thus it is natural to assume that the mapping F is a Fredholm mapping of class C^r, $r \geq 1$, and index $m \geq 1$ from an open subset S of a real Banach space X into another such space Y. We denote by $DF(x)$ the (Frechet) derivative of F at the point $x \in S$. A point $x \in S$ is a regular point of F if $DF(x)$ maps X onto Y, and a point $y \in Y$ is a regular value of F if the solution set

$$F^{(-1)}(y) = \{x \in S, \quad F(x) = y\}$$

contains only regular points. Then for any regular value $y \in Y$ the set $M \equiv M_y = F^{(-1)}(y)$ is an m-dimensional C^r-manifold in X without boundary (see e.g. [14]).

For all computations on such a manifold M we need an efficient computational scheme for fixing local coordinate systems at any point of M. Among the many possibilities, a simple linear scheme appears to be most advantageous. In order to motivate the idea, let M be a one-dimensional C^1-manifold in R^3. At a given point $x^o \in M$ we choose a one-dimensional subspace T and a two-dimensional plane $W \subset R^3$, as shown in Figure 1, such that for sufficiently small $t \in T$ the plane $x^o + t + W$ intersects M in a unique point which we call $x(t)$. In this way, we obtain a mapping $t \to x(t)$ from some (small) open neighborhood of the origin in R^1 onto a neighborhood of x^o in M. This will be the desired local coordinate system of M at x^o.

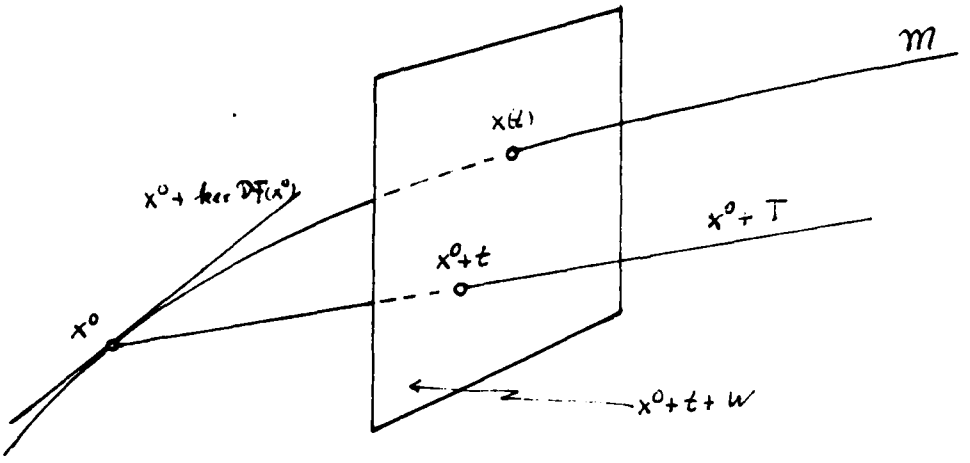

Figure 1

Clearly, T and W cannot be chosen arbitrarily. Certainly the direct sum $T \oplus W$ should be all of R^3 and, in order to get unique intersections $x(t)$, we should avoid that W contains the tangent manifold $\ker DF(x^0)$ of M at x^0. If $D_w F(x^0)$ denotes the partial derivative of F at x^0 with respect to W, then this means that we should enforce $\ker D_w F(x^0) = \{0\}$.

The approach carries over directly to the general case. With a slight notational change the following result was proved in [15]:

Theorem 2.1: Let y be a regular value of F and $x^0 \in M_y$. Suppose that T, W are subspaces of X such that $X = T \oplus W$, $\dim T = m$, and $\ker D_w D(x^0) = \{0\}$. Set $x^0 = t^0 + w^0$, $t^0 \in T$, $w^0 \in T$. Then there exist open neighborhoods $V \subset T$ of t^0 and $U \subset X$ of x^0 and a unique C^r-function $w: V \to W$ such that $w(t^0) = w^0$ and

$$M_y \cap U = \{x \in X;\ x = t + w(t),\ t \in V\}.$$

This result means that a basis for the m-dimensional space T may serve as a local coordinate system on M_y near x^0. Of course, if our original decomposition of X into the state space Z and parameter space Λ satisfies $\ker D_z F(x^0) = \{0\}$ then Λ itself may be used to parametrize M near x^0. Generally, any $x^0 \in S$, where $\ker D_z F(x^0) = \{0\}$, is called a <u>non-singular</u> point of F with respect to the original (natural) parametrization; otherwise x^0 is a <u>singular point</u>. In connection with mechanical problems the most frequently occurring singular points are turning points and simple bifurcation points (buckling points). Generally, if $x^0 \in S$ is a nonsingular point, then the partial derivative $D_z F(x^0)$ is an isomorphism of the state space Z onto the range space Y.

3. ERROR ESTIMATION

We consider a nonlinear mapping $F: S \subset X \to Y$ which satisfies the conditions discussed in Section 2 and assume that a natural decomposition of $X = Z \oplus \Lambda$ into a state space Z and m-dimensional parameter space Λ has been given. If $0 \in Y$ is a regular value then we know that the solution set of the equation (1.1) is indeed an m-dimensional C^r-manifold M in X.

As noted before, in applications the equation (1.1) usually represents some boundary value problem. Hence for the computation, it becomes necessary to replace (1.1) by some finite-dimensional (discretized) approximating equation. But since the parameter space Λ is already finite dimensional, it is only the state variable z that has to be discretized. Thus, the approximating equations, in general, have the form

$$F_h(z_h,\lambda) = 0 \tag{3.1}$$

where now F_h maps a discretized space $X_h = Z_h \oplus \Lambda$ to another such space Y_h.

If F_h again satisfies the needed differentiability conditions and $0 \in Y_h$ is a regular value for it, then the solution set of (3.1) forms an m-dimensional differentiable manifold M_h in X_h. Usually, in finite element computations we have $X_h \subset X$ and our task then is to assess the approximation error between these manifolds measured, for instance, in the norm of X. The development of a rigorous theory of these errors is a fairly recent undertaking. For a one-dimensional parameter space Λ a priori estimates were first developed in [13], [17] and then [14]. The latter results were generalized in [15] to a parameter space Λ of arbitrary finite dimension. All these results involve a family of approximate problems (3.1) which converge in some sense to the original problem (1.1) when the real discreti-

zation index $h > 0$ tends to zero. Then it is shown that for sufficiently small h and in a neighborhood of some point of the solution manifold M of (1.1) the approximate problems also possess solution manifolds M_h for which the distance to M in X can be estimated. A different approach was taken in [16]. There only a single discretized equation (3.1) is considered instead of a converging family of such equations, and estimates are obtained which are local in nature analogous to the local error estimates in the numerical solution of initial value problems for ordinary differential equations.

These a priori estimates are of considerable theoretical interest. But for the computational task outlined in the Introduction we require a posteriori estimates which measure the error of the specific computed points on the approximate solution manifold M_h. However, before we turn to these a posteriori estimates, we need to clarify how these errors are to be defined.

Without any further information, we may compare a computed point x^h on M_h with any point x^o on M. But then the distance $||x^o-x^h||_X$ can hardly be expected to represent a good measure of the quality of the computation. In order to correlate points better we need to choose a local coordinate system at the desired exact point x^o on the manifold M. As discussed in the previous section, this means that a coordinate space $T \subset X$ and complementary space $W \subset X$ are selected for which Theorem 2.1 holds. Then, when the approximation is sufficiently good, the manifold M_h will be close to M and the same local coordinate system can also be used in a neighborhood on M_h of the point x^h for which $x^o-x^h \in W$. This is schematically shown in Figure 2.

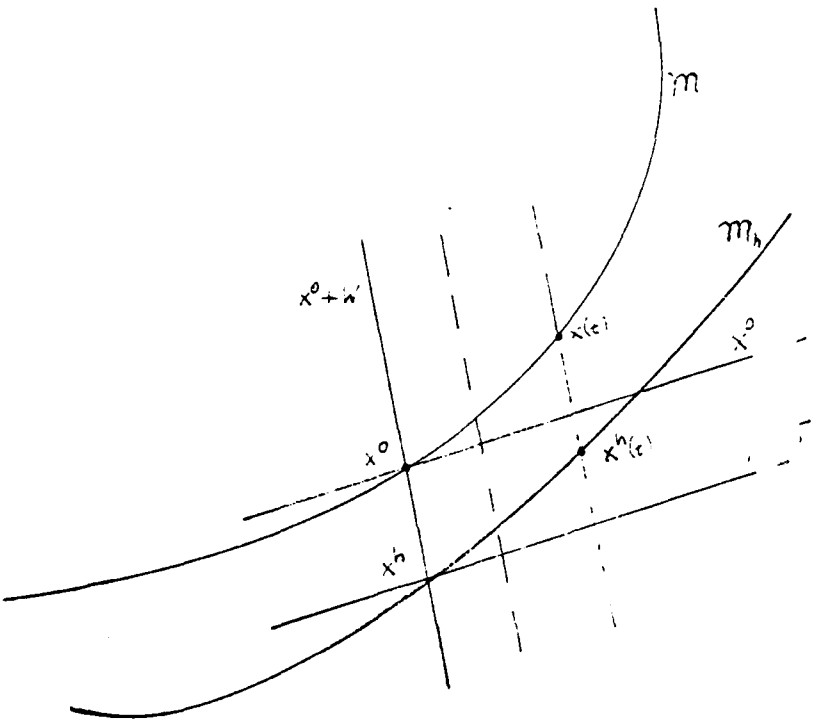

Figure 2

Thus the resulting error estimate depends on the choice of the local coordinate system on M. This is an important point which cannot be overlooked. With a change of the local coordinate system the error-norms change. If x is a non-singular point of M then, of course, we may define the local coordinate system in terms of the natural parameter space Λ and the state space Z. In other words, we then compare $x^o = (z^o,\lambda^o)$ on M with the point $x^h = (z^h,\lambda^o)$ on M_h for which the parameter vector λ^o is the same. Certainly, at singular points of M, such as the limit point $\bar{x}$ in Figure 3, this choice fails. Moreover, as the figure indicates, even at non-singular points x^o near $\bar{x}$ the error-norms $||x^o-x^h||_\chi$ based on the natural coordinate system may be unduly large.

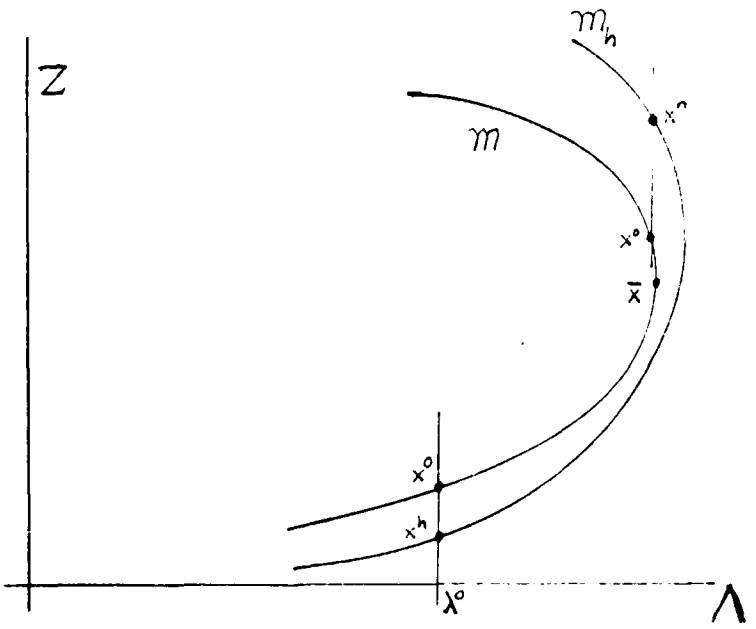

Figure 3

All of the cited articles on a priori error estimations utilize appropriate local coordinate systems at the various types of points. For example, the three papers of [13] treat separately the case of non-singular points, limit points and simple bifurcation points and use a suitable coordinate at each of these points. In [14] and [15] general local coordinate systems in the sense of Theorem 2.1 are utilized to avoid the need of distinguishing between the different types of points.

4. A POSTERIORI ESTIMATES

For the finite-element solution of various classes of linear problems the theory and application of reliable, a posteriori error estimates has advanced considerably in recent years (see e.g. [2], [3], [5], [6], [7], [8], [10]). Not surprisingly, in the nonlinear case -- where even a priori estimates were developed only recently -- the available results on a posteriori estimates are few. An interesting approach was considered in [19], [20], [21], and in [10] and [25] it was shown that for certain model problems in one space dimension it is possible to generalize the techniques of the linear theory. While the resulting estimates did prove to be reliable, their computational cost was still somewhat high.

We sketch here a new approach -- first outlined in [27] -- which produces very effective and reliable a posteriori estimates for a broad class of nonlinear problems and which turns out to be computationally very inexpensive.

We use again the setting of the previous sections and assume that the solution set of the original problem (1.1) is an m-dimensional, differentiable manifold M in $X = Z \times \Lambda$ and that M_h represents the corresponding solution manifold of some discretized equation (3.1) in $X_h = Z_h \times \Lambda \subset X$. As we saw in Section 3, any error estimate depends on the particular choice of the local coordinate system on M. The a posteriori estimates discussed here can be developed for any local coordinate system for which Theorem 2.1 holds. But in order to avoid certain technical details, which may obscure the ideas, we restrict ourselves here to the case of a non-singular point $x^0 = (z^0,\lambda^0) \in M$ and the choice of the natural coordinate system based on the parameter space Λ and the state space Z.

We assume that F is of class C^r, $r \geq 2$, on its open domain S in X. If $x^0 \in M$ is a non-singular point, then -- by definition -- the partial

derivative $D_z F(x^0)$ is non-singular and hence the same is true at any point $\bar{x}^0 = (\bar{z}^0, \lambda^0)$ in some neighborhood of x^0 in S. Hence we can apply a Newton step to the equation $G(z) = F(z,\lambda^0)$ starting from $\bar{z}^0$. The first iterate $\bar{z}^1$ is obtained from the solution w of the linearized equation

$$F(\bar{z}^0,\lambda^0) + D_z F(\bar{z}^0,\lambda^0)w = 0 \tag{4.1}$$

by setting $\bar{z}^1 = \bar{z}^0 + w$. By the Newton-Kantorovich theorem (see e.g. [23]) it follows that

$$\frac{?}{1+\sqrt{2}}\,||w|| \leq ||z^0-\bar{z}^0|| \leq 2||w||, \tag{4.2}$$

provided only that $\bar{z}^0$ is within the attraction ball specified by that theorem (see, especially, the formulation given in [24]).

In our setting, $\bar{x}^0 = (\bar{z}^0,\lambda^0) \in M_h$ is the computed approximation of the desired point $x^0 = (z^0,\lambda^0)$. Hence the required error $||z^0-\bar{z}^0||$ can be estimated in terms of the norm $||w||$ of the solution w of the linearized equation (4.1). Of course, (4.1) is still an infinite-dimensional problem which can only be solved approximately. But here we turn out to be exactly in the setting of the theory of linear a posteriori error estimates and hence can apply the relevant results.

Rather than elaborate on the general theory we illustrate the technique on the following one-dimensional problem

$$\frac{d}{ds} A\left(\frac{\partial z}{\partial s}\right) + B(z,s,\lambda) = 0, \quad \forall\, s \in I = (0,1), \tag{4.3}$$

$$z(0) = z(1) = 0$$

with sufficiently smooth coefficient functions A, B. A weak formulation is

$$N(z,\lambda)v \equiv \int_0^1 [A(z')v' - B(z,s,\lambda)v]ds = 0, \quad \forall\ v \in H_0^1(I) \tag{4.4}$$

and the corresponding linearized problem (4.1) has the form

$$L[z,\lambda]wv \equiv N(z,\lambda)v + \int_0^1 (DA(z')w'v' - D_u B(z,s,\lambda)wv)ds = 0,$$

$$\forall\ v \in H_0^1(I). \tag{4.5}$$

For simplicity, suppose that piecewise linear elements are used on some mesh

$$\Delta: 0 = s_0 < s_1 < s_2 < \ldots < s_{n+1} = 1, \quad n = n(\Delta).$$

In other words, we restrict consideration to the finite dimensional subspace

$$K(\Delta) = \{z \in H_0^1(I);\ \ z(s) = \sum_{i=1}^{n} x_i \phi_i(s),\ \ 0 \le s \le 1\}$$

where ϕ_i denotes the standard, piecewise linear "hat function" with $\phi_i(s_j) = \delta_{ij}$, $i,j = 1,\ldots,n$. Then the exact solution z^0 and the finite-element solution $\bar{z}^0$ are the unique functions $z^0 \in H_0^1(I)$ and $\bar{z}^0 \in K(\Delta)$ such that (4.4) holds for all v in $H_0^1(\Omega)$ and $K(\Delta)$, respectively.

We wish to estimate the norm of the solution w of (4.5) at $\bar{x}^0$; that is, of the problem

$$L[\bar{z}^0,\lambda^0]wv = 0, \quad \forall\ v \in H_0^1(I). \tag{4.6}$$

Evidently, the zero-function $w^0 \equiv 0$ is the solution of (4.6) when v is restricted to $K(\Delta)$. Hence, w represents the error of the finite-element solution of (4.6), and our problem of estimating $||w||$ is exactly the problem of computing an a posteriori error estimate of the finite element solution w^0 of the linearized problem (4.6).

Since, by (4.2), any approximation of $||w||$ represents an a posteriori error estimate of the finite element error $||z^0-\bar{z}^0||$ of the nonlinear problem, it remains to apply the theory of linear a posteriori estimates to the problem (4.6). In the case of our model problem, a simple approach is to use a quadratic finite element approximation $w = \bar{w}(s)$, $0 \leq s \leq 1$, of the solution of (4.6); that is,

$$\bar{w}(s) = \rho_i \bar{w}_i(s) \quad \text{for} \quad s_{i-1} \leq s \leq s_i,$$

$$\bar{w}_i(s) = 4\,\frac{(s-s_{i-1})(s_i-s)}{(s_i-s_{i-1})^2}, \quad i = 1,\ldots,n+1. \tag{4.7}$$

On each one of the $n+1$ elements of Δ the evaluation of the corresponding unknown ρ_i represents a very simple calculation. Hence, say, the quantities

$$\eta_i = \left(\int_{s_{i-1}}^{s_i} (\rho_i \bar{w}_i'(s))^2 ds\right)^{1/2}, \quad i = 1,\ldots,n+1 \tag{4.8}$$

represent error indicators on these elements and our a posteriori estimate becomes

$$\varepsilon = \left(\sum_{i=1}^{n+1} \eta_i^2\right)^{1/2}. \tag{4.9}$$

Other forms of the error indicators and other norms may be used as well. For more details and proofs we refer to [3], [5], [7], [8].

We shall return to the model problem (4.4) in Section 6. As an example of the reliability of the estimates developed here we consider the two-dimensional problem

$$N(z,\lambda)v \equiv \int_\Omega [A_1(z_s,z_t)v_s + A_2(z_s,z_t)v_t - C(s,t,\lambda)v]dsdt = 0$$

$$\forall\ v \in H_0^1(\Omega) \tag{4.10}$$

where Ω is the unit square $[0,1] \times [0,1]$ in R^2. More specifically, we use

$$A_1(z_s,z_t) = a(z_s^2+z_t^2)z_s$$

$$A_2(z_s,z_t) = a(z_s^2+z_t^2)z_t$$

$$a(\sigma) = 1 - \frac{1}{2+\sigma^2}$$

and choose the coefficient function C such that the exact solution has the form

$$z^0(s,t) = \lambda \frac{s(1-s)t(1-t)}{\gamma + (s-0.75)^2 + (t-0.25)^2} \tag{4.11}$$

with some constant $\gamma > 0$.

The linearized problem now has the form

$$N(z,\lambda)v + \int_\Omega (v_s,v_t)M(s,t)\begin{pmatrix} z_s \\ z_t \end{pmatrix} dsdt = 0 \tag{4.12}$$

where

$$M(s,t) = \begin{pmatrix} D_1A_1(z_s,z_t) & D_2A_1(z_s,z_t) \\ D_1A_2(z_s,z_t) & D_2A_2(z_s,z_t) \end{pmatrix}$$

and D_iA_j, $i,j = 1,2$, denotes the derivative of the coefficient function A_j with respect to its i-th variable. The problem (4.12) has the form used in the FEARS-system (see [36]) and hence for the computation of $||w||$ we can apply the a posteriori error estimates developed for that class of linear problems (see e.g. [3], [22]).

The tables below present some computational results obtained in this case. Bilinear elements on square, uniform meshes with the indicated mesh size h and number of degrees of freedom n were used throughout. The continuation process was applied to the one-dimensional solution manifold passing through the origin for $\lambda = 0$. The points with parameter values $\lambda = 1,2,3,4,5$ were chosen as target points. In all cases the energy norm for (4.12) was used.

The table reflects our general experience that the effectivity of the estimates is excellent. The performance corresponds to that reported for the linear case (loc.cit.)

The solution (4.11) has a singularity at (0.75,0.25) when the constant γ is zero. Thus when γ tends to zero we expect the errors to increase. This is indeed the case but the performance of the error estimation remains excellent for errors up to about 10-15%. In Table 2 we give only some results for $\gamma = 0.1$ and the case $h = 1/16$; that is, $n = 225$.

Table 1: $\gamma = 0.5$

h	n	$\|\|e\|\|$	ε	$\frac{\|\|e\|\|}{\|\|u\|\|}$ %	$\frac{\varepsilon}{\|\|u\|\|}$ %	$\frac{\varepsilon}{\|\|e\|\|}$ %
$\lambda = 1$, $\|\|u\|\| = 0.1646$						
1/8	49	.2025(-1)	.2069(-1)	12.30	12.57	102.2
1/16	225	.1013(-1)	.1017(-1)	6.152	6.172	100.3
1/24	529	.6756(-1)	.6763(-1)	4.102	4.106	100.1
$\lambda = 2$, $\|\|u\|\| = 0.3647$						
1/8	49	.4204(-1)	.4396(-1)	11.56	12.09	104.6
1/16	225	.2102(-1)	.2120(-1)	5.763	5.812	100.9
1/24	529	.1401(-1)	.1406(-1)	3.840	3.853	100.3
$\lambda = 3$, $\|\|u\|\| = 0.6465$						
1/8	49	.6903(-1)	.7711(-1)	10.73	11.98	111.7
1/16	225	.3445(-1)	.3543(-1)	5.332	5.482	102.8
1/24	529	.2296(-1)	.2324(-1)	3.551	3.594	101.2
$\lambda = 4$, $\|\|u\|\| = .9553$						
1/8	49	.1003	.1171	10.54	12.31	116.7
1/16	225	.5012(-1)	.5231(-1)	5.250	5.478	104.4
1/24	529	.3341(-1)	.3405(-1)	3.496	3.564	101.9
$\lambda = 5$, $\|\|u\|\| = 1.246$						
1/8	49	.1329	.1582	10.70	12.73	119.0
1/16	225	.6632(-1)	.6968(-1)	5.323	5.592	105.0
1/24	529	.4420(-1)	.4521(-1)	3.456	3.627	102.3

Table 2: $\gamma = 0.1$

$\|\|e\|\|$	ε	$\frac{\|\|e\|\|}{\|\|u\|\|}$ %	$\frac{\varepsilon}{\|\|u\|\|}$ %	$\frac{\varepsilon}{\|\|e\|\|}$ %
$\lambda = 1, \quad \|\|u\|\| = 0.8614$				
0.6990(-1)	0.710(-1)	8.115	8.244	101.6
$\lambda = 2, \quad \|\|u\|\| = 1.733$				
0.1525	0.1542	8.801	8.897	101.1
$\lambda = 3, \quad \|\|u\|\| = 2.552$				
0.2285	0.2302	8.957	9.022	100.7
$\lambda = 4, \quad \|\|u\|\| = 3.368$				
0.3042	0.3036	9.032	9.016	99.83
$\lambda = 5, \quad \|\|u\|\| = 4.186$				
0.3805	0.3783	9.090	9.037	99.42

5. CONTINUATION PROCESSES ON MANIFOLDS

Suppose again that M denotes the m-dimensional solution manifold of a given parametrized equation (1.1). In line with the comments in the Introduction we are interested in computing a sufficient number of points on M which may be used, for instance, as the basis for further postprocessing. All practically useful methods for this purpose compute sequences of points along prescribed one-dimensional submanifolds N of M, although there is certainly room for some different approaches.

There are various ways of defining such submanifolds N. In many applications the usual technique is to specify a parameter combination with one degree of freedom. For instance, in a structural problem the parameter vector may represent a general load vector. Then the chosen parameter combination may determine a load direction while the remaining degree of freedom is the load intensity.

The restriction to the submanifold N is equivalent with the construction of a modified parametrized equation for which the parameter space is one-dimensional (see e.g. [15]). Thus after discretization the problem reduces to a form

$$G(z,\lambda) = 0 \tag{5.1}$$

where $G\colon R^{n+1} \to R^n$ is a given, sufficiently differentiable function of $n+1$ variables and n components.

The one-dimensional solution manifold N of (5.1) may have several connected components and our objective is to determine numerically the component N_0 of N that contains a specified starting point $x^0 \in N$. Most commonly used processes for accomplishing this

task belong to the class of predictor-corrector continuation methods. Starting from x^0 these methods produce a sequence $x^0, x^1, x^2, \ldots$ of points on N_0. For any $k \geq 0$ the computations involved in the step from x^k to x^{k+1} correspond essentially to the construction of the local coordinate systems discussed in Section 2.

The situation is sketched in Figure 4. We calculate first a suitably oriented tangent vector p^k of N_0 at x^k. Then a unit vector t^k with $(p^k)^T t^k \neq 0$ is chosen to define the parametrization subspace $T = \text{span}(t^k)$ of a local coordinate system at x^k. Typical choices are

$$t^k = p^k \qquad \text{(pseudo-arclength choice)} \tag{5.2}$$

and

$$t^k = e^{i_k} \qquad \text{(local variable choice)}$$

where $e^1, \ldots, e^{n+1}$ denote the unit basis vectors of R^{n+1}. The orthogonal complement of T is used as the space W. Now a suitable step along the tangent direction is chosen. This fixes the predicted point $\bar{x}^k = x^k + h_k p^k$ and with it the $(n-1)$-dimensional plane $\bar{x}^k + W$ that passes through $\bar{x}^k$ and is orthogonal to t^k. Finally, a corrector iteration is applied which -- when started at $\bar{x}^k$ -- produces in $\bar{x}^k + W$ a sequence of iterates that converges to the desired next point x^{k+1} on N_0. If the iteration fails a new attempt is made with a reduced stepsize h_k.

In recent years the literature on these continuation processes or incremental methods, as they are also called, has been growing at a rapid pace. Accordingly, there is no need to discuss here any algorithmic details. For some surveys of these processes we refer, for instance, to [30], [34] and for a description of a particular general program to [28], [29].

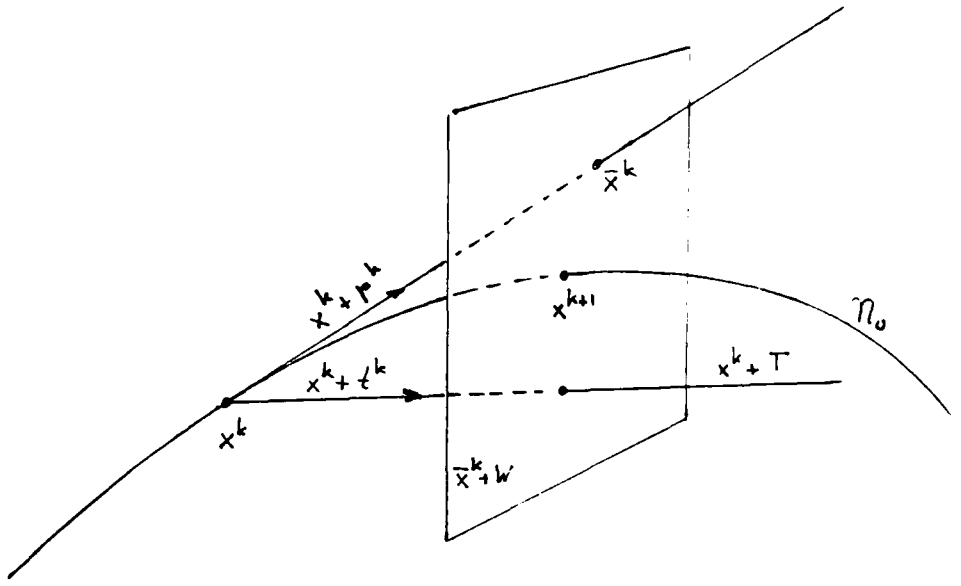

Figure 4

At each step, these methods use heuristic techniques to choose various quantities for which only incomplete information is available, as, for instance, the parametrization direction t^k and the steplength h_k. Thus, broadly speaking, they may be called feedback or adaptive methods. In [26] a precise definition of these terms was developed which applies to many of the adaptive procedures in numerical analysis, and in [4] it was used to prove various results about adaptive mesh-refinement processes for linear finite element computations. There is certainly a need to develop such results also for the continuation methods here under discussion. But, so far, no attempt along this line appears to have been made.

We shall not go into the details of the theory in [26] but identify only some of the main questions. Most of the processes under consideration can be modeled as a discrete, state-space system. We denote the discrete time set by $\mathbb{N} = \{0,1,2,\ldots\}$ and the state space by X. A pair (k,x)

with $k \in \mathbb{N}$, $x \in X$ is called an event and interpreted to mean that at time k the system is in state x. The system is assumed to work on any problem p in a class P. Its operation is described by a state transition function τ: $\mathbb{N} \times X \times P \to X$ which provides that when (k,x) is the current event then feedback from the given problem p will lead to a transition to the state $x' = \tau(k,x,p)$. Thus, for any problem $p \in P$ and starting state $x_0 \in X$, the system produces a trajectory of events

$$\omega(p,x_0) = \{(0,x_0),(1,x_1),(2,x_2),\ldots\}, \quad x_{k+1} = \tau(k,x_k,p), \quad k \geq 0.$$

The entire system Σ is specified by the three sets $\mathbb{N}$, X, and P and the function τ. In view of the interpretation of the dependence of τ upon the problem p as a feedback from that problem, we call Σ a general feedback system.

As stated before, many computational procedures can be modeled as such general feedback systems. Interest then centers on measuring their performance. A fairly general performance measure for Σ may be defined as a mapping μ: $\Omega(\Sigma) \to M$ from the set

$$\Omega(\Sigma) = \{\omega(p,x_0); \quad p \in P, \quad x_0 \in X\}$$

of all possible trajectories of Σ into a given partially ordered set M of performance indices. Recall that in a partially ordered set M an element $m^* \in M$ is minimal if there is no $m \in M$ such that $m \leq m^*$; that is, if for any $m \in M$ either $m \geq m^*$ or m and m^* are not comparable. Accordingly, in [26] a feedback system Σ is called an adaptive system under the performance measure μ if there exists a non-empty subset $Q(\mu) \subset P \times X$ such that $\mu(\omega(p,x_0))$ is minimal in M for any $(p,x_0) \in Q(\mu)$. The size

of the set $Q(\mu)$ may be taken as a measure of the robustness of Σ (see e.g. [35]).

A simple, albeit very frequently used type of performance measure distinguishes only between acceptable and unacceptable performance. Here we use $M = \{0,1\}$ with the natural ordering and call the trajectory $\omega = \omega(p,x_0)$ acceptable or unacceptable if $\mu(\omega) = 0$ or $\mu(\omega) = 1$, respectively. Hence, the feedback system is adaptive under μ if the set

$$Q(\mu) = \{(p,x_0) \in P \times X, \quad \mu(\omega(p,x_0)) = 0\}$$

turns out to be non-empty.

Clearly, the continuation processes discussed above are feedback systems under this definition. But, surprisingly, there is little discussion in the literature how to specify suitable performance measures for such processes, let alone how to prove that the methods are adaptive for any one of them.

There are, of course, many possible performance measures that might be considered for continuation methods. If a specific target points x^* is to be reached on the given one-dimensional manifold N, then we may define μ as a measure of the total number of points needed to step from x^0 to x^* or of the total work involved in reaching the target. But in many applications no such target point is desired or even meaningful. In that case, a possible choice of a performance measure might be a "velocity" that indicates how fast the process is moving along N_0. Already simplified model studies provide here sometimes rather startling results. For example, suppose that the corrector iteration is guaranteed to converge whenever the predicted point is within a prescribed distance $\varepsilon > 0$ of N_0. Then for various model curves as N_0 one can derive asymptotic relationships for the distance s between successive steps. For instance, when the pseudo arc-

length choice (5.2) is used for the local parametrization, then, under certain assumptions, it can be shown that

$$s = O(\frac{\varepsilon}{\kappa}) \quad \text{as} \quad \varepsilon \to 0$$

where κ is the curvature of N_0. On the other hand, when the local variable choice (5.3) is used then, in general, it follows that

$$s = O(\varepsilon) \quad \text{as} \quad \varepsilon \to 0.$$

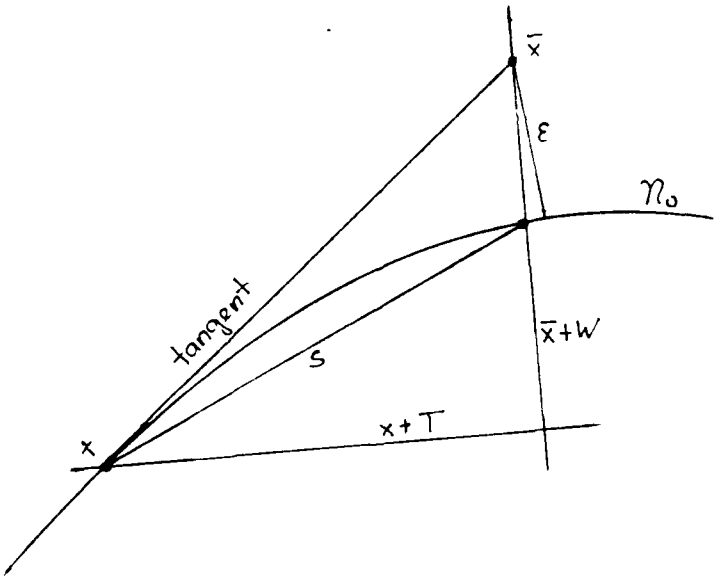

Figure 5

Hence, it should be expected that along strongly curved segments of N_0 the pseudo-arclength process will take many small steps while there is no effect upon the local-variable method. Indeed, this can be observed in practical situations.

These represent only some early results in a more detailed study of suitable performance measures for continuation methods. But they indicate that there is certainly a need for systematic studies in this area which can provide a basis for an assessment of the efficiency of the various techniques utilized in practical programs.

6. ADAPTIVE ERROR CONTROLS

When a continuation process is used for problems where the error estimates of Section 4 are applicable, then, in most cases, the discretization errors show marked variations along any computed one-dimensional sub-manifold. In fact, it may even happen that there are solutions of the discretized problem which do not approximate exact solutions. A simple example of such spurious solutions arises, for instance, in the case of the classical Euler-Bernoulli rod problem (see e.g. [9]).

As noted in the Introduction, for our problems it is certainly desirable to provide facilities in the continuation procedures that can control the discretization errors along the computed submanifolds. The basic control mechanism is here the adaptive refinement or de-refinement of the mesh used in the discretization. The continuation process is applied in its normal form but at each computed point a posteriori error estimates are determined. Then, an appropriate procedure decides when the errors at any point x^k are unacceptable. In that case a new mesh Δ^+ is created from the mesh Δ used in the computation of x^k by uniformly subdividing some elements of Δ and coalescing certain contiguous clusters of others. Then a new point $(x^k)^+$ is determined by interpolation and the continuation process for the new discretized problem is started from $(x^k)^+$.

Certainly, this type of combined continuation and mesh-refinement procedure is a feedback process in the sense of the previous section. The question is how to define the decision process and the desired performance measures so that the procedure indeed becomes adaptive. This is as yet an open problem. We shall outline here only some possible approaches that appear to be very promising.

Our primary aim is to compute a sequence of points $x^0, x^1, \ldots$ which

approximate points on the desired manifold N_o of the original problem in such a way that the error estimates $\varepsilon^o, \varepsilon^1, \ldots$ at these points satisfy

$$\varepsilon^k \leq \text{tol}_k \equiv \delta_{abs} + \delta_{rel}||x^k||, \quad k = 0,1,\ldots \tag{6.1}$$

with given tolerance coefficients δ_{abs} and δ_{rel}. The secondary aim is to avoid frequent re-meshing and re-starting. More ideally the decision procedure should be such that the total work required for computing a sufficient number of points along a prescribed segment of N_o is less than that required for other choices of re-meshing points and associated meshes for which (6.1) is satisfied.

We restrict this discussion to the case of the problem (4.3). The corresponding linearized problem (4.4) has the general form

$$\int_o^1 [a(s)w'v' - b(s)wv]ds = \int_o^1 c(s)vds, \quad \forall\ v \in H_o^1(I) \tag{6.2}$$

considered in [7]. Any continuous, strictly monotonically increasing function ξ on $I = [0,1]$ with $\xi(0) = 0$, $\xi(1) = 1$, together with the specifications

$$\xi(s_j) = \frac{j}{N}, \quad j = 0,1,\ldots,N=n+1$$

defines a family of meshes $\Delta(\xi,n)$, $n = 0,1,\ldots$, on I. Let $w \in H_o^1(I)$ be the solution of (6.2) and consider the partition function

$$\xi_o(s) = \gamma_o \int_o^s [a(s)(w''(s))^2]^{1/3}ds, \quad s \in I, \tag{6.3a}$$

$$\gamma_o = \{\int_o^1 [a(s)(w''(s))^2]^{1/3}ds\}^{-1}. \tag{6.3b}$$

Then it was shown in [7] that under suitable conditions the family of meshes $\Delta(\xi_o,n)$ generated by ξ_o is asymptotically optimal with

$$ {}_I||e||_E^2 = \frac{1}{12(n+1)^2\gamma_o^3}(1+O(\bar{h})) \quad \text{as} \quad \bar{h} \to 0 \tag{6.4} $$

where $\bar{h} = \max\{s_j - s_{j-1},\ j = 1,\ldots,N\}$. In other words, for any other admissible partition function ξ the error for the mesh $\Delta(\xi,n)$ is not less than that for $\Delta(\xi_o,n)$ for all sufficiently small $\bar{h}$.

Moreover, it was shown in [7] that for any mesh Δ the error under the energy norm can be expressed as

$$ {}_I||e||_E^2 = \sum_{j=1}^{n+1} \varepsilon_j^2 (1+O(\bar{h})) \quad \text{as} \quad \bar{h} \to 0 \tag{6.5} $$

where

$$ (12\varepsilon_j^2)^{1/3} = \int_{s_{j-1}}^{s_j} [a(s)(w''(s))^2]^{1/3} ds \ (1+O(1)) \quad \text{as} \quad \bar{h} \to 0 \tag{6.6} $$

This suggests the definition of the piecewise constant function ψ on I for which

$$ \psi(s) = \frac{12\varepsilon_j^2}{h_j^3} \qquad s_{j-1} < s < s_j. \tag{6.7} $$

Evidently, the value of ψ on each subinterval represents some average of $a(w'')^2$ on that interval, and we have

$$ \int_{s_{j-1}}^{s_j} [a(s)(w''(s))^2]^{1/3} ds = \int_{s_{j-1}}^{s_j} \psi^{1/3}(s) ds \ (1+O(1)) \quad \text{as} \quad \bar{h} \to 0. \tag{6.8} $$

If we use instead of the ε_j in (6.7) the computed error indicators, such as (4.8), then we obtain an approximation $\bar{\psi}$ of ψ and with it, from (6.8) and (6.3), an approximate optimal partition function $\overline{\xi_0}$. This provides us with a basic mesh-refinement strategy. A point x^k is declared unacceptable when $\varepsilon^k > \tau\ tol_k$ where tol_k is the tolerance defined by (6.1) and τ is some factor, say, $\tau = 0.75$. From the error indicators at x^k the approximate optimal partition function $\overline{\xi_0}$ and its associated factor $\overline{\gamma_0}$ (see (6.3a) and (6.3b)) can be computed. Then (6.4) suggests the use of the relation

$$\tau\ \varepsilon^k = \frac{1}{12(\bar{n}+1)^2\ \overline{\gamma_0}^3}$$

for obtaining an "ideal" mesh size $\bar{n}$, and with it an associated mesh $\Delta(\overline{\xi_0},\bar{n})$. Now the desired new mesh Δ^+ at x^k can be generated as an approximation of $\Delta(\overline{\xi_0},\bar{n})$; that is, we subdivide certain intervals and re-combine others so as to match $\Delta(\overline{\xi_0},\bar{n})$ as closely as possible. This can be accomplished in various ways and we shall not elaborate upon these procedures. But note that in general the size $n(\Delta^+)$ of the new mesh need not be exactly equal to $\bar{n}$.

As an example for the operation of this procedure we consider the simple model problem (4.4) with the coefficients

$$A(\sigma) = \sigma/(1+\sigma), \quad B(z,s,\lambda) = \lambda$$

in which case the exact solution is

$$z(s) = -s + \frac{1}{\lambda} \ln[(e^{\lambda}-1)s + 1], \quad 0 \le s \le 1.$$

For growing λ this solution increases rapidly within a small interval near $s = 0$. Table 3 gives the results of the above procedure when started with $x^0 = 0$ at $\lambda = 0$. The tolerance was computed with $\delta_{abs} = .0075$, $\delta_{rel} = .05$ and the decision factor was $\tau = .75$.

Figure 6 illustrates the changing meshes during the course of the process.

As the example indicates the procedure performs as expected. This is our general experience for a number of problems of varying complexity. The simplicity of the approach certainly makes it very attractive. At the same time, there are several aspects that may be worthy of improvement:

(i) The function $\bar{\psi}$ used in the definition of the approximate, optimal partition function $\bar{\xi}_0$ incorporates only information at the current point and does not attempt to predict the future course of the process.

(ii) The decision factor τ upon which the acceptance or rejection of a point is based and which features in the determination of the "ideal" mesh $\Delta(\bar{\xi}_0,\bar{n})$ does not change with the conditions during the computation.

(iii) In its present form, it is not clear how to generalize the procedure to problems with higher space dimension.

Preliminary results indicate that the procedure can be improved to account for these points by utilizing some of the concepts and approaches developed in [11] and [12] for the case of parabolic equations. A prototype software system, for the adaptive finite element solution of a class of two-dimensional, parametrized non-linear problems is now under construction which will incorporate such a more general decision procedure. An outline of this system -- called NFEARS -- has been given in [32].

Table 3

λ	N_{used}	N_{ideal}	error estim %	exact error %	tolerance	decision
0	32	—	0	0		proceed
0.110	32	5	0.1005(-2)	0.1361(-2)	0.9102(-2)	proceed
0.444	32	13	0.4205(-2)	0.1013(-1)	0.1391(-1)	proceed
1.337	32	22	0.1814(-1)	0.1814(-1)	0.2736(-1)	proceed
2.238	32	33	0.5570(-1)	0.5586(-1)	0.4248(-1)	refine
	33	24	0.3077(-1)	0.3077(-1)	0.4261(-1)	proceed
2.350	33	26	0.3456(-1)	0.3465(-1)	0.4466(-1)	proceed
2.685	33	32	0.4947(-1)	0.5242(-1)	0.5105(-1)	proceed
3.589	33	39	0.1451	0.1466	0.7130	refine
	37	27	0.4777(-1)	0.4776(-1)	0.7193(-1)	proceed
3.700	37	28	0.5248(-1)	0.5251(-1)	0.7484(-1)	proceed
4.036	37	32	0.7163(-1)	0.7606(-1)	0.8399(-1)	proceed
4.938	37	45	0.2082	0.2094	0.1147	refine
	45	44	0.1112	0.1109	0.1153	proceed
5.049	45	48	0.1267	0.1267	0.1198	refine
	44	31	0.7810(-1)	0.7857(-1)	0.1202	proceed
5.161	44	31	0.7620(-1)	0.8644(-1)	0.1249	proceed
5.497	44	38	0.1193	0.1254	0.1398	

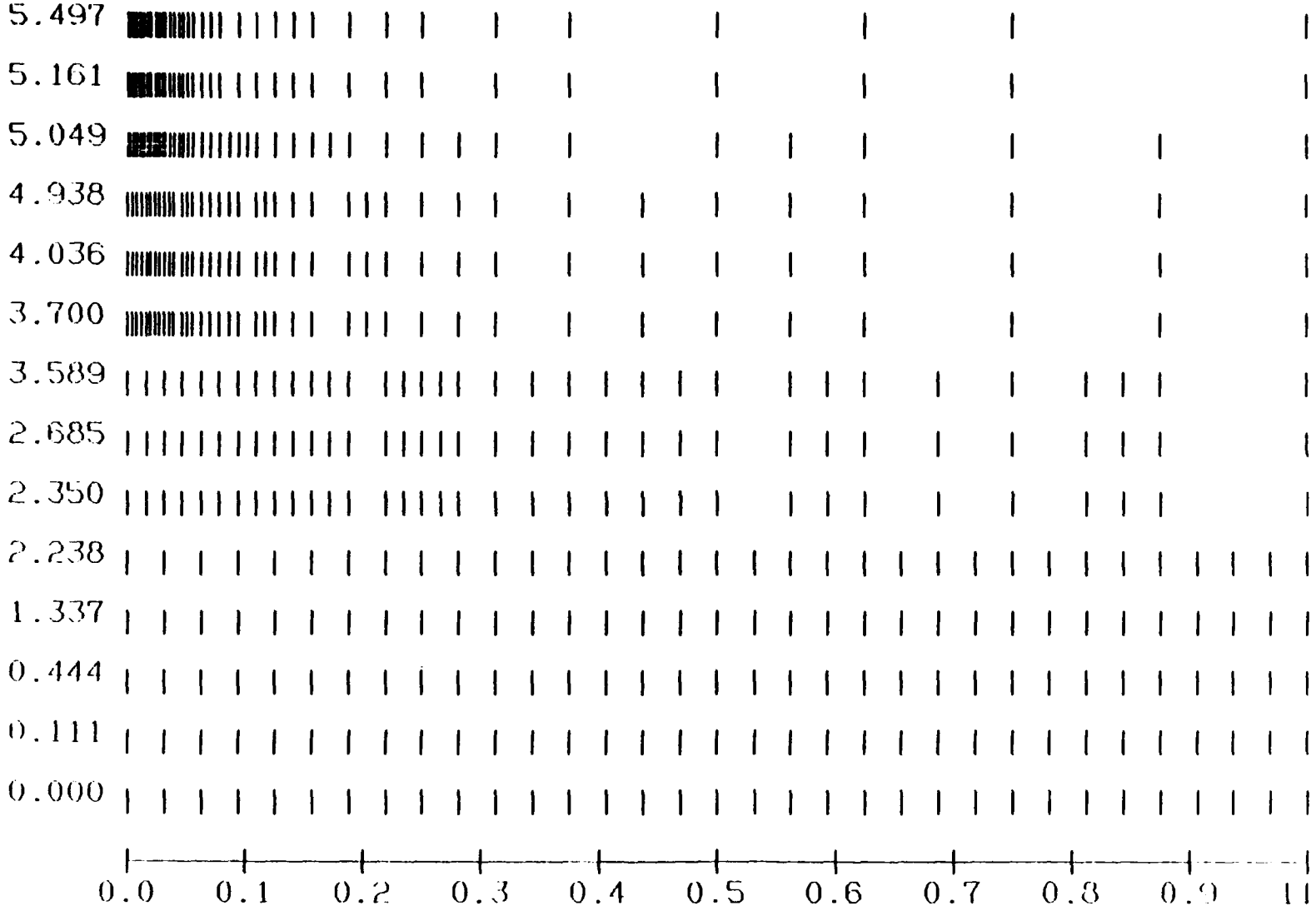
5.497
5.161
5.049
4.938
4.036
3.700
3.589
2.685
2.350
2.238
1.337
0.444
0.111
0.000
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0

Figure 6

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