

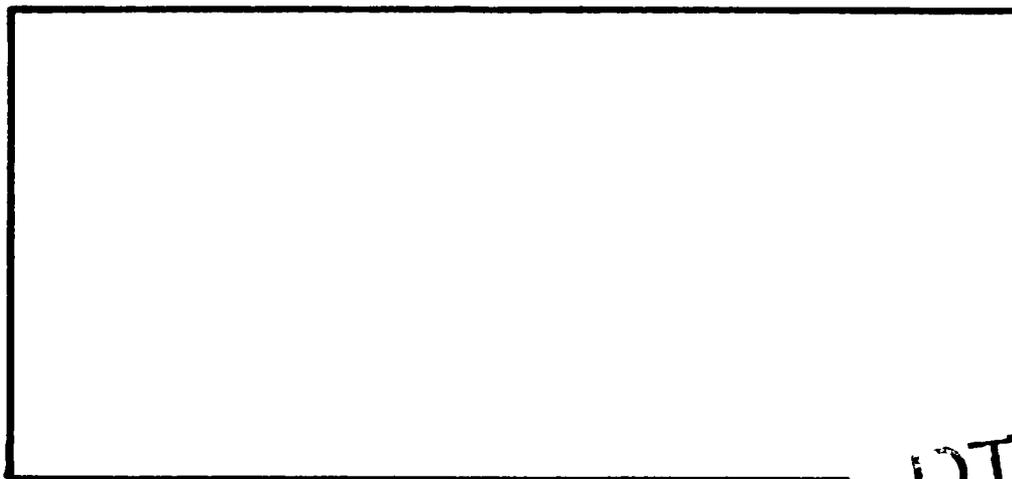
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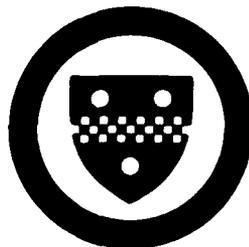
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Technical Report ICMA-81-30

October 1981

A Program for a Locally-Parametrized
Continuation Process*)

by

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*) This work was supported in part by the National Science Foundation under Grant MCS-78-05299 and the Office of Naval Research under Contract N00014-77-C-0623.

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1. INTRODUCTION

The study of many equilibrium phenomena leads to non-linear equations which involve a number of intrinsic parameters. Interest then centers rarely on the determination of a few specific solutions of the equations for fixed parameter values but rather on an assessment of the behavior of these solutions under general variations of the parameters. For example, in structural analysis the parameters may characterize load points and load directions, material properties, geometrical data, etc. The set of all solutions and associated parameter values has been called the equilibrium surface of the structure (see eg. [31]). This equilibrium surface provides considerable insight into the behavior of the structure and the stability properties (see eg. [23], [32] for further discussions and various examples). From a numerical viewpoint the question then is to analyze computationally the shape and characterize particular features of this equilibrium surface.

In nonlinear mechanics the principal tools for such a computational analysis are the so-called incremental methods. These procedures were developed more or less independently in the engineering literature. But they are now also recognized to be closely related to the continuation methods used for some time in mathematics in general and in numerical analysis in particular. The literature in this area is extensive: we refer only to [21] for a discussion about the connection between incremental approaches for structural problems and continuation methods, to [8] for a historical overview of uses of continuation techniques in mathematics and to [2], [35] for some literature survey of numerical aspects of continuation methods.

Not surprisingly there are differences between the methods used in structural engineering and numerical analysis and neither is directly suited to the analysis of an equilibrium surface. In the numerical analysis liter-

ature continuation methods are usually considered only as tools for determining a specific solution y^* of a given nonlinear operator equation $Gy = 0$. For this the equation is imbedded into a one-parameter family $H(y,t) = 0$ which has a solution $y = y(t)$ for each fixed t in some interval, say, $0 \leq t \leq 1$. (See eg. [15] for a survey of such imbeddings.) If $y(t)$ depends continuously on t and satisfies $y(0) = y^0$ and $y(1) = y^*$, where y^0 is a known point, then the numerical process constructs a sequence of points in the proximity of the path $y(t)$, $0 \leq t \leq 1$, starting at y^0 and ending at the desired point y^* . On the other hand, in structural mechanics incremental methods usually are designed to follow numerically a specific load curve parametrized by a load intensity. Hence, while in the imbedding approach the parameter is essentially artificial, in the incremental procedures it has an intrinsic meaning for the application, and, even more importantly, there is no longer a fixed endpoint which is the aim of the computation, but the load curve itself is of interest.

For a numerical analysis of a given equilibrium surface we need to consider continuation-methods in a broader sense as a collection of numerical procedures for completing at least the following three basic tasks:

- (i) Follow numerically any curve on the surface specified by a particular combination of parameter values with one degree of freedom.
- (1.1) (ii) On any such curve determine the exact location of target points where a given state variable has a specified value.
- (iii) On such a curve identify and compute exactly the critical points where stability may be lost.

Beyond this various more special tasks may arise as, for example, the following ones:

- (iv) From any one of the critical points determined under (iii) follow a path in the critical boundary.
- (1.2)
- (v) On any one of the curves (i) determine the location of bifurcation points and the paths intersecting at that point.

Methods which are either directly applicable or can be readily adapted to completing these various tasks have been proposed by various authors. In particular, for (i) the literature is very large and we refer here only to the mentioned surveys [2], [35]. Methods relating to (iii) were described, for instance, in [1], [20], [22], [33], [34], and for (iv) and (v) we refer to [28] and [10], [25], respectively, where also further references are given.

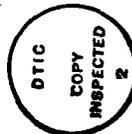
So far only a few library programs for performing these various tasks have been published. Without claim for completeness we mention here [14], [38]. Each one of these programs has the objective of computing a specified solution curve of a nonlinear equation by a continuation approach along the lines sketched above. In this paper, we present a new library package specifically written with the objective of completing the three basic tasks (1.1) (i), (ii), (iii). The package can be expanded to incorporate facilities for (1.2) (iv), (v), but this will not be addressed here. The package is based on the continuation approaches introduced in [26], [27] and incorporates some of the concepts of steplength determination discussed in [7]. At the same time, new techniques of parameter adaptation are utilized here based on a prediction of changes in the curvature of the continuation path.

As with all programming packages further improvements are possible. For example, it is planned to introduce an automatic first step selection and a function-scaling option. Special versions incorporating facilities for the tasks (1.2) are also being designed. But since all these changes are built on the present package the presentation of a documentation of PITCON in its basic form appeared desirable and justified.

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2. BASIC FORMULATION

Generally, after suitable discretizations, the equilibrium problems mentioned in the introduction lead to a finite-dimensional, non-linear equation of the form

$$(2.1) \quad G(y,p) = 0$$

where $y \in R^m$ is a vector of state variables, $p \in R^r$ a vector of parameters, and $G: R^m \times R^r \rightarrow R^m$ a given function. Then we are interested in the features of the set

$$(2.2) \quad E(G) = \{(y,p) \in R^m \times R^r; G(y,p) = 0\}$$

of all solutions of (2.1). Under well-known conditions $E(G)$ represents an r -dimensional manifold in $R^m \times R^r$.

In most applications, interest centers on tracing paths on $E(G)$ which are characterized by $r-1$ relations between the parameters. In other words, we are given a suitable mapping $K: R^r \rightarrow R^{r-1}$ and wish to compute the subset of $E(G)$ defined by the augmented equations

$$(2.3) \quad \begin{aligned} G(y,p) &= 0, \\ Kp &= 0. \end{aligned}$$

In this formulation we should include the parameters in the list of variables, in which case, (2.3) represents a system with one more variable than equations. Then, for ease of notation, it is reasonable to combine the vectors y and p into one vector x of dimension $n = m+r$. Moreover, from the viewpoint of our package of library programs it is natural to assume that both mappings

G and K of (2.3) are provided for by the user. In other words, we may write (2.3) as one equation

$$(2.4) \quad Fx = 0$$

with a user-specified mapping $F: \mathbb{R}^n \rightarrow \mathbb{R}^{n-1}$. Note, however, that in this underdetermined equation (2.4) no one variable is explicitly identified as continuation variable as is typical in the incremental and continuation methods mentioned in the introduction.

We assume here that the given mapping F has the following properties:

- (i) F is continuously differentiable on \mathbb{R}^n .
- (2.5) (ii) The derivative $DF(x)$ of F is locally lipschitzian on \mathbb{R}^n .
- (iii) The regularity set $R(F) = \{x \in \mathbb{R}^n; \text{rank } DF(x) = n-1\}$ is non-empty and therefore an open subset of \mathbb{R}^n .

From (2.5) it follows (see [26]) that the tangent map specified by

$$(2.6) \quad T: R(F) \rightarrow \mathbb{R}^n, \quad DF(x)Tx = 0, \quad \|Tx\|_2 = 1, \quad \det \begin{pmatrix} DF(x) \\ (Tx)^T \end{pmatrix} > 0$$

is uniquely determined and locally lipschitzian on $R(F)$. Furthermore, (2.5) implies that the regular solution set $E(F) \cap R(F)$ of F is either empty or a one-dimensional C^1 -manifold in the open set $R(F)$. Our objective is to determine numerically a non-empty connected component E^* of $E(F) \cap R(F)$. It is well-known (see eg. [17]) that such a component E^* is diffeomorphic either to the circle or to some interval (that is, some connected subset) of \mathbb{R}^1 . Hence, E^* is uniquely determined by any one of its points $x^0 \in E(F) \cap R(F)$

and we denote this by writing $E^*(F, x^0)$. Note that for any $x^1 \in E^*(F, x^0)$ we have $E^*(F, x^1) = E^*(F, x^0)$.

A parametrization by arclength of $E^*(F, x^0)$ is a solution of the initial value problem

$$(2.7) \quad \dot{x} = Tx, \quad x(0) = x^0.$$

Note that, since T is locally Lipschitzian, (2.7) has a unique solution which cannot terminate inside $R(F)$. Evidently standard ODE-solvers may be applied to solve (2.7) numerically. This has been pursued for some time in the literature (see eg. [3], [6], [13], [37]). Independent of this, the choice of the arclength for the parametrization of $E^*(F, x^0)$ has been proposed by many authors. Notably H. B. Keller and his co-workers (see eg. [10], [11]) have advocated this choice for some time. It is also the basis of incremental procedures given in [5], [29] and has been more or less implicit in various papers in the field.

Our programs here are based more generally on the structure of $E^*(F, x^0)$ as a one-dimensional manifold and use a local parametrization at each point computed along $E^*(F, x^0)$. A natural class of such local parameters are the n components of the vector x . We call a process based on this choice of parametrization a locally-parametrized continuation method.

3. OUTLINE OF THE PROCESS AND BASIC STEPS

As noted before, our objective is to determine numerically a non-empty component $E^*(F, x^0)$ of the regular solution set $E(F) \cap R(F)$. For the discussion it is useful to consider a parametrization by arclength of $E^*(F, x^0)$, that is, a function $x: J \rightarrow E^*(F, x^0)$ which maps some interval $J \subset \mathbb{R}^1$ diffeomorphically onto some open subset of $E^*(F, x^0)$ such that $\|\dot{x}(s)\|_2 = 1$ for $s \in J$. We may assume also that $x(0) = x^0$, $0 \in J$.

The process described here belongs to the class of predictor-corrector continuation methods. Starting from x^0 it produces a sequence of approximations $x^k \doteq x(s_k)$, $k = 0, 1, \dots$, corresponding to some sequence $0 = s_0 < s_1 < s_2 < \dots$ of arclength values. Note, however, that in general the values s_1, s_2, \dots are only approximately computable and are of limited interest in most applications.

In our program the principal steps performed during one continuation step are as follows:

1. Initialization.
2. Check for and computation of target point, if desired.
3. Calculation of tangent vector and determination of new local continuation parameter.
- (3.1) 4. Check for and computation of limit point, if desired.
5. Steplength computation.
6. Computation of predicted point and corrector iteration.
7. Storage of data and return.

The sequencing of these steps is dictated by the data-flow. For the description of the details it will be advantageous not to adhere to this

sequence. Instead, in the remainder of this section, we discuss the basic steps 3. and 6. Then the next section introduces the new steplength computation used in step 5. and section 5 covers steps 2. and 4. The data-handling steps 1. and 7. should be self-explanatory from the documentation of the program itself.

Let e^1, \dots, e^n be the natural basis vectors of R^n . Then it is readily verified that (see eg. [26])

$$(3.2) \quad \det \begin{pmatrix} DF(x) \\ (e^i)^T \end{pmatrix} = [(e^i)^T Tx] \det \begin{pmatrix} DF(x) \\ (Tx)^T \end{pmatrix}, \quad \forall x \in R(F), \quad i = 1, \dots, n,$$

where the matrix occurring on the right is non-singular. Hence, for any index i , $1 \leq i \leq n$, such that $(e^i)^T Tx \neq 0$, the solution $v \in R^n$ of the linear system

$$(3.3) \quad \begin{pmatrix} DF(x) \\ (e^i)^T \end{pmatrix} v = e^n$$

is uniquely defined. Evidently, then

$$(3.4) \quad Tx = \sigma \frac{v}{\|v\|_2},$$

and, in line with (2.6), we should set

$$(3.5) \quad \sigma = \text{sign}(v^T e^i) \text{sign} \det \begin{pmatrix} DF(x) \\ (e^i)^T \end{pmatrix}.$$

As long as the solution path remains completely in $R(F)$ this is satisfactory.

But frequently in applications we may encounter a bifurcation point $x^* \notin R(F)$ where several solution paths terminate. For example, using arclength representations we may find solutions $x^j: J_j \subset \mathbb{R}^1 \rightarrow R(F)$, $j = 1, \dots, 4$, for which $x^j(s)$ tends to x^* when s tends to one of the endpoints of J_j . Moreover, it often happens that there are pairs of these solutions, say, x^1 and x^2 for which $\lim \dot{x}^1(s) = -\lim \dot{x}^2(s)$ at x^* , (see Fig. 1). In other words, if we disregard the direction of the solutions, they appear to form one smooth curve through x^* . In such a case, when the process moves along x^1 toward x^* it usually "jumps" over x^* onto x^2 . Then, unless we reverse the sign of σ in (3.4) the tangent will again point toward x^* and the process reverses direction.

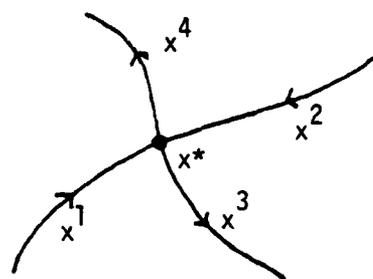


Figure 1

In order to avoid this problem suppose that the point x in (3.4) is the k -th approximation computed along the curve. Then σ is determined as follows

$$(3.6) \quad \sigma = \begin{cases} \text{dir}, & \text{if } k = 0 \\ +1, & \text{if } \text{sign } v^T e^i = \text{sign}(Tx^{k-1})^T e^i \\ -1, & \text{otherwise} \end{cases}$$

where dir is a user specified direction at the starting point. By comparing this value of σ with that of (3.5) we can detect if the process did jump over a bifurcation point of odd multiplicity. Obviously, bifurcation points of even multiplicity cannot be found this way.

Once the tangent Tx^k has been obtained we determine the indices j_1 and j_2 of the largest and second largest component of Tx^k in modulus,

respectively. The relation (3.2) certainly suggests that the index i_k , $1 \leq i_k \leq n$, of the new local continuation variable be set equal to j_1 . However, if we are approaching a limit point in the j_1 -th variable then this choice may be disadvantageous. Accordingly, if the following three conditions are simultaneously satisfied

$$(3.7) \quad \begin{aligned} & \text{(i)} \quad |(e^{j_1})^T T_x^k| < |(e^{j_1})^T T_x^{k-1}|, \\ & \text{(ii)} \quad |(e^{j_2})^T T_x^k| > |(e^{j_2})^T T_x^{k-1}|, \\ & \text{(iii)} \quad |(e^{j_2})^T T_x^k| \geq \mu |(e^{j_1})^T T_x^k|, \end{aligned}$$

with a fixed μ , $0 < \mu < 1$, then we set $i_k = j_2$. Of course, if we don't have a previous tangent vector this check has to be bypassed. The new continuation index i_k will be used for the computation of the next point x^{k+1} and its tangent T_x^{k+1} . For the tangent computation at x^0 a continuation index is assumed to be given by the user.

With the tangent T_x^k and the steplength $h_k > 0$ determined by the steplength algorithm of section 4 we compute now the predicted point $\hat{x}^k = x^k + h_k T_x^k$. Then any appropriate iterative method for the solution of the augmented equation

$$(3.8) \quad \hat{F}x \equiv \begin{pmatrix} Fx \\ (e^{i_k})^T (x - \hat{x}^k) \end{pmatrix} = 0$$

starting from \hat{x}^k may be used as a corrector process. In the program we use either the regular Newton method or its modified form in which the Jacobian at the starting point is held fixed.

Let $y^0 = \hat{x}^k, y^1, y^2, \dots$ be the iterates produced in this way. The process has to incorporate provisions for monitoring the convergence and for aborting the iteration as soon as divergence is suspected. In the program non-convergence is declared if any one of the following three conditions is true

$$(3.9) \quad \begin{aligned} & \text{(i)} \quad \|\hat{F}y^j\| \geq \theta \|\hat{F}y^{j-1}\| \quad \text{for some } j \geq 1, \\ & \text{(ii)} \quad \|y^j - y^{j-1}\| \geq \theta \|y^{j-1} - y^{j-2}\| \quad \text{for some } j \geq 2, \\ & \text{(iii)} \quad j \geq j_{\max}. \end{aligned}$$

For the constant θ we use $\theta = 1.05$ except in the first check of (3.9) (i) where $\theta = 2$ is chosen. The maximal iteration count j_{\max} depends on the method. For the regular Newton process we set $j_{\max} = 10$ and double this for the modified method. In the case of non-convergence the predictor step is reduced by a given factor, for example 1/3, unless the resulting step is below a given minimal steplength.

Convergence is declared if either one of the two conditions holds for an iterate:

$$(3.10) \quad \begin{aligned} & \text{(i)} \quad \|\hat{F}y^j\| \leq 8 \epsilon_{\text{mach}} \quad \text{for some } j \geq 0, \\ & \text{(ii)} \quad (\|\hat{F}y^j\| \leq \epsilon_{\text{abs}}) \quad \text{and} \quad (\|y^j - y^{j-1}\| \leq \epsilon_{\text{abs}} + \epsilon_{\text{rel}} \|y^j\|) \quad \text{for some } j \geq 1. \end{aligned}$$

The tolerances $\epsilon_{\text{abs}}, \epsilon_{\text{rel}}$ are user specified and ϵ_{mach} is the smallest floating point number such that $1. = 1. + \epsilon_{\text{mach}}$. In both tests (3.9) and (3.10) the maximum norm is used.

4. THE STEPLENGTH ALGORITHM

For the points x^k , $k = 0, 1, \dots$, approximating the continuation curve $x: J \rightarrow E^*(F, x^0)$ the achievable error $||x^k - x(s_k)||$ is solely determined by the termination criterion (3.10) of the corrector process. In contrast to this the standard ODE-solvers involve a corrector equation obtained by extrapolation for which the solutions are not, in general, on the exact curve. As a consequence the available error for the ODE-solvers depends on the history of the process up to that point, and this in turn has a strong influence on the step-selection. On the other hand, for our continuation process any step $h_k > 0$ along the Euler line is acceptable in principle if only the corrector converges from the predicted point \hat{x}^k . Moreover, in [26] it was shown that any compact segment of the continuation curve in $R(F)$ has an ϵ -neighborhood for some $\epsilon > 0$ in which Newton's method will converge to the curve.

This suggests that we estimate the radius of convergence of the corrector process at the computed points and extrapolate these radii to the next point about to be determined. In practice the estimate of a convergence radius at some continuation point would have to be based on the corrector iterates which led to that point. Unfortunately, as was proved in [7], this represents insufficient information for obtaining such an estimate. On the other hand, an approach was presented in [7] which allows for an assessment of the convergence quality of the particular sequence of corrector iterates.

For details of this approach we refer to the cited article. In brief, let $\{y^i\}$ be a given sequence with limit y^* generated by an iterative process and denote the errors by $e_i = ||y^i - y^*||$, $i = 0, 1, \dots$. The definition of any convergence measure is based on a hypothetical model of the behavior of the errors. For example, if $\{y^i\}$ converges linearly it is reasonable to assume that

$$(4.1) \quad 0 \leq e_{i+1} \leq \lambda e_i, \quad i = 0, 1, \dots$$

with some constant λ , $0 < \lambda < 1$, depending on $\{y^i\}$. Suppose now that the process was terminated with the iterate y^{i^*} . Then

$$(4.2) \quad \tilde{\lambda} = \tilde{\omega}^{1/(i^*-1)}, \quad \tilde{\omega} = \frac{\|y^{i^*} - y^{i^*-1}\|}{\|y^{i^*} - y^0\|}, \quad i^* \geq 2,$$

represents a computable estimate of λ .

In the setting of our continuation process suppose now that the y^i , $i = 0, 1, \dots$, are the corrector iterates leading from the current predicted point $\hat{x}^k = y^0$ to the new continuation point $x^{k+1} = y^{i^*}$. Then

$$(4.3) \quad \delta_k = \|\hat{x}^k - x^{k+1}\| = \|y^0 - y^{i^*}\|$$

is the correction-distance. For the modified Newton method the convergence is indeed linear, and a reasonable aim in the construction of the steps along the curve is to ensure that the number of corrector iterates remains about constant. In other words, we aim at taking always, say, m^* corrector steps. Hence, under the heuristic assumption that the error model (4.1) remains valid for some interval of starting errors e_0 around δ_k , we should have begun with an "ideal starting error" $\delta_k^* = \theta_k \cdot \delta_k$ such that

$$(4.4) \quad \tilde{\lambda}^{m^*} \delta_k^* = \tilde{\lambda}^{i^*} \delta_k$$

and therefore

$$(4.5) \quad \theta_k = \bar{\lambda}^{i^*-m^*} \equiv \bar{\omega}^{(i^*-m^*)/(i^*-1)}.$$

In our program we use $m^* = 10$ for the modified Newton method and enforce always that $0.125 \leq \theta_k \leq 8$.

This technique is also readily applicable for Newton's method. In [7] two different hypothetical error models for the Newton process were discussed. Here we use only one of these models, namely the one arising in the attraction theorem formulated in [24]. In essence, under certain conditions about the equation and the desired limit y^* of the Newton process there exists a radius $r^* > 0$ such that for any starting point y^0 in the ball $B(y^*, r^*)$ the relative errors $\varepsilon_i = e_i/r^*$, $i = 0, 1, \dots$, satisfy

$$(4.6) \quad 0 \leq \varepsilon_{i+1} \leq \phi(\varepsilon_i), \quad i = 0, 1, \dots, \quad \phi(t) = \frac{t^2}{3-2t}, \quad 0 \leq t \leq 1.$$

The radius r^* depends on global information about the equation and is not accessible. If $0 < \varepsilon_0 < 1$ and the $\{\varepsilon_i\}$ satisfy (4.6) then we have

$$(4.7) \quad \varepsilon_i \leq \eta_i \equiv \phi^i(\eta_0) \equiv \frac{3}{1 + 2 \cosh 2^i \alpha}, \quad i = 0, 1, \dots, \quad \eta_0 = \varepsilon_0,$$

where α is the unique positive solution of

$$(4.8) \quad \psi(\alpha) = \eta_0, \quad \psi(\alpha) = \frac{3}{1 + 2 \cosh \alpha}.$$

Moreover, for any ω , $0 < \omega < 1$, and $i^* \geq 2$ the equation

$$(4.9) \quad \frac{1}{\psi(\alpha)} \phi^{i^*-1}(\psi(\alpha)) \equiv \frac{1 + 2 \cosh \alpha}{1 + 2 \cosh 2^{i^*-1} \alpha} = \omega$$

has a unique solution $\alpha > 0$.

Now suppose that $\{y^i\}$ denotes the sequence of Newton iterates and that the process was terminated at y^{i^*} . As in the linear case we use the approximation

$$(4.10) \quad \tilde{\omega} = \frac{||y^{i^*} - y^{i^*-1}||}{||y^{i^*} - y^0||} \doteq \frac{e_{i^*-1}}{e_0} = \frac{\epsilon_{i^*-1}}{\epsilon_0} \leq \frac{\eta_{i^*-1}}{\eta_0}$$

and compute with this $\tilde{\omega}$ the solution $\tilde{\alpha}$ of (4.9) which gives the estimate $\tilde{\eta}_0 = \psi(\tilde{\alpha})$ of ϵ_0 . Now we proceed as before and obtain the factor

$$(4.11) \quad \theta_k^* = \frac{\delta_k^*}{\delta_k} = \frac{\tilde{\eta}_0'}{\tilde{\eta}_0}$$

for the ideal starting error by determining the unique solution $\tilde{\eta}_0'$, $0 < \tilde{\eta}_0' < 1$, of

$$(4.12) \quad \phi^{m^*}(\tilde{\eta}_0') = \phi^{i^*}(\tilde{\eta}_0).$$

Since the iterates ϕ^i are explicitly known the various equations are not difficult to solve numerically. However, for the computation it is more advantageous to introduce a least squares fit of θ_k as a function of $\tilde{\omega}$ for all relevant values of i^* . In the program we use $m^* = 4$ and the approximations for θ_k given in Table 1. Note that as before we restrict θ_k to the interval $0.125 \leq \theta_k \leq 8$.

j*	$\tilde{\omega} \in [a, b]$		θ_k
	a	b	
2	0.8735115	1	1
	0.1531947	0.8735115	$0.9043128 - 0.7075675 \ln \omega$
	0.03191815	0.1531947	$-4.667383 - 3.677482 \ln \omega$
	0	0.03191815	8
3	0.4677788	1	1
	0.6970123(-3)	0.4677788	$0.8516099 - 0.1953119 \ln \omega$
	0.1980863(-5)	0.6970123(-3)	$-4.830636 - 0.9770528 \ln \omega$
	0	0.1980863(-5)	8
4	0	1	1
5	0.3339946(-10)	1	$1.040061 + 0.03793395 \ln \omega$
	0	0.3339946(-10)	0.125
6	0.1122789(-8)	1	$1.042177 + 0.04450706 \ln \omega$
	0	0.1122789(-8)	0.125
≥ 7	0	1	0.125

Table 1

We turn now to the algorithm for the determination of the steplength $h_k > 0$ along the Euler line $\pi(t) = x^k + t T x^k$ used for the prediction. In order to estimate the distance between $\pi(t)$ and the exact curve $x = x(s)$ we introduce the quadratic Hermite-Birkhoff interpolation polynomial

$$(4.13) \quad q(t) = x^k + t T x^k + \frac{1}{2} t^2 w^k, \quad w^k = \frac{1}{\Delta s_k} (T x^k - T x^{k-1}), \quad \Delta s_k = \|x^k - x^{k-1}\|_2$$

for which

$$(4.14) \quad q(0) = x^k, \quad q'(0) = T x^k, \quad q'(-\Delta s_k) = T x^{k-1}.$$

Since

$$(4.15) \quad w^k = \int_0^1 x''(s_k - \sigma \Delta s_k) d\sigma = x''(s_k - \bar{\sigma} \Delta s_k), \quad 0 < \bar{\sigma} < 1,$$

the quantity

$$(4.16) \quad \|w^k\|_2 = \frac{2}{\Delta s_k} |\sin \frac{1}{2} \alpha_k|, \quad \alpha_k = \arccos ((T x^k)^T T x^{k-1})$$

represents an approximation of the curvature of the exact point at some point between $x(s_{k-1})$ and $x(s_k)$.

It is tempting to derive from q a prediction of the curvature to be expected during the next continuation step. However, a closer computation shows that the value of the curvature of q assumes its maximum $\|w^k\|_2 / \cos^2 \frac{1}{2} \alpha_k$ at $t = -\frac{1}{2} \Delta s_k$ and that for increasing t this value decreases rapidly. For example, at $t = 0$ the curvature of q equals only $\|w^k\|_2 |\cos \frac{1}{2} \alpha_k|$ and for positive t no reasonable predictive information can be gained this way.

The relation (4.15) suggests the use of the simple linear extrapolation

$$(4.17a) \quad \gamma_k^{\text{tent}} = \|w^k\|_2 + \frac{\Delta s_k}{\Delta s_k + \Delta s_{k-1}} (\|w^k\|_2 - \|w^{k-1}\|_2)$$

for a prediction of the curvature during the next continuation step. However, this value may become negative and accordingly we use instead

$$(4.17b) \quad \gamma_k = \max(\gamma_{\min}, \gamma_k^{\text{tent}})$$

with a given small $\gamma_{\min} > 0$.

Most of the data discussed so far are sketched in Figure 2. In order to derive a formula for the desired predictor step h_k we note that

$$(4.18) \quad \|q(t) - \pi(t)\|_2 = \frac{1}{2} t^2 \|w^k\|_2$$

represents an estimate of the distance between the Euler line and the exact curve. In fact, for smooth curves the error of this estimate is asymptotically of order three in $\max(|t|, \Delta s_k)$ as this quantity tends to zero. Hence, if we want this distance to be at most equal to a tolerance $\epsilon > 0$ then we should choose the next step as

$$(4.19) \quad t = \sqrt{\frac{2\epsilon}{\|w^k\|_2}}.$$

It is natural to replace the curvature $\|w^k\|_2$ by the predicted value γ_k of (4.17) and to relate the tolerance ϵ to the "ideal starting error" δ_k^* obtained earlier. As Figure 2 indicates it is unreasonable to expect $\epsilon > \Delta s_k$. Hence, we use instead

$$(4.20) \quad \epsilon_k = \begin{cases} \epsilon_{\min} \Delta s_k & \text{if } \delta_k^* \leq \epsilon_{\min} \Delta s_k \\ \Delta s_k & \text{if } \delta_k^* \geq \Delta s_k \\ \delta_k^* & \text{otherwise} \end{cases}$$

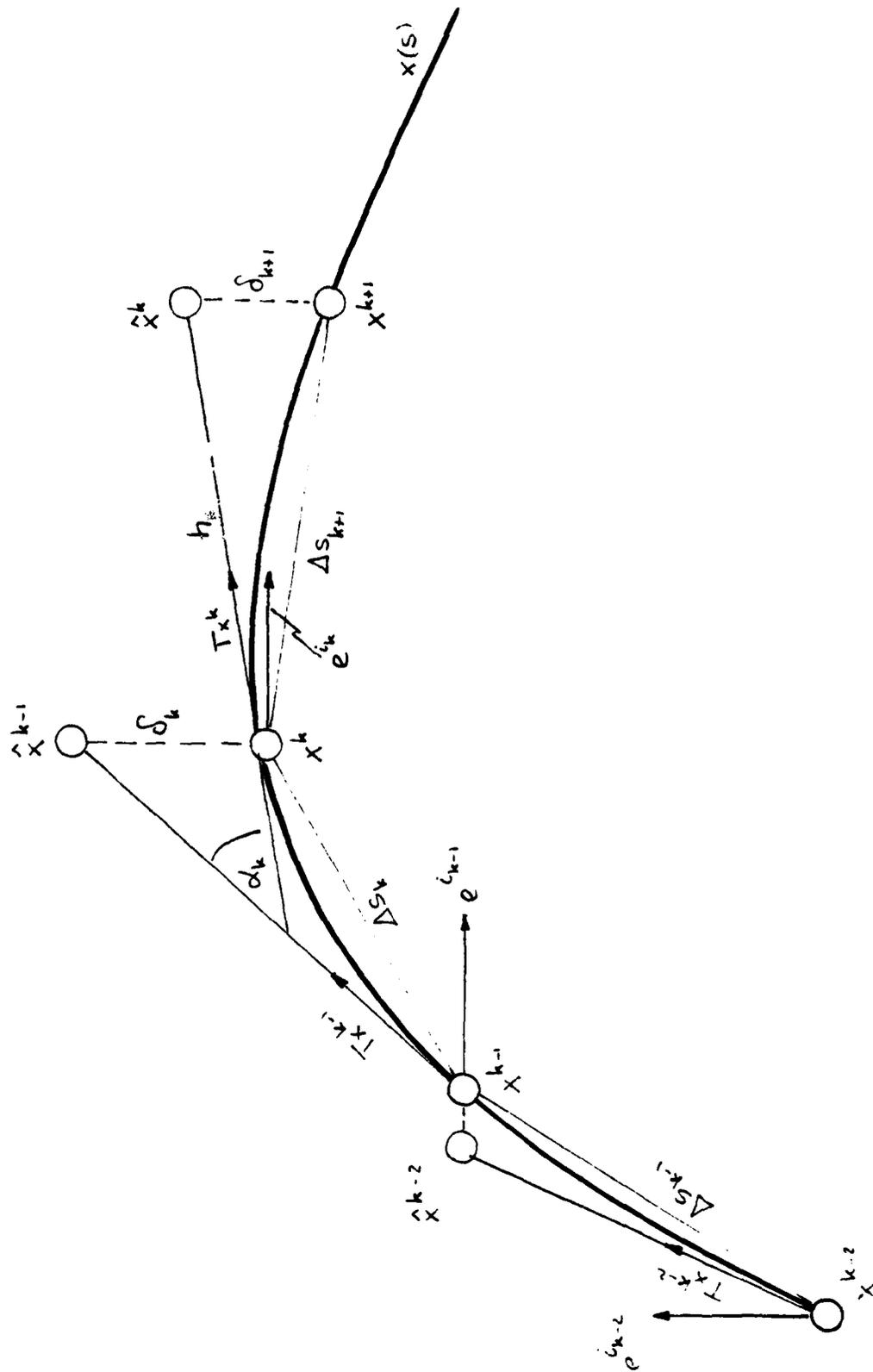


Figure 2

with a small $\epsilon_{\min} > 0$, e.g., $\epsilon_{\min} = 0.01$. Then a tentative predicted step is given by

$$(4.21) \quad h_k^{(1)} = \sqrt{\frac{2\epsilon_k}{\gamma_k}}.$$

From the form (3.8) of the augmented equation we see that the corrector iterates remain in a hyperplane perpendicular to the basis vector e^i_k through the predicted point. Then Figure 2 suggests that we adjust the predicted steplength h_k so as to ensure that h_k will be approximately equal to Δs_{k+1} . There is no need to enforce this too rigidly. It suffices to define a new tentative step by the requirement

$$(e^i)^T \pi(h_k^{(2)}) = (e^i)^T q(h_k^{(1)})$$

whence,

$$(4.22) \quad h_k^{(2)} = h_k^{(1)} \left[1 + \frac{h_k^{(1)}}{2\Delta s_k} \left(1 - \frac{(e^i)^T T x^{k-1}}{(e^i)^T T x^k} \right) \right].$$

This formula may involve subtractive cancellation and has to be evaluated in double precision.

The final value h_k of the steplength is now obtained from $h_k^{(2)}$ by enforcing three different bounding requirements. First of all, if the previous continuation step from x^{k-1} to x^k was obtained only after a failure of the correction process and a corresponding reduction of the predicted step, then we should not allow h_k to exceed Δs_k . Secondly, as in the ODE solvers we need to control both the relative growth and the absolute size of the pre-

dicator step. Thus, we require that

$$(4.23) \quad \frac{1}{\kappa} \Delta s_k \leq h_k \leq \kappa \Delta s_k, \quad h_{\min} \leq h_k \leq h_{\max}$$

where κ is some factor, say, $\kappa = 3$, and h_{\min} , h_{\max} depend on the machine as well as the requirements of the problem. It should be obvious how the final step h_k is obtained from $h_k^{(2)}$ on the basis of these restrictions.

5. THE COMPUTATION OF TARGET AND LIMIT POINTS

By generating a sequence of solution points on a given curve, the continuation process reveals the shape of the curve, but there are often other items of interest that need to be studied as well. Our program is designed to pause during the continuation steps in order to seek out special points that the user has requested, namely, target and limit points.

A target point $x \in E^*(F, x^0)$ is a point on the solution curve for which the component $x_i = (e^i)^T x$ with given index $i = IT$ has a prescribed value $\bar{x}_i = XIT$. Limit or turning points with respect to a given index $i = LIM$ are points $x \in E^*(F, x^0)$ where the i -th component $(e^i)^T Tx$ is zero. More specifically, since it is computationally unreasonable to attempt to compute zeroes of even order, we are concerned only with limit points on the continuation curve where $(e^i)^T Tx(s)$ changes sign.

It might be mentioned that bifurcation points represent another interesting, special class of points. But in that case we are not only interested in the specific location of the point but also in the solution curves that branch off from it. This is exactly the task (1.2) (v) listed earlier. The corresponding procedures (loc. cit.) would add considerably to the complexity of our program, and, since their utility tends to be of a more specialized nature, it was decided not to cover task (1.2) (v) (nor (1.2) (iv)) in the present program.

As indicated before, the determination of a target or limit point represents an interruption in the normal flow of the continuation program. After at least one step has been taken, the program has available an old point x^{k-1} , a new point x^k and the tangent vector Tx^{k-1} . Normally, then we turn to the computation of Tx^k , of the new steplength, and finally of the next point x^{k+1} . But if the index IT or LIM is non-zero then these

computations are postponed for the search of a target or limit point, respectively. We discuss these cases separately:

Target points: Suppose that a non-zero value of $i = IT$ and associated value $\bar{x}_i = XIT$ have been given. If \bar{x}_i lies between $(e^i)^T x^{k-1}$ and $(e^i)^T x^k$, then it is assumed that a solution point $x \in E^*(F, x^0)$ with $(e^i)^T x = \bar{x}_i$ is nearby. In this case a point

$$(5.1) \quad y(t) = (1-t)x^{k-1} + tx^k, \quad 0 \leq t \leq 1,$$

on the secant between x^{k-1} and x^k is determined such that $(e^i)^T y(t) = \bar{x}_i$. Now with the augmenting equation $(e^i)^T x = \bar{x}_i$ the corrector process is applied, and, if it terminates successfully the resulting point is taken as the desired target. Otherwise, a failure is indicated for the target routine. In either case, the routine returns and on the next call the continuation loop will pick up from where it was interrupted. Note that in effect the target routine uses the IT -th variable for the local parametrization of the curve between x^{k-1} and x^k . This may be an inferior choice of parameter for the corrector but it allows us to enforce that the resulting target point $x \in E^*(F, x^0)$ indeed satisfies $(e^i)^T x = \bar{x}_i$. Clearly, for very large continuation steps we have no guarantee that all target points will be detected or that a target computation will succeed. Thus, the utility of the target routine will depend on the maximal allowed stepsize that has been chosen.

Limit points: If the limit point index $i = LIM$ is non-zero, then a limit point determination is carried out after a target point search has been successfully or unsuccessfully completed, provided it was called for at all.

Recall that we still have as current information the vectors x^{k-1} , x^k , and Tx^{k-1} . Now the new tangent Tx^k is evaluated and if $\text{sign}(e^{\hat{i}})^T Tx^{k-1} \neq \text{sign}(e^{\hat{i}})^T Tx^k$ for $i = \text{LIM} (\neq 0)$ then a limit point search is begun. For this the index \hat{i} of the largest component in modulus of the secant direction $x^k - x^{k-1}$ is chosen as a local parametrization of the curve between x^{k-1} and x^k . More specifically, suppose that $x: [s_{k-1}, s_k] \rightarrow E^*(F, x^0)$ represents the segment of the curve between x^{k-1} and x^k . Then \hat{i} is assumed to be the index of a local coordinate for which there exists a bijective parameter transformation $\phi: [0, 1] \rightarrow [s_{k-1}, s_k]$ such that $(e^{\hat{i}})^T y(t) = (e^{\hat{i}})^T x(\phi(t))$, $0 \leq t \leq 1$, where $y(t)$ is defined by (5.1).

Hence, we may consider the function

$$(5.2) \quad g: [0, 1] \rightarrow \mathbb{R}^1, \quad g(t) = (e^{\hat{i}})^T Tx(\phi(t)), \quad 0 \leq t \leq 1,$$

and our problem is to determine a zero of g . Since by assumption $\text{sign } g(0) \neq \text{sign } g(1)$, a rootfinder of the Dekker-Brent type can be applied. For the evaluation of $g(t)$ we use the augmenting equation $(e^{\hat{i}})^T x = (e^{\hat{i}})^T y(t)$ and apply the corrector process with $y(t)$ as starting point. If it terminates successfully with some x then Tx can be evaluated and we set $g(t) = (e^{\hat{i}})^T Tx$. Hence, g is certainly costly to compute and we require an efficient rootfinder to speed the convergence of the limit point routine. A specially modified version of the routine given in [4] is used in our program. Clearly, as in the case of target points, we may fail to detect a limit point if the continuation steps are too large and in such a situation the rootfinder may also fail to converge. In addition, the evaluation of g may run into difficulties when the desired limit point is near a bifurcation point.

6. SOME NUMERICAL EXAMPLES

The programs described here have been used extensively with excellent success on problems from many different areas. We include here only a few numerical examples to illustrate the operation of the programs.

Example 1. In order to present some details of the performance of the programs we consider first a very small problem which was originally formulated in [9] and subsequently used as a test case by many authors. The mapping F has here the form

$$(6.1) \quad Fx = \begin{pmatrix} x_1 - x_2^3 + 5x_2^2 - 2x_2 + 34x_3 - 47 \\ x_1 + x_2^3 + x_2^2 - 14x_2 + 10x_3 - 39 \end{pmatrix}, \quad \forall x \in \mathbb{R}^3.$$

For the starting point $x^0 = (15, -2, 0)^T$ the solution curve passes through $x^* = (5, 4, 1)^T$ and this point is chosen as target.

Tables 2 and 3 show runs with the full Newton method and modified Newton method, respectively as corrector process. A starting step $h_0 = 0.3$ and maximum step $h_{\max} = 25.0$ were used. The performance for the two correctors is practically the same although the step-prediction exhibits certain differences due to our assessment of the corrector distance. Clearly, the use of the modified Newton process is much less expensive and hence preferable as Table 4 shows which summarizes the total number of function and Jacobian calls including those for the target calculation. Comparative performance data given in [7] for this problem involved 22 continuation steps, 15 step reductions and 128 Jacobian evaluations. The procedure discussed in [19] required 25 continuation steps but no further details were provided in the paper.

Step	Continuation point			Contin. Variable	Total Correct. Steps	Comments
	x_1	x_2	x_3			
0	15.000	-2.00000	0.00000	x_3	—	
1	14.705	-1.9421	0.065381	x_1	2	
2	14.285	-1.7291	0.26874	x_3	3	
3	16.906	-1.2094	0.54684	x_2	2	
4	24.918	-0.59908	0.55514	x_1	3	
5	48.974	0.71803	-0.080758	x_1	3	
6	57.928	1.2846	-0.40736	x_1	4	Step red.
7	60.052	1.5709	-0.54035	x_1	4	Step red.
8	61.666	2.0010	-0.66683	x_2	2	
9	-5.1039	4.1510	1.3464	x_2	2	Target passed
TOTAL					25	
Computation of target					4	

Table 2

Step	Continuation point			Contin. Variable	Total Correct Steps	Comments
	x_1	x_2	x_3			
0	15.000	-2.0000	0.00000	x_3	—	
1	14.710	-1.9421	0.065381	x_1	3	
2	14.285	-1.7291	0.26874	x_3	4	
3	16.906	-1.2094	0.54685	x_2	1	
4	24.918	-0.59906	0.55514	x_1	6	
5	48.975	0.71810	-0.080804	x_1	5	
6	57.289	1.2847	-0.40742	x_1	6	Step red.
7	60.053	1.5711	-0.54042	x_1	5	Step red.
8	61.666	2.0013	-0.66689	x_2	2	
9	-4.4239	4.1413	1.3229	x_2	1	Target passed
TOTAL					33	
Computation of target					8	

Table 3

	Corrector Process	
	Newton	Mod. Newton
Function calls	41	53
Jacobian calls	38	21

Table 4

It may be noted that the solution curve has two limit points each with respect to x_1 and x_3 . The two step reductions are almost unavoidable here since the curve has a long straight segment followed by a very sharp bend. The target computation is relatively expensive since the last step is extremely large due to another straight curve segment.

Example 2. Maneuvering airplanes, especially at high angles of attack, sometimes undergo sudden jumps in their response to the pilot's control inputs. The problem has been discussed extensively in the literature, see, for example, [18], [30], [39]. Without going into further details we use here a simplified version of a system of five equilibrium equations involving the roll rate (x_1), pitch rate (x_2), yaw rate (x_3), (incremental) angle of attach (x_4), side slip angle (x_5), elevator angle (x_6), aileron angle (x_7), and rudder angle (x_8). More specifically, for the particular aircraft discussed in [18] these equations have the dimensionless form

$$(6.1) \quad Fx \equiv Ax + \phi(x) = 0, \quad \forall x \in R^8$$

where

$$A = \begin{pmatrix} -3.933 & 0.107 & 0.126 & 0 & -9.99 & 0 & -45.83 & -7.64 \\ 0 & -0.987 & 0 & -22.95 & 0 & -28.37 & 0 & 0 \\ 0.002 & 0 & -0.235 & 0 & 5.67 & 0 & -0.921 & -6.51 \\ 1.0 & 0 & 0 & -1.0 & 0 & -0.168 & 0 & 0 \\ 0 & 0 & -1.0 & 0 & -0.196 & 0 & -0.0071 & 0 \end{pmatrix}$$

and

$$\phi(x) = \begin{pmatrix} -0.727 x_2 x_3 + 8.39 x_3 x_4 - 684.4 x_4 x_5 + 63.5 x_4 x_7 \\ 0.949 x_1 x_3 + 0.173 x_1 x_5 \\ -0.716 x_1 x_2 - 1.578 x_1 x_4 + 1.132 x_4 x_7 \\ -x_1 x_2 \\ x_1 x_4 \end{pmatrix}.$$

Figure 3 shows some solution curves on the three-dimensional equilibrium surface in R^8 . More specifically, in all cases we fixed a value of x_6 (elevator deflection) and chose the rudder deflection $x_8 = 0$. The paths $x_6 > \omega_1$, $x_8 = 0$ with $\omega_1 \approx -0.0061771$ have two limit points, for $\omega_1 > x_6 > \omega_2$, $x_8 = 0$, with $\omega_2 \approx -0.012498$ a third limit point appears, and for $\omega_2 > x_6$, $x_8 = 0$ only one limit point remains. A similar picture arises for negative roll rates.

In all cases the programs easily detected and computed the various limit points (see Table 5). But the example also shows that even with a large number of search paths it is difficult to provide a full picture of the location of the critical boundary, that is, of the curves of limit points with respect to x_1 for $x_8 = 0$ and varying x_6, x_7 . In Figure 3 the corresponding branches of limit point curves are shown as dotted lines. They were obtained with a code for the

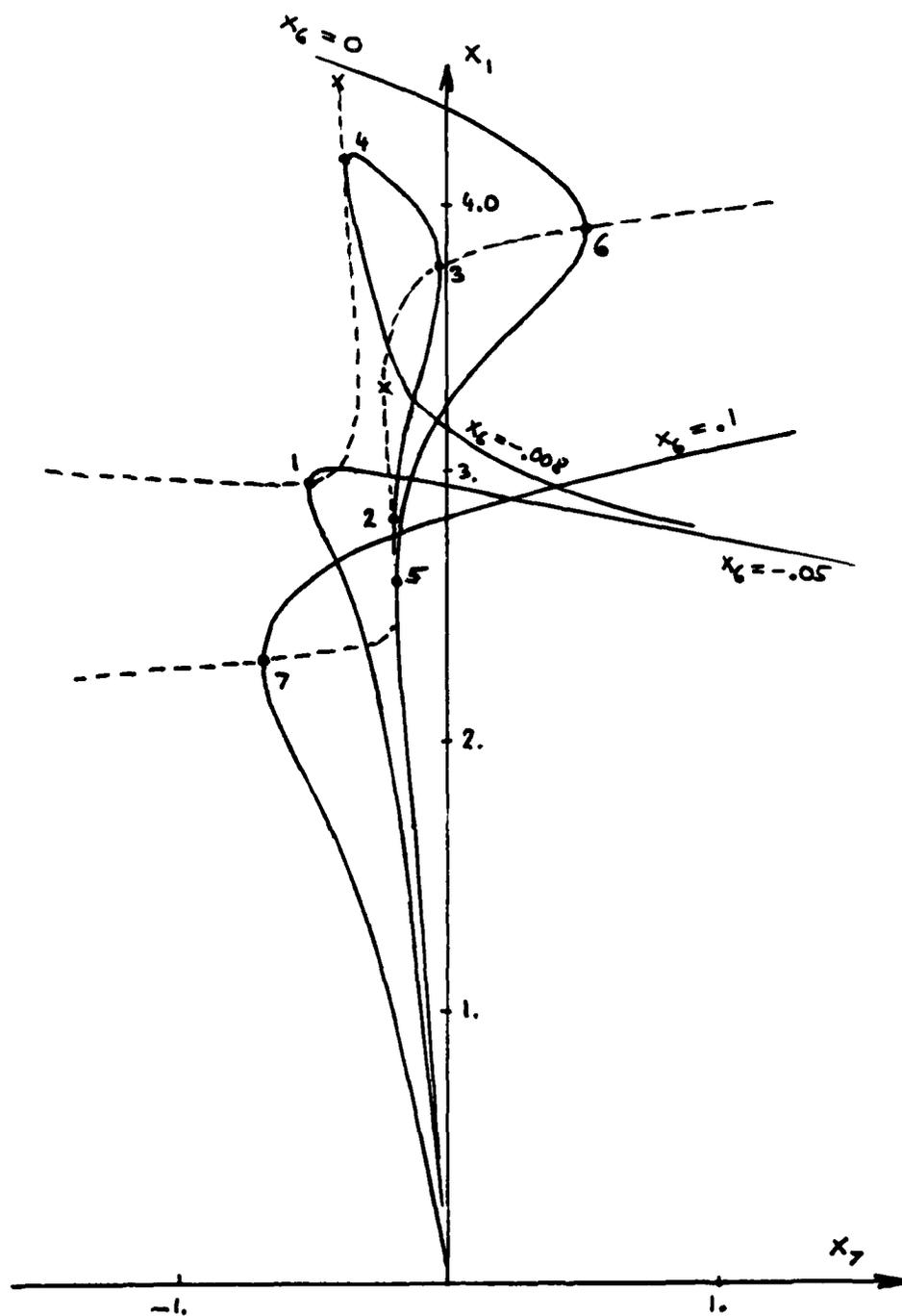


Figure 3

earlier mentioned task (1.3) (iv) (see [28]).

	x_1	x_2	x_3	x_4	x_5	x_6	x_7
1	2.9649	0.82557	0.073661	0.041309	0.26735	-0.05	0.50481
2	2.8174	-0.17629	0.089926	0.026429	-0.071476	-0.008	-0.20497
3	3.7579	-0.65542	0.38658	0.092521	-0.19867	-0.008	0.006208
4	4.1638	0.089131	0.094806	0.022889	0.016232	-0.008	-0.37766
5	2.5873	-0.22355	0.054682	0.013676	-0.091687	0.0	-0.18691
6	3.9005	-1.1482	0.58156	0.13352	-0.32859	0.0	0.51016
7	2.2992	-1.4102	-0.061849	-0.079009	-0.58630	0.1	-0.68972
8	4.4565	-4.4909	1.6164	0.33091	-1.0857	0.1	10.0212

Table 5

Example 3. As an example for the numerical investigation of the equilibrium surface of a mechanical structure, we consider a clamped, thin, shallow, circular arch which has been used as a test case by various authors (see eg. [12], [16], [36]). Let U and W be the radial and axial displacements, R the arch radius, A the cross-sectional area, H the thickness, and E Young's modulus. With the dimensional displacements $u = U/H$, $w = W/H$, the total potential energy -- non-dimensionalized by dividing by $EAR(H/R)^2$ --

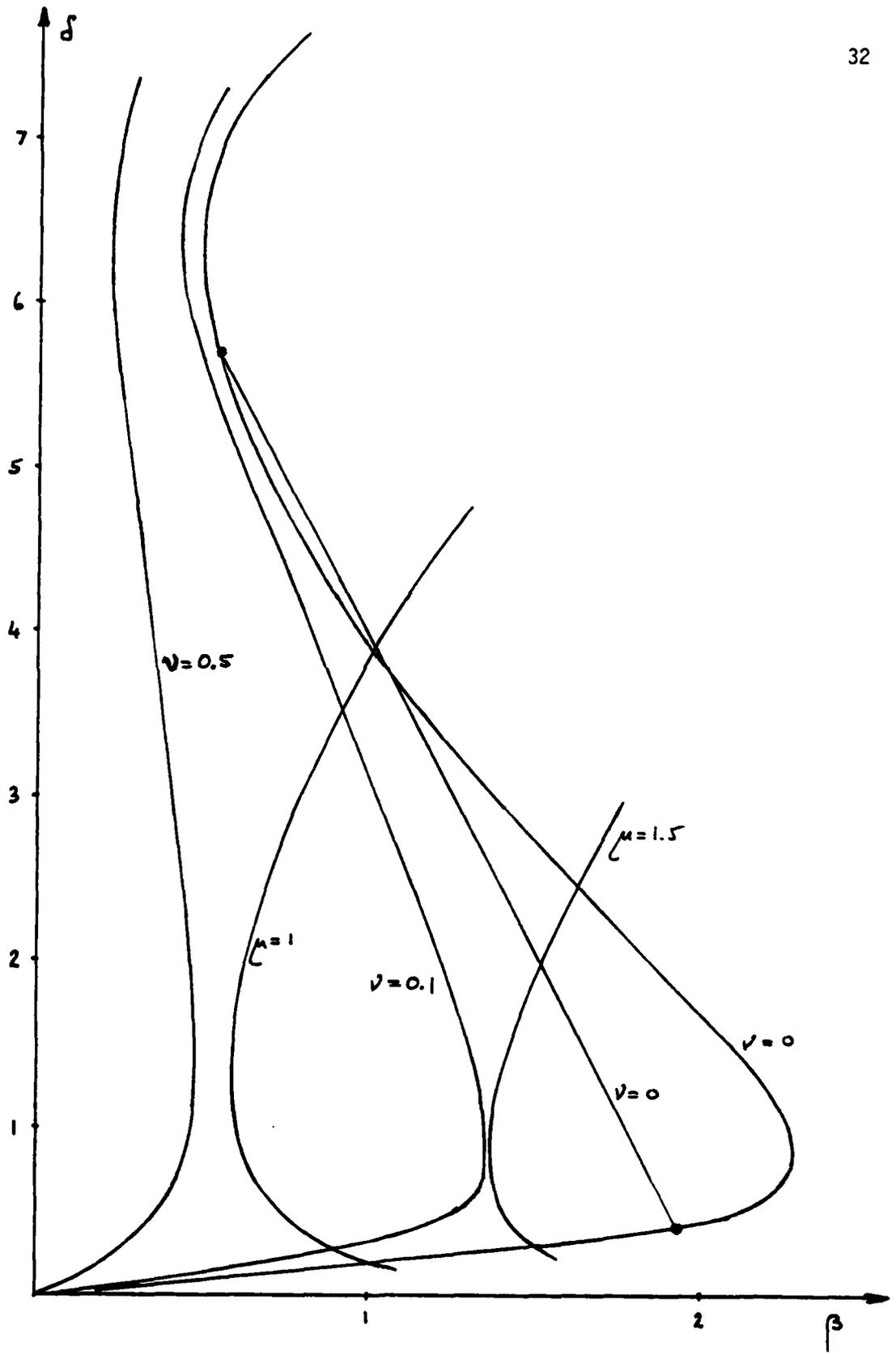


Figure 4

is given by

$$(6.2) \quad \int_{-\theta_0}^{\theta_0} \left\{ \left[\left(\frac{dw}{d\theta} - u \right) + \frac{1}{2} \frac{H}{R} \left(\frac{du}{d\theta} \right)^2 \right]^2 + \alpha_1 \left(\frac{d^2u}{d\theta^2} \right)^2 - \alpha_2 p u \right\} d\theta.$$

Here $p = p(\theta)$ is the dimensionless radial load, and α_1, α_2 are dimensionless constants. Each end is assumed to be pinned, that is, we have the boundary conditions

$$(6.3) \quad u(\pm \theta_0) = 0, \quad w(\pm \theta_0) = 0, \quad \frac{d^2u}{d\theta^2}(\pm \theta_0) = 0.$$

The finite element approximation introduced in [36] was applied. More specifically, we used a uniform mesh with eight elements, $\theta_0 = 15$ and the constants $\alpha_1 = 3.8716 \times 10^{-6}$, $\alpha_2 = 1.65504 \times 10^{-1}$ corresponding to the data in [16]. Moreover, the following load function $p = p(\mu, \nu)$ was chosen

$$(6.4) \quad p(\mu, \nu) = \begin{cases} \mu(1 + 7\nu), & \text{for element 4} \\ \mu(1 - \nu), & \text{otherwise} \end{cases}$$

corresponding to a base load $\beta = \mu(1 - \nu)$ and an excess load $8\mu\nu$ in element 4 such that the average load is always μ .

Several curves on the equilibrium surface corresponding to constant values of μ or ν were computed. Figure 4 shows the projection of these curves into the (β, δ) -plane where δ represents the radial displacement of the center point. For uniform loads, that is, $\nu = 0$, we encounter two bifurcation points on the primary curve which are connected by two "buckling" curves that have the same projection in the (β, δ) -plane.

7. THE PITCON CODE

```

SUBROUTINE PITCON(NVAR,I M,IT,XIT,KSTEP,IPC,H,TRET,IMOD,IPVT,
1 HMAX,HMIN,HFACT,ABSERR,ERR,WORK,ISIZE)
C*****
C
C PITCON.FOR
C
C 29 OCT 1981 VERSION OF PITCON,
C THE UNIVERSITY OF PITTSBURGH CONTINUATION PACKAGE.
C THIS VERSION USES SINGLE PRECISION AND FULL MATRIX STORAGE.
C
C THIS PACKAGE WAS PREPARED WITH THE PARTIAL SUPPORT OF
C THE NATIONAL SCIENCE FOUNDATION, UNDER GRANT MCS-78-05299,
C
C BY WERNER C. RHEINBOLDT AND JOHN V. BURKARDT
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C UNIVERSITY OF PITTSBURGH, PITTSBURGH, PA 15261.
C
C AN EARLIER VERSION OF THE PACKAGE WAS WRITTEN IN COOPERATION WITH
C GEORGE D BYRNE,
C COMPUTING TECHNOLOGY AND SERVICES
C EXXON RESEARCH AND ENGINEERING COMPANY
C LINDEN, NEW JERSEY, 07036
C
C THIS PACKAGE COMPUTES POINTS ALONG A SOLUTION CURVE OF AN
C UNDERDETERMINED SYSTEM OF NONLINEAR EQUATIONS OF THE FORM  $Fx=0$ .
C THE CURVE IS SPECIFIED TO PASS THROUGH A GIVEN STARTING SOLUTION
C  $x$  OF THE SYSTEM. HERE  $x$  DENOTES A REAL VECTOR OF NVAR
C COMPONENTS AND  $Fx$  A REAL VECTOR OF NVAR-1 COMPONENTS.
C NORMALLY EACH CALL TO PITCON PRODUCES A NEW POINT FURTHER ALONG
C THE SOLUTION CURVE IN A USER-SPECIFIED DIRECTION.
C AN OPTION ALLOWS THE SEARCH FOR AND COMPUTATION OF TARGET POINTS,
C THAT IS, SOLUTION POINTS  $x$  FOR WHICH  $x(IT) = XIT$  FOR SOME USER
C SPECIFIED VALUES OF IT AND XIT.
C A FURTHER OPTION ALLOWS THE SEARCH FOR AND COMPUTATION OF LIMIT
C POINTS FOR SPECIFIED COORDINATE LIM, THAT IS, SOLUTION POINTS FOR
C WHICH THE LIM-TH COMPONENT OF THE TANGENT VECTOR IS ZERO.
C
C EXPLANATIONS OF THE ALGORITHMS USED IN THIS PACKAGE MAY
C BE FOUND IN THE FOLLOWING REFERENCES:
C
C WERNER RHEINBOLDT,
C SOLUTION FIELD OF NONLINEAR EQUATIONS AND CONTINUATION METHODS
C SIAM JOURNAL OF NUMERICAL ANALYSIS, 17, 1980, PP 221-237
C
C COR DEN HEIJER AND WERNER RHEINBOLDT,
C ON STEPLENGTH ALGORITHMS FOR A CLASS OF CONTINUATION METHODS,
C SIAM JOURNAL OF NUMERICAL ANALYSIS 18, 1981, PP 925-947
C
C WERNER RHEINBOLDT,
C NUMERICAL ANALYSIS OF CONTINUATION METHODS FOR NONLINEAR
C STRUCTURAL PROBLEMS,
C COMPUTERS AND STRUCTURES, 13, 1981, PP 103-114
C
C OUTLINE OF THE MATHEMATICAL PROCEDURE
C
C THE FUNCTION  $F$  DEFINING THE SYSTEM OF EQUATIONS IS SUPPOSED TO
C BE CONTINUOUSLY DIFFERENTIABLE. THE REGULARITY SET  $R(F)$  OF  $F$  IS
C THE SET OF ALL POINTS  $x$  IN NVAR-DIMENSIONAL SPACE WHERE THE
C DERIVATIVE  $DF(x)$  HAS MAXIMAL RANK. THE STARTING POINT IS ASSUMED
C TO BE IN  $R(F)$ . FOR ANY INDEX IP WITH 1.LE.IP.LE.NVAR, LET

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PTCN0060
PTCN0061
PTCN0062
PTCN0063
PTCN0064
PTCN0065
PTCN0066
PTCN0067
PTCN0068
PTCN0069
PTCN0070

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C STEP 3: TANGENT AND LOCAL CONTINUATION PARAMETER CALCULATION. IF THE LOOP WAS SUSPENDED AT THE LAST CALL TO FITCON TO ALLOW THE RETURN OF A LIMIT POINT, THEN THE TANGENT HAS ALREADY BEEN CALCULATED AND A LIMIT POINT CHECK IS SUPERFLUOUS, SO THE PROGRAM SKIPS TO STEP 5. OTHERWISE, A VECTOR IN THE TANGENT PLANE AT XC IS COMPUTED. SUPPOSE THAT THE PREVIOUS CONTINUATION PARAMETER INDEX WAS IPL, WHERE ON THE FIRST STEP IPL IS USER-SUPPLIED. THE NEW TANGENT IS NORMALIZED, AND THE IPL-TH COMPONENT IS FORCED TO HAVE THE SAME SIGN AS THE IPL-TH COMPONENT OF THE PREVIOUS TANGENT (OR ON FIRST STEP, THE SAME SIGN AS THE USER INPUT DIRECTION DIR.) THEN THE LOCAL CONTINUATION PARAMETER IPC IS DETERMINED. IPC IS SET TO THE LOCATION OF THE LARGEST COMPONENT OF THE TANGENT VECTOR UNLESS A LIMIT POINT FOR THIS CHOICE APPEARS TO BE APPROACHING, IN WHICH CASE THE LOCATION OF THE SECOND LARGEST COMPONENT MAY BE TRIED. ONCE IPC IS SET, THE QUANTITIES TCIPC, TCLIM, HSFCLC, ALPHLC AND DIR ARE COMPUTED, WHOSE MEANINGS ARE EXPLAINED BELOW.

C STEP 4: LIMIT POINT CHECK. IF LIM.NE.0, THE LIM-TH COMPONENTS OF THE OLD AND NEW TANGENTS ARE COMPARED. IF THESE DIFFER IN SIGN, A LIMIT POINT LIES BETWEEN XL AND XC. THE PROGRAM ATTEMPTS TO FIND THIS LIMIT POINT. IF FOUND, IT STORES THE LIMIT POINT IN XR, THE TANGENT AT XR IN TL, SETS IRET=2, AND RETURNS, TEMPORARILY INTERRUPTING THE NORMAL LOOP.

C STEP 5: STEP LENGTH COMPUTATION. THE PROGRAM COMPUTES HTANCF, THE STEPSIZE TO BE USED ALONG THE TANGENT TO OBTAIN THE PREDICTED POINT XPRED:=XC+HTANCF*TC, THE STARTING POINT FOR THE CORRECTOR PROCESS. IN COMPUTING HTANCF, CERTAIN CURVATURE AND STEPSIZE DATA ARE UPDATED.

C STEP 6: PREDICTION AND CORRECTION STEP. WITH THE PREDICTED POINT XPRED=XC+HTANCF*TC AS A STARTING POINT, THE CORRECTOR PROCESS IS APPLIED TO CORRECT THE POINT UNTIL ABS(F(XCOR)).LE.ABSERR AND XSTEP, THE LAST CORRECTOR STEP, SATISFIES XSTEP.LE.ABSERR+RELERR*ABS(XCOR). IF THE SIZE OF A CORRECTOR STEP IS TOO LARGE, OR IF A CORRECTION STEP INCREASES THE FUNCTION VALUE, OR THE MAXIMUM NUMBER OF STEPS ARE TAKEN WITHOUT CONVERGENCE, THE STEPSIZE HTANCF IS REDUCED AND THE CORRECTOR STEP IS ATTEMPTED AGAIN. IF THE STEPSIZE SHRINKS BELOW HMIN, THE PROGRAM SETS AN ERROR FLAG AND RETURNS.

C STEP 7: STORING INFORMATION BEFORE RETURN. AFTER A SUCCESSFUL CONTINUATION STEP, THE PROGRAM REARRANGES ITS STORAGE SO THAT THE ENTRIES CORRESPONDING TO XC AND XF HOLD THE PROPER DATA, COMPUTES CORDIS, THE SIZE OF THE CORRECTION TO THE PREDICTED POINT, AND MODIFIES CORDIS TO A VALUE THAT WOULD CORRESPOND TO AN OPTIMAL NUMBER OF CORRECTOR STEPS.

C ON NORMAL RETURN, THE VECTOR XR (THE FIRST NVAR ENTRIES OF RWORK), CONTAINS A SOLUTION POINT ON THE CURVE F(XR)=0, AND IS EITHER A CONTINUATION POINT, A TARGET POINT, OR A LIMIT POINT, WHICH IS INDICATED BY THE VALUE OF IRET. IF IRET IS NEGATIVE, AN ERROR HAS OCCURRED. IF A LIMIT POINT IS RETURNED, THE TANGENT VECTOR AT THE LIMIT POINT IS CONTAINED IN THE LOCATION TL IN RWORK. ON FIRST CALL, THE USER MUST SET SOME OF THE SCALAR PARAMETERS, AND THE STARTING POINT XR. THEREAFTER, ONLY IT AND XJT SHOULD BE CHANGED BY THE USER DURING A PROBLEM RUN. IF A NEW PROBLEM IS TO BE RUN (WHETHER A DIFFERENT FUNCTION, OR THE SAME FUNCTION WITH DIFFERENT STARTING POINT OR ERROR CONTROLS) THE PROGRAM MAY BE RESET BY USING KSTEP=-1 OR 0, AT WHICH TIME THE SCALARS AND THE POINT XR MUST BE SET AGAIN. NOTE THAT IN THIS CASE THE STATISTICAL DATA IN THE COMMON BLOCKS /COUNT1/ AND /COUNT2/ WILL BE RESET TO 0 AS WELL.

PTCN0141
 PTCN0142
 PTCN0143
 PTCN0144
 PTCN0145
 PTCN0146
 PTCN0147
 PTCN0148
 PTCN0149
 PTCN0150
 PTCN0151
 PTCN0152
 PTCN0153
 PTCN0154
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 PTCN0188
 PTCN0189
 PTCN0190
 PTCN0191
 PTCN0192
 PTCN0193
 PTCN0194
 PTCN0195
 PTCN0196
 PTCN0197
 PTCN0198
 PTCN0199
 PTCN0200
 PTCN0201
 PTCN0202
 PTCN0203
 PTCN0204
 PTCN0205
 PTCN0206
 PTCN0207
 PTCN0208
 PTCN0209
 PTCN0210

DEFINITIONS AND DEFAULTS OF PITCON PARAMETERS

NVAR = THE NUMBER OF VARIABLES IN THE NONLINEAR SYSTEM. NVAR IS THE DIMENSION OF THE PIVOT VECTOR IPVT, AND THE SIZE OF THE VECTORS XR, XC, XF, TL AND TC WHICH ARE CONTAINED IN RWORK. RWORK ALSO CONTAINS STORAGE FOR THE MATRIX FFRYM WHICH IS OF SIZE NVAR X NVAR. NVAR MUST BE GREATER THAN 1, AND MUST NOT BE CHANGED DURING THE COURSE OF A PROBLEM RUN. NVAR HAS NO DEFAULT VALUE.

LIM = LIMIT POINT FLAG AND INDEX. IF (LIM.EQ.0), LIMIT POINTS ARE NOT TO BE LOOKED FOR. OTHERWISE, THE USER SHOULD SET LIM TO THE INDEX OF THE VARIABLE FOR WHICH LIMIT POINTS ARE TO BE SOUGHT. LIM DEFAULTS TO ZERO. LIM MUST SATISFY 0.LE.LIM.LE.NVAR.

IT = TARGET POINT FLAG AND INDEX. IF (IT.EQ.0), TARGET POINTS ARE NOT TO BE LOOKED FOR. OTHERWISE, THE USER SHOULD SET IT TO THE INDEX OF THE VARIABLE FOR WHICH TARGET VALUES XIT ARE DESIRED. IT HAS THE DEFAULT VALUE ZERO. IT MAY BE RESET BY THE USER AT ANY TIME DURING A RUN. IT MUST SATISFY 0.LE.IT.LE.NVAR.

XIT = THE VALUE OF THE TARGET VECTOR COMPONENT SOUGHT, IF IT.NE.0. TARGET POINTS XR SATISFY XR(IT)=XIT. XIT HAS NO DEFAULT.

KSTEP = THE NUMBER OF CONTINUATION STEPS TAKEN. THIS DOES NOT INCLUDE FAILURES, TARGET POINTS OR LIMIT POINTS. THE PROGRAM INCREMENTS KSTEP EACH TIME A NEW POINT XF IS COMPUTED. ON THE FIRST CALL TO PITCON FOR A PARTICULAR PROBLEM, THE USER SHOULD SET KSTEP TO 0 OR -1. IF KSTEP=-1, THE PROGRAM WILL CHECK THE ACCURACY OF THE STARTING POINT XR, AND IF NECESSARY, ATTEMPT TO CORRECT IT USING NEWTON'S METHOD. IF KSTEP=0, THE PROGRAM PERFORMS NO CHECK ON THE STARTING POINT, AND PROCEEDS TO THE CONTINUATION LOOP. IF THE USER WISHES TO RUN A DIFFERENT PROBLEM THEN A CALL TO PITCON WITH KSTEP=-1 OR 0 WILL RESET THE CODE, DESTROYING THE INFORMATION FROM THE PREVIOUS RUN. KSTEP DEFAULTS TO -1.

IPC = THE COMPONENT OF XC TO BE USED AS CONTINUATION PARAMETER. ON THE FIRST CALL ONLY, THE USER OUGHT TO SET IPC OR ALLOW THE DEFAULT VALUE IPC=NVAR. AFTER THE FIRST CALL, THE DETERMINATION OF IPC IS DONE BY THE PROGRAM USING INFORMATION ABOUT THE TANGENT VECTOR AT XC.

H = SUGGESTED STARTING STEP SIZE ALONG THE TANGENT TO THE CURVE. IF H=0.0 ON THE INITIAL CALL, H DEFAULTS TO (HMAX+HMIN)/2 IF H IS NEGATIVE ON THE FIRST CALL, THE MINUS SIGN IS ABSORBED BY DIR AND INDICATES THAT THE DIRECTION OF THE FIRST STEP SHOULD BE IN THE NEGATIVE IPC DIRECTION. AFTER THE FIRST STEP, STEPSIZE IS CONTROLLED BY THE PROGRAM. UPON RETURN WITH A CONTINUATION POINT (IRET=0), H IS OVERRITTEN BY HTANCF, THE STEPSIZE USED IN REACHING THE NEW POINT.

IRET = A RETURN FLAG TO INDICATE ERRORS OR THE TYPE OF POINT RETURNED IN XR. NONNEGATIVE VALUES OF IRET REPRESENT NORMAL RETURNS. NEGATIVE VALUES OF IRET INDICATE THAT SOME ERROR OR DIFFICULTY HAS BEEN ENCOUNTERED. VALUES OF IRET BETWEEN -1 AND -4 ARE SIMPLY REPORTS THAT AN ATTEMPT TO COMPUTE A LIMIT OR TARGET POINT FAILED. THESE DO NOT AFFECT FURTHER CONTINUATION STEPS, AND THE USER NEED NOT MODIFY ANY VARIABLES BEFORE PROCEEDING. VALUES OF IRET OF -5 AND -6 REFER TO DANGEROUS SITUATIONS THAT MAY BE CORRECTABLE. VALUES OF IRET FROM -7 TO -10 ARE SERIOUS, FATAL ERRORS. THE USER SHOULD HALT THE PROGRAM AND EXAMINE HIS INPUT AND THE INTERIM RESULTS. IRET SHOULD BE ZERO ON THE FIRST CALL FOR A PROBLEM. THE SPECIFIC VALUES OF IRET AND THEIR MEANINGS ARE:

IRET=2: NORMAL RETURN WITH LIMIT POINT IN XR AND TANGENT AT XR CONTAINED IN TL.

IRET=1: NORMAL RETURN WITH TARGET POINT IN XR.

PTCN0211
 PTCN0212
 PTCN0213
 PTCN0214
 PTCN0215
 PTCN0216
 PTCN0217
 PTCN0218
 PTCN0219
 PTCN0220
 PTCN0221
 PTCN0222
 PTCN0223
 PTCN0224
 PTCN0225
 PTCN0226
 PTCN0227
 PTCN0228
 PTCN0229
 PTCN0230
 PTCN0231
 PTCN0232
 PTCN0233
 PTCN0234
 PTCN0235
 PTCN0236
 PTCN0237
 PTCN0238
 PTCN0239
 PTCN0240
 PTCN0241
 PTCN0242
 PTCN0243
 PTCN0244
 PTCN0245
 PTCN0246
 PTCN0247
 PTCN0248
 PTCN0249
 PTCN0250
 PTCN0251
 PTCN0252
 PTCN0253
 PTCN0254
 PTCN0255
 PTCN0256
 PTCN0257
 PTCN0258
 PTCN0259
 PTCN0260
 PTCN0261
 PTCN0262
 PTCN0263
 PTCN0264
 PTCN0265
 PTCN0266
 PTCN0267
 PTCN0268
 PTCN0269
 PTCN0270
 PTCN0271
 PTCN0272
 PTCN0273
 PTCN0274
 PTCN0275
 PTCN0276
 PTCN0277
 PTCN0278
 PTCN0279
 PTCN0280

C SIZE NVAR X NVAR. THE MEANINGS OF THESE COMPONENTS OF RWORK ARE DESCRIBED BELOW. THE USER SHOULD SET A VALUE TO XRPTCN0352
 C ON FIRST CALL, BUT NO OTHER PORTIONS OF RWORK SHOULD BE SET. AFTER THE FIRST CALL FOR A PROBLEM, NO ENTRIES OF RWORK PTCN0353
 C SHOULD BE ALTERED. PTCN0354
 C (XR) = ON FIRST CALL, A USER SUPPLIED STARTING POINT, WHICH MAY BE IMPROVED BY THE PROGRAM IF KSTEP=-1. ON NORMAL RETURN FROM PTCN0355
 C PITCON, XR WILL HOLD THE MOST RECENTLY FOUND POINT, WHETHER A CONTINUATION POINT, TARGET POINT, OR LIMIT POINT. PTCN0356
 C (XC) = THE PREVIOUS CONTINUATION POINT. PTCN0357
 C (XF) = THE CURRENT CONTINUATION POINT. PTCN0358
 C (TL) = PREVIOUS VALUE OF TANGENT VECTOR. NOTE THAT THIS CORRESPONDS TO A POINT XL WHICH HAS BEEN DISCARDED. ON A LIMIT POINT RETURN, TL WILL CONTAIN INSTEAD THE TANGENT AT THE LIMIT POINT. ON A TARGET POINT RETURN, TL WILL HAVE BEEN OVERRITTEN BY THE FUNCTION VALUE AT THE TARGET POINT. PTCN0359
 C (TC) = THE TANGENT VECTOR AT THE PREVIOUS CONTINUATION POINT. PTCN0360
 C (FPRYM) = MATRIX STORAGE AREA FOR SETTING UP AND SOLVING THE LINEAR SYSTEMS INVOLVING DFA(X,IP). PTCN0361
 C ISIZE = USER SET DIMENSION FOR VECTOR RWORK, WHICH MUST BE AT LEAST OF SIZE NVAR*(NVAR+5). PTCN0362
 PTCN0363
 PTCN0364
 PTCN0365
 PTCN0366
 PTCN0367
 PTCN0368
 PTCN0369
 PTCN0370
 PTCN0371
 PTCN0372
 PTCN0373
 PTCN0374
 PTCN0375
 PTCN0376
 PTCN0377
 PTCN0378
 PTCN0379
 PTCN0380
 PTCN0381
 PTCN0382
 PTCN0383
 PTCN0384
 PTCN0385
 PTCN0386
 PTCN0387
 PTCN0388
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 PTCN0399
 PTCN0400
 PTCN0401
 PTCN0402
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 PTCN0416
 PTCN0417
 PTCN0418
 PTCN0419
 PTCN0420

NOMENCLATURE FOR STEP DEPENDENT VARIABLES

THE PROGRAM ACCUMULATES INFORMATION THAT IS ASSOCIATED WITH SEVERAL PREVIOUS CONTINUATION POINTS OR THE STEPS MADE BETWEEN THEM. IN INTERPRETING THE CODE OR ITS OUTPUT, IT IS IMPORTANT TO KNOW WHERE SUCH QUANTITIES APPLY. THE FOLLOWING DESCRIPTION OF SOME OF THE VARIABLES IS VALID ONLY UPON A NORMAL RETURN WITH A CONTINUATION POINT. THE POINTS 'XLL' AND 'XL' WILL HAVE BEEN DISCARDED BY THE PROGRAM, BUT SOME QUANTITIES ASSOCIATED WITH THEM STILL SURVIVE.

QUANTITIES ASSOCIATED WITH STEP FROM 'XLL' TO 'XL':

HSECLL = SIZE OF SECANT FROM 'XLL' TO 'XL', EUCLIDEAN NORM(XLL-XL)

QUANTITIES ASSOCIATED WITH THE POINT 'XL':

IPL = THE LOCATION OF THE FIRST OR SECOND LARGEST COMPONENT OF THE TANGENT VECTOR AT 'XL'.
 TLLIM = VALUE OF LIM-TH COMPONENT OF TANGENT VECTOR AT 'XL'.
 TL = TANGENT VECTOR AT 'XL', ALTHOUGH LIMIT OR TARGET POINT CALCULATIONS COULD HAVE OVERRITTEN THIS VECTOR.

QUANTITIES ASSOCIATED WITH INTERVAL FROM 'XL' TO XC:

ALPHLC = THE ANGLE BETWEEN THE TANGENTS AT 'XL' AND XC.
 CURVLC = ESTIMATED CURVATURE BETWEEN 'XL' AND XC.
 HSECLC = SIZE OF SECANT BETWEEN 'XL' AND XC, EUCLIDEAN NORM(XL-XC)

QUANTITIES ASSOCIATED WITH THE POINT XC:

DETA = BINARY MANTISSA OF DETERMINANT OF DFA(XC,IPL), DIVIDED BY IPL-TH COMPONENT OF TANGENT AT XC.
 DIR = SIGN OF DETA, DETERMINES SENSE OF CONTINUATION.
 IEXP = BINARY EXPONENT OF DETERMINANT OF DFA(XC,IPL).
 IPC = LOCATION OF FIRST OR SECOND LARGEST COMPONENT OF TANGENT VECTOR AT XC.
 TC = TANGENT VECTOR AT XC.
 TCLIM = VALUE OF LIM-TH COMPONENT OF TANGENT AT XC.
 TCIPC = VALUE OF TC(IPC)

QUANTITIES ASSOCIATED WITH THE INTERVAL FROM XC TO XF:

CURVCF = ESTIMATED CURVATURE BETWEEN XC AND XF.
 HTANCF = STEPSIZE USED ALONG TANGENT TO GET PREDICTED POINT

C	WHICH WAS CORRECTED TO SOLUTION POINT XF.	PTCN0421
C		PTCN0422
C	QUANTITIES ASSOCIATED WITH THE POINT XF:	PTCN0423
C		PTCN0424
C	CORDIS = SIZE OF THE TOTAL CORRECTION FROM PREDICTED POINT	PTCN0425
C	X=XC+HTANCF*TC TO CORRECTED POINT XF.	PTCN0426
C	NOTE THAT THIS HAS BEEN MODIFIED TO AN 'OPTIMAL' VALUE.	PTCN0427
C	CURVXF = A PREDICTED VALUE OF THE CURVATURE AT XF.	PTCN0428
C	FNRMXF = MAXIMUM NORM OF FUNCTION VALUE AT XF.	PTCN0429
C	FPRYM = DFA(XF,IPC) HAS ACTUALLY BEEN LAST EVALUATED AT THE	PTCN0430
C	PENULTIMATE CORRECTOR ITERATE (IF IMOD.NE.1). IT WILL BE	PTCN0431
C	EVALUATED AT XF AS SOON AS THE NEXT LOOP BEGINS AND THE	PTCN0432
C	TANGENT IS NEEDED.	PTCN0433
C	XSTEP = SIZE OF THE LAST CORRECTOR STEP TAKEN IN CONVERGING TO XF.	PTCN0434
C		PTCN0435
C		PTCN0436
C	SUBROUTINES IN THIS PACKAGE	PTCN0437
C		PTCN0438
C		PTCN0439
C	PITCON(NVAR,LIM,IT,XIT,KSTEP,IPC,H,IRET,IMOD,IPVT,	PTCN0440
C	HMAX,HMIN,HFACT,ABSERR,RELERR,RWORK,ISIZE)	PTCN0441
C		PTCN0442
C	DRIVING ROUTINE OF CONTINUATION CODE. INITIALIZES INFORMATION,	PTCN0443
C	DETERMINES WHETHER LIMIT, TARGET OR CONTINUATION POINT WILL	PTCN0444
C	BE SOUGHT THIS STEP, COMPUTES STEPLENGTHS, CONTROLS CORRECTOR	PTCN0445
C	PROCESS, AND HANDLES ERROR RETURNS.	PTCN0446
C		PTCN0447
C	CORRECT(NVAR,X,IHOLD,WORK,IERR,IMOD,FPRYM,IPVT,ABSERR,RELERR,	PTCN0448
C	XSTEP,NEQN,FNRM)	PTCN0449
C		PTCN0450
C	USES A FORM OF NEWTON'S METHOD TO SOLVE THE AUGMENTED NONLINEAR	PTCN0451
C	SYSTEM FA(X)=0 WITH AUGMENTING EQUATION X(IHOLD)=R, THAT IS, X(IHOLD)	PTCN0452
C	IS HELD FIXED DURING THE CORRECTION PROCESS.	PTCN0453
C		PTCN0454
C	TANGNT(NVAR,XC,IPC,TC,IRET,ICALL,FPRYM,IPVT,NEQN,DETA,IEXP)	PTCN0455
C		PTCN0456
C	APPLIES ALGORITHM DESCRIBED ABOVE TO SOLVE DFA(XC,IPL)*TC=E(NVAR)	PTCN0457
C	AND THEN NORMALIZES TANGENT VECTOR, CORRECTS SIGN, AND SETS	PTCN0458
C	IPC AND DIR.	PTCN0459
C		PTCN0460
C	ROOT(A,FA,B,FB,C,FC,KOUNT,IFLAG)	PTCN0461
C		PTCN0462
C	ROOT FINDER USED TO LOCATE LIMIT POINT. THIS ROUTINE IS A MODIFIED	PTCN0463
C	VERSION OF THE FORTRAN FUNCTION ZERO GIVEN IN THE BOOK:	PTCN0464
C	'ALGORITHMS FOR MINIMIZATION WITHOUT DERIVATIVES'	PTCN0465
C	BY RICHARD P BRENT, PRENTICE HALL, 1973.	PTCN0466
C		PTCN0467
C	SOLVE(NVAR,X,Y,IP,DETA,IEXP,IERR,ICALL,IMOD,FPRYM,IPVT)	PTCN0468
C		PTCN0469
C	SETS UP AND SOLVES THE SYSTEM DFA(X,IP)*Y(OUTPUT)=Y(INPUT)	PTCN0470
C	WHERE DFA(X,IP) IS THE JACOBIAN OF FA AT X,	PTCN0471
C	AND Y IS A RIGHT HAND SIDE SUPPLIED BY THE CALLING ROUTINE.	PTCN0472
C		PTCN0473
C	**NOTE** SUBROUTINE SOLVE USES FULL MATRIX STORAGE TO SOLVE THE	PTCN0474
C	SYSTEM. THE USER MAY WISH TO REPLACE THIS ROUTINE WITH ONE MORE	PTCN0475
C	SUITED TO HIS PROBLEM.	PTCN0476
C		PTCN0477
C	USER SUPPLIED SUBROUTINES	PTCN0478
C		PTCN0479
C		PTCN0480
C	FCTN(NVAR,X,FX)	PTCN0481
C		PTCN0482
C		PTCN0483
C	EVALUATES THE NVAR-1 COMPONENT FUNCTION FX GIVEN X AN NVAR COMPONENT	PTCN0484
C	VECTOR. THIS FUNCTION DESCRIBES THE NONLINEAR SYSTEM. THE AUGMENTING	PTCN0485
C	EQUATION IS HANDLED BY THE CONTINUATION PACKAGE.	PTCN0486
C		PTCN0487
C	FPRIME(NVAR,X,FPRYM)	PTCN0488
C		PTCN0489
C	EVALUATES THE NVAR-1 BY NVAR JACOBIAN MATRIX FPRYM (X)	PTCN0490

AT X AND STORES IT IN THE NVAR BY NVAR ARRAY FPRYM,
SO THAT FPRYM(J,J) CONTAINS (DF(X) (I)/ DX (J)).
THE LAST ROW OF FPRYM (FOR THE AUGMENTING EQUATION) IS INSERTED
BY THE ROUTINE SOLVE.

LINPAK ROUTINES USED

LINPAK REFERENCE:

LINPACK USER'S GUIDE,
J J DONGARRA, J R BUNCH, C B MOLER AND G W STEWART,
SOCIETY FOR INDUSTRIAL AND APPLIED MATHEMATICS,
PHILADELPHIA, 1979.

ISAMAX(N,SX,INCX)

INTEGER FUNCTION RETURNS THE POSITION OF LARGEST ELEMENT OF SX

SAXPY(N,SA,SX,INCX,SY,INCY)

SETS VECTOR SY(I) = SA*SX(I)+SY(I)

SCOPY(N,SX,INCX,SY,INCY)

SETS SY(I)=SX(I)

SDOT(N,SX,INCX,SY,INCY)

SDOT = SUM(I=1 TO N) SX(I)*SY(I)

SNRM2(N,SX,INCX)

SNRM2 = EUCLIDEAN NORM OF SX(I)

****NOTE**** SNRM2 HAS MACHINE DEPENDENT CUTOFF CONSTANTS

SSCAL(N,SA,SX,INCX)

SETS SX(I)=SA*SX(I)

SGEFA(A,LDA,N,IPVT,INFO)

FACTORS MATRIX A WHOSE LEADING DIMENSION WAS DECLARED AS LDA
AND WHOSE ACTUAL USED DIMENSION IS N, SETS UP PIVOT INFORMATION
IN VECTOR IPVT AND WARNS OF ZERO PIVOTS.

SGESL(A,LDA,N,IPVT,B,JOB)

ACCEPTS OUTPUT OF SGEFA, AND A RIGHT HAND SIDE B, AND SOLVES
SYSTEM A*X=B, RETURNING X IN B. FOR MODIFIED NEWTON'S METHOD, ONCE
MATRIX IS FACTORED BY SGEFA, ONLY SGESL IS CALLED FOR SUCCESSIVE
RIGHT HAND SIDES

LABELED COMMON BLOCKS

/COUNT1/ COUNTS NUMBER OF CALLS FROM ... TO ... AS FOLLOWS:

ICRSL = CORECT TO SOLVE

ITNSL = TANGNT TO SOLVE

NSTCR = PITCON TO CORECT FOR IMPROVED STARTING POINT

NCNCR = PITCON TO CORECT FOR CONTINUATION POINT

NTRCR = PITCON TO CORECT FOR TARGET POINTS

NLMCR = PITCON TO CORECT FOR LIMIT POINT

NLMRT = PITCON TO ROOT FOR LIMIT POINT

NOTE THAT NSTCR, NCNCR, NTRCR, NLMCR AND NLMRT COUNT THE NUMBER
OF ITERATIVE STEPS (NEWTON OR ROOTFINDING) AND NOT JUST THE NUMRER
OF SUBROUTINE CALLS.

/COUNT2/ KEEPS PERFORMANCE AND WORK STATISTICS

IFEVAL = NUMBER OF CALLS TO FCTN

IPEVAL = NUMBER OF CALLS TO FPRIME

ISOLVE = NUMBER OF CALLS TO SOLVE

NRED = NUMBER OF STEPSIZE REDUCTIONS MADE BEFORE PREDICTOR

PTCN0491
PTCN0492
PTCN0493
PTCN0494
PTCN0495
PTCN0496
PTCN0497
PTCN0498
PTCN0499
PTCN0500
PTCN0501
PTCN0502
PTCN0503
PTCN0504
PTCN0505
PTCN0506
PTCN0507
PTCN0508
PTCN0509
PTCN0510
PTCN0511
PTCN0512
PTCN0513
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PTCN0541
PTCN0542
PTCN0543
PTCN0544
PTCN0545
PTCN0546
PTCN0547
PTCN0548
PTCN0549
PTCN0550
PTCN0551
PTCN0552
PTCN0553
PTCN0554
PTCN0555
PTCN0556
PTCN0557
PTCN0558
PTCN0559
PTCN0560

POINT CONVERGED TO THE NEW CONTINUATION POINT. PTCN0561
 NRDSUM = TOTAL NUMBER OF STEPSIZE REDUCTIONS PTCN0562
 KN = NUMBER OF CORRECTOR ITERATION STEPS TAKEN IN MOST RECENT PTCN0563
 CALL TO CORRECT. PTCN0564
 KNSUM = TOTAL NUMBER OF CORRECTOR ITERATION STEPS. PTCN0565
 PTCN0566
 PTCN0567
 PTCN0568
 PTCN0569
 PTCN0570
 PTCN0571
 PTCN0572
 PTCN0573
 PTCN0574
 PTCN0575
 PTCN0576
 PTCN0577
 PTCN0578
 PTCN0579
 PTCN0580
 PTCN0581
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 PTCN0595
 PTCN0596
 PTCN0597
 PTCN0598
 PTCN0599
 PTCN0600
 PTCN0601
 PTCN0602
 PTCN0603
 PTCN0604
 PTCN0605
 PTCN0606
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 PTCN0619
 PTCN0620
 PTCN0621
 PTCN0622
 PTCN0623
 PTCN0624
 PTCN0625
 PTCN0626
 PTCN0627
 PTCN0628
 PTCN0629
 PTCN0630

/OUTPUT/
 IWRITE = USER ACCESSIBLE OUTPUT INDICATOR.
 IWRITE=0, NO OUTPUT PRINTED BY PITCON.
 IWRITE=1, ERROR MESSAGES PRINTED BY PITCON.
 IWRITE=2, CERTAIN OUTPUT WILL BE PRINTED BY PITCON.

/POINT/ CONTAINS DATA ABOUT THE SOLUTION CURVE
 DETA = BINARY MANTISSA OF THE DETERMINANT OF THE AUGMENTED JACOBIAN
 IEXP = BINARY EXPONENT OF THE DETERMINANT OF THE AUGMENTED JACOBIAN
 CURVCF = ESTIMATED CURVATURE BETWEEN XC AND XF.
 CORDIS = NORM OF THE CORRECTOR STEP FROM PREDICTED POINT TO CORRECTED
 POINT, USING MAXIMUM ABSOLUTE VALUE AS THE NORM.
 THIS QUANTITY IS MODIFIED TO AN 'OPTIMAL' VALUE.
 ALPHLC = ANGLE BETWEEN OLD AND NEW TANGENTS TL AND TC
 HSECLC = EUCLIDEAN NORM OF SECANT BETWEEN XL AND XC.
 FNRMXF = MAXIMUM NORM OF FUNCTION VALUE AT NEW CONTINUATION POINT.

/TOL/
 EPMACH= SMALLEST NUMBER SUCH THAT $1.0 + \text{EPMACH} > \text{EPMACH}$
 $\cdot \text{SEBETA} \cdot (1 - \text{TAU})$ FOR ROUNDED, TAU-DIGIT ARITHMETIC
 BASE BETA. TWICE THIS VALUE FOR TRUNCATED ARITHMETIC.
 THIS IS THE RELATIVE MACHINE PRECISION.
 EPMACH= $2 \cdot (-27)$ FOR DEC-10.
 EPSATE= $8 \cdot \text{EPMACH}$
 EPSQRT= SQUARE ROOT OF EPMACH

PROGRAMMING NOTES

THE USER MUST -

1. WRITE SUBROUTINES
 SUPPLY A CALLING PROGRAM, AND THE TWO ROUTINES FCTN AND FPRIME
 AS DESCRIBED ABOVE.
2. SET STORAGE AREAS
 DECLARE A REAL VECTOR RWORK OF SIZE ISIZE, $\text{ISIZE} \geq \text{NVAR} \cdot (\text{NVAR} + 5)$
 AND AN INTEGER VECTOR IPVT OF SIZE NVAR.
3. PASS CERTAIN NON-DEFAULTABLE VALUES
 PASS NVAR GREATER THAN ZERO, $\text{ISIZE} \geq \text{NVAR} \cdot (\text{NVAR} + 5)$
 AND SET IRET=0, KSTEP=-1 OR KSTEP=0 ON FIRST CALL
 FOR A NEW PROBLEM.

THE USER SHOULD -

1. STORE A STARTING POINT XR IN THE FIRST NVAR LOCATIONS OF RWORK
 BEFORE CALLING PITCON.
 IF SUCH A VALUE IS NOT GIVEN, THE CODE MAY BE UNABLE TO PRODUCE ONE.
2. CAREFULLY MONITOR THE VALUE OF IRET SO THAT ANY SERIOUS ERROR
 IS CAUGHT BEFORE ANOTHER CALL IS MADE TO PITCON.
3. CHOOSE A VALUE OF IMOD FOR THE TYPE OF CORRECTOR PROCESS TO
 BE USED.

THE USER MAY -

1. MONITOR THE PASSING OF BIFURCATION POINTS BY SAVING THE OLD
 VALUE OF DETA AND COMPARING IT TO THE CURRENT VALUE. IF THERE
 IS A CHANGE IN SIGN, THEN A BIFURCATION POINT HAS BEEN PASSED.


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TERR=0
IF (IRET.EQ.-1) IRET=2
IF (IRET.EQ.-2.OR.IRET.EQ.-3.OR.IRET.EQ.-4) IRET=1
IF (IRET.EQ.-5.OR.IRET.EQ.-6) IRET=0
IF CODE WAS CALLED AGAIN AFTER FATAL VALUE OF IRET,
THEN RETURN WITH ERROR VALUE IRET=-10.
IF (IRET.LT.0) GO TO 440
PERFORM ONE-TIME ONLY INITIALIZATIONS
IF (IDONE.NE.0) GO TO 10
SET THE MACHINE DEPENDENT VARIABLE EPMACH, THE SMALLEST NUMBER
SO THAT (1.0+EPMACH.GT.1.0)
FOR DEC PDP-10 IN SINGLE PRECISION:
EPMACH=7.4505806E-9
FOR TRM 360 OR 370 IN SHORT (SINGLE) PRECISION:
EPMACH=9.53674E-7
FOR CDC 6600 OR 7400 IN SINGLE PRECISION:
EPMACH=7.105427406E-15
SET EPSATE=8*EPMACH, EPSQRT=SQRT(EPMACH)
EPSATE=8.0*EPMACH
EPSQRT=SQRT(EPMACH)
ALFMIN=2.0*ACOS(1.0-EPMACH)
IF (KSTEP.LT.-1.OR.KSTEP.GT.0) KSTEP=-1
KSTEPO=-2
TOONE=1
PERFORM INITIALIZATIONS AND CHECKS FOR NEW PROBLEM ONLY
10 IF (KSTEP.GT.0) GO TO 30
IF (KSTEPO.EQ.-1.AND.KSTEP.EQ.0) GO TO 30
IF (NVAR.LE.1) GO TO 440
IF (ISIZE.LT.(NVAR)*NVAR) GO TO 440
IXR=1
JXR=0
IXC=IXR+NVAR
JXC=JXR+NVAR
IXF=IXC+NVAR
JXF=JXC+NVAR
ITL=IXF+NVAR
JTL=JXF+NVAR
ITC=ITL+NVAR
JTC=JTL+NVAR
IFP=ITC+NVAR
JFP=JTC+NVAR
BETA=0.0
TCIPC=0.0
CORDIS=0.0
CURVCF=0.0
HSECLL=0.0
HSECLC=0.0
XITD=0.0
ITD=0
NEQN=NVAR-1
NRED=0
KNSUM=0
NRDSUM=0
ICRSI=0
ITNSI=0

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IF (IERR.EQ.0) GO TO 320
IF (IERR.EQ.-1) GO TO 370
IF (IERR.EQ.-2) GO TO 360
IF (IERR.EQ.-3) GO TO 380
C*****
C
C 3. TANGENT AND LOCAL CONTINUATION PARAMETER CALCULATION. UNLESS THE
C TANGENT AND LIMIT POINT CALCULATIONS WERE ALREADY PERFORMED (BECAUSE
C THE LOOP WAS INTERRUPTED FOR A LIMIT POINT), SET UP AND SOLVE
C THE EQUATION FOR THE TANGENT VECTOR. FORCE THE TANGENT VECTOR TO BE
C OF UNIT LENGTH, AND FORCE THE IPL-COMPONENT TO HAVE THE SAME SIGN AS
C THE IPL-TH COMPONENT OF THE PREVIOUS TANGENT VECTOR, OR (ON FIRST
C STEP) THE SAME SIGN AS THE USER INPUT DIRECTION DIR. SET THE LOCAL
C PARAMETER IPC TO THE LOCATION OF THE LARGEST COMPONENT
C OF THE TANGENT VECTOR, UNLESS A LIMIT POINT IN THAT DIRECTION
C APPEARS TO BE APPROACHING AND ANOTHER CHOICE IS AVAILABLE.
C*****
C
C 40 IF (IRET.NE.2) GO TO 50
C IRET=0
C GO TO 160
C
C STORE OLD TANGENT IN TL, COMPUTE NEW TANGENT FOR XC
C
C 50 JPL=IPC
C IF (KSTEP.GT.0) CALL SCOPY(NVAR,RWORK(ITC),1,RWORK(ITL),1)
C ICALL=1
C CALL TANGT(NVAR,RWORK(IFX),IPC,RWORK(ITC),IRET,ICALL,RWORK(IFP),
C 1 IPUT,NEQN,DETA,IEXP)
C IF (IRET.EQ.-2) GO TO 430
C IF (IRET.EQ.-1) GO TO 410
C
C SUBROUTINE TANGT RETURNED IPC, THE LOCATION OF THE LARGEST COMPONENT
C OF THE TANGENT VECTOR. THIS WILL BE USED FOR THE LOCAL
C PARAMETERIZATION OF THE CURVE UNLESS A LIMIT POINT IN IPC SEEMS
C TO BE COMING. TO CHECK THIS, WE COMPARE TC(IPC)=TC(IPC) AND THE
C SECOND LARGEST COMPONENT TC(JPC)=TC(JPC). IF TCJPC IS NO LESS
C THAN .1 OF TCIPC, AND TC(JPC) IS LARGER THAN TL(JPC),
C WHEREAS TC(IPC) IS LESS THAN TL(IPC), WE WILL RESET THE
C LOCAL PARAMETER IPC:=JPC.
C
C TL IPL=TCIPC
C TCIPC=RWORK(JTC+IPC)
C JPC=IPC
C IF (ABS(TCIPC).GE.ABS(RWORK(JTL+IPC))) GO TO 60
C IF (TLIPL.EQ.0.0) GOTO 60
C RWORK(JTC+IPC)=0.0
C JPC=ISAMAX(NVAR,RWORK(ITC),1)
C TCJPC=RWORK(JTC+JPC)
C RWORK(JTC+IPC)=TCIPC
C IF (ABS(TCJPC).LT.TENM1*ABS(TCIPC)) GO TO 60
C IF (ABS(TCJPC).LT.ABS(RWORK(JTL+JPC))) GOTO 60
C IPC=JPC
C IF (IWRITE.GE.2) WRITE(6,610)
C 60 TC IPL=RWORK(JTC+IPL)
C DTLIPL=DBLE(RWORK(JTL+IPC))
C DETA=DETA/TCIPL
C
C ADJUST SIGN OF TANGENT
C COMPARE THE SIGN OF TC(IPL) WITH SIGN OF TL(IPL)
C (BUT ON FIRST STEP, COMPARE SIGN OF TC(IPL) WITH USER INPUT DIR).
C IF THESE SIGNS DIFFER, CHANGE THE SIGN OF TC TO FORCE AGREEMENT,
C AND THE SIGN OF DETA.
C THEN RECORD DIR:= SIGN OF DETERMINANT = SIGN(DETA).
C
C STLIPL=DIR
C IF (TLIPL.NE.0.0) STLIPL=SIGN(1.0,TLIPL)
C IF (SIGN(1.0,TC(IPL)).EQ.STLIPL) GO TO 70

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CALL SSCAL(NVAR,-1.0,RWORK(JTC),J)
DETA=-DETA
TCIPL=-TCIPL
70 TCIPC=RWORK(JTC+IPC)
TCJPC=RWORK(JTC+JPC)
DTCTPC=DBLE(TCIPC)
DIR=SIGN(1.0,DETA)
IF (LIM.EQ.0) GO TO 80
TLLIM=TCLIM
TCLIM=RWORK(JTC+LIM)
C
C COMPUTE ALPHLC, THE ANGLE BETWEEN TANGENT AT XL AND TANGENT AT XC
C AND HSECLC, THE EUCLIDEAN NORM OF SECANT FROM XL TO XC.
C
80 IF(KSTEP.LE.0) GO TO 160
COSALF=0.000
DO 90 J=1,NVAR
    COSALF=COSALF+DBLE(RWORK(JTC+J))*DBLE(RWORK(JTL+J))
90 RWORK(JXR+J)=RWORK(JXF+J)-RWORK(JXC+J)
HSECLL=HSECLC
HSECLC=SNRM2(NVAR,RWORK(JXR),J)
ALPHLC=SNGL(COSALF)
IF (ALPHLC.GT.1.0)ALPHLC=1.0
IF (ALPHLC.LT.-1.0)ALPHLC=-1.0
ALPHLC=ACOS(ALPHLC)
IF (WRITE,GE,2)WRITE(6,550)ALPHLC
C
C *****
C
C 4. LIMIT POINT CHECK. IF (LIM.NE.0) CHECK TO SEE IF
C OLD AND NEW TANGENTS DIFFER IN SIGN OF LIM-TH COMPONENT.
C IF SO, ATTEMPT TO COMPUTE A POINT XR BETWEEN XC AND XF
C FOR WHICH TANGENT COMPONENT VANISHES
C *****
C
C IF (LIM.LE.0.OR.KSTEP.LE.0) GO TO 160
C
C CHECK FOR LIMIT INTERVAL
C
C IF (SIGN(1.0,TCLIM).EQ.SIGN(1.0,TLLIM)) GO TO 160
C
C TEST FOR ACCEPTABLE ENDPOINTS
C
C ATLLM=ABS(TLLIM)
C IF (ATLLM.GT.0.5*ABSERR) GO TO 110
C
C IF XC IS LIMIT POINT, TL ALREADY CONTAINS TANGENT AT XC
C
100 CALL SCOPY(NVAR,RWORK(JXC),1,RWORK(JXR),1)
    GO TO 310
110 ATCLIM=ABS(TCLIM)
    IF (ATCLIM.GT.0.5*ABSERR) GO TO 130
120 CALL SCOPY(NVAR,RWORK(JXF),1,RWORK(JXR),1)
    CALL SCOPY(NVAR,RWORK(JTC),1,RWORK(JTL),1)
    GO TO 310
C
C TEST FOR SMALL INTERVAL
C
130 XCLIM=RWORK(JXC+LIM)
    XFLIM=RWORK(JXF+LIM)
    DEL=ABS(XFLIM-XCLIM)
    XABS=AMAX1(ABS(XCLIM),ABS(XFLIM))
    IF (DEL.GT.(ABSERR+RELEERR*XABS)) GO TO 140
    IF (ATLLM.GT.ATCLIM) GO TO 120
    GO TO 100
C
C BEGIN ROOT-FINDING ITERATION WITH INTERVAL (0,1) AND
C FUNCTION VALUES TL(LIM), TC(LIM).
C

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140 KOUNT=0
    A=0.0
    FA=TLLIM
    TSN=TCLIM
    C=1.0
    FC=TCLIM
C
C SET IPLIM TO THE INDEX OF MAXIMUM ENTRY OF SECANT
C (EXCEPT THAT IPLIM MUST NOT EQUAL LIM)
C AND SAVE THE SIGN OF THE MAXIMUM COMPONENT IN DIRLIM
C SO THAT NEW TANGENTS MAY BE PROPERLY SIGNED.
C
    CALL SCOPY(NVAR,RWORK(IXF),1,RWORK(JXR),1)
    CALL SAXPY(NVAR,-1.0,RWORK(IXC),1,RWORK(JXR),1)
    RWORK(JXR+LIM)=0.0
    IPLIM=ISAMAX(NVAR,RWORK(JXR),1)
    DIRLIM=SIGN(1.0,RWORK(JXR+IPLIM))
C
C CALL ROOTFINDER FOR APPROXIMATE ROOT SN, SET X=SN*XF+(1-SN)*XC
C CALL CORRECTOR TO RETURN TO CURVE ON LINE X(IPLIM)=CONSTANT,
C COMPUTE TANGENT THERE, AND SET FUNCTION VALUE TO TANGENT(LIM)
C
150 CALL ROOT(A,FA,SN,TSN,C,FC,KOUNT,IFLAG)
    NLNRT=NLNRT+1
    IF(IFLAG.LT.-1)GO TO 350
    IF(IFLAG.EQ.-1.OR.IFLAG.EQ.0)GO TO 310
    CALL SCOPY(NVAR,RWORK(IXF),1,RWORK(JXR),1)
    CALL SSCAL(NVAR,SN,RWORK(JXR),1)
    SCALER=1.0-SN
    CALL SAXPY(NVAR,SCALER,RWORK(IXC),1,RWORK(JXR),1)
    CALL CORECT(NVAR,RWORK(JXR),IPLIM,RWORK(ITL),TERR,(MOO,RWORK(JFP)
    1 ,IPUT,ABSERR,RELEERR,XSTPLM,NEQN,FNRH)
    NLNCR=NLNCR+KN
    IF(IERR.NE.0)GO TO 350
    ICALL=1
    IPT=IPLIM
    CALL TANGNT(NVAR,RWORK(JXR),IPT,RWORK(ITL),IRET,ICALL,
    1 RWORK(JFP),IPUT,NEQN,DETLIM,IEXLIM)
    IF(IRET.LT.0)GO TO 350
C
C ADJUST THE SIGN OF THE TANGENT SO THAT THE IPLIM-TH COMPONENT
C HAS THE SAME SIGN AS THE IPLIM-TH COMPONENT OF THE SECANT
C
    JF (DIRLIM.NE.SIGN(1.0,RWORK(JTL+IPLIM)))
    1 CALL SSCAL(NVAR,-1.0,RWORK(ITL),1)
C
C SEE IF WE CAN ACCEPT THE NEW POINT BECAUSE TANGENT(LIM) IS SMALL
C OR MUST 'ACCEPT' THE POINT BECAUSE THE VALUES ARE NOT DECREASING
C RAPIDLY ENOUGH, OR IF WE CAN GO ON.
C
    TSHOLD=TSN
    TSN=RWORK(JTL+LIM)
    IF (ABS(TSN).LE.0.5*ABSERR) GO TO 310
    GO TO 150
C
C *****
C 5. STEP LENGTH COMPUTATION. COMPUTE STEPLENGTH HTANCE
C
C THE FORMULAS UNDERLYING THE ALGORITHM ARE
C
C LET
C
C ALPHLC = MAXIMUM OF ARCCOS(TL,TC) AND ALFMIN = 2*ARCCOS(1-EPHACH)
C HSECLC = NORM(XL-XC)
C HSECLL = NORM(XL-XLL)
C ABSIN = ARS(SIN(.5*ALPHLC))
C CURVLC = LAST VALUE OF CURVCF
C CURVCF = 2*ABSIN/HSECLC
C CORDIS = OPTIMIZED CORRECTOR DISTANCE TO CURRENT CONTINUATION POINT.

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HTANCF=AMIN1(HTANCF,TEMP)
HTANCF=AMAX1(HTANCF,HMIN)
HTANCF=AMIN1(HTANCF,HMAX)
PTCN1121
PTCN1122
PTCN1123
PTCN1124
C*****PTCN1125
C
C 6. PREDICTION AND CORRECTION STEPS. USING XR=XC+HTANCF*TC
PTCN1126
C AS STARTING POINT, CORRECT XR WITH A FULL OR MODIFIED NEWTON
PTCN1127
C ITERATION. IF CORRECT FAILS, REDUCE STEPSIZE USED FOR PREDICTOR
PTCN1128
C POINT, AND TRY AGAIN. CORRECTION WILL ONLY BE ABANDONED IF STEPSIZE
PTCN1129
C FALLS BELOW HMIN.
PTCN1130
PTCN1131
PTCN1132
C*****PTCN1133
C
C 190 KSTEP0=KSTEP
PTCN1134
C KSTEP=KSTEP+1
PTCN1135
C NRED=0
PTCN1136
C 200 CALL SCOPY(NVAR,RWORK(IXF),1,RWORK(IXR),1)
PTCN1137
C CALL SAXPY(NVAR,HTANCF,RWORK(ITC),1,RWORK(IXR),1)
PTCN1138
C 210 IF(IWRITE.GE.2)WRITE(6,570)HTANCF
PTCN1139
C IF(IWRITE.GE.3)WRITE(6,580)(RWORK(JXR+I),I=1,NVAR)
PTCN1140
C CALL CORRECT(NVAR,RWORK(IXR),IPC,RWORK(ITL),IERR,IMOD,RWORK(IFP),
PTCN1141
C 1 IPVT,ABSERR,RELERR,XSTEP,NEQN,FNRMXF)
PTCN1142
C NCHCR=NCHCR+KN
PTCN1143
C IF (IERR.EQ.0) GO TO 230
PTCN1144
C IF (IERR.EQ.-1) GO TO 420
PTCN1145
C
PTCN1146
C NO CONVERGENCE, TRY A SMALLER STEPSIZE
PTCN1147
C
PTCN1148
C HTANCF=HRED*HTANCF
PTCN1149
C IF (HTANCF.LT.HMIN) GO TO 390
PTCN1150
C NRED=NRED+1
PTCN1151
C IF (IERR.EQ.-2) GO TO 220
PTCN1152
C GO TO 200
PTCN1153
C 220 CALL SAXPY(NVAR,-1.0,RWORK(IXC),1,RWORK(IXR),1)
PTCN1154
C CALL SSCAL(NVAR,HRED,RWORK(IXR),1)
PTCN1155
C CALL SAXPY(NVAR,1.0,RWORK(IXC),1,RWORK(IXR),1)
PTCN1156
C GO TO 210
PTCN1157
C
PTCN1158
C *****PTCN1159
C
C 7. SUCCESSFUL STEP, STORE INFORMATION BEFORE RETURN.
PTCN1160
C UPDATE OLD AND CURRENT CONTINUATION POINTS.
PTCN1161
C COMPUTE CORDIS, THE SIZE OF THE CORRECTOR STEP. COMPUTE
PTCN1162
C A FACTOR THETA WHICH RESCALES CORDIS TO A VALUE WHICH WOULD
PTCN1163
C CORRESPOND TO A DESIRABLE NUMBER OF CORRECTOR STEPS
PTCN1164
C (4 FOR FULL NEWTON, 10 FOR MODIFIED NEWTON).
PTCN1165
C SEE REFERENCE DEN HEIJER AND RHEINBOLOT, LOC. CIT.
PTCN1166
C *****PTCN1167
C
C 230 NRDSUM=NRDSUM+NRED
PTCN1168
C IF(NRED.NE.0.AND.IWRITE.GE.2)WRITE(6,590)NRED
PTCN1169
C
C COMPUTE CORRECTOR STEP = XC+HTANCF*TC-XF
PTCN1170
C SET CORDIS = MAX NORM OF CORRECTOR STEP
PTCN1171
C
PTCN1172
C CALL SCOPY(NVAR,RWORK(IXF),1,RWORK(IXC),1)
PTCN1173
C CALL SAXPY(NVAR,-1.0,RWORK(IXR),1,RWORK(IXC),1)
PTCN1174
C CALL SAXPY(NVAR,HTANCF,RWORK(ITC),1,RWORK(IXC),1)
PTCN1175
C IMAX=ISAMAX(NVAR,RWORK(IXC),1)
PTCN1176
C CORDIS=ABS(RWORK(JXC+IMAX))
PTCN1177
C IF(KN.EQ.0) CORDIS=0.0
PTCN1178
C
PTCN1179
C MODIFY CORDIS TO A VALUE THAT WOULD CORRESPOND TO THE
PTCN1180
C DESIRED NUMBER OF CORRECTOR STEPS
PTCN1181
C
PTCN1182
C IF(CORDIS.EQ.0,0)GO TO 300
PTCN1183
C OMEGA=XSTEP/CORDIS
PTCN1184
C THETA=0.0
PTCN1185
PTCN1186
PTCN1187
PTCN1188
PTCN1189
PTCN1190

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C      IF (IMOD.EQ.1) GOTO 260
C C C FULL NEWTON METHOD FOR CORRECTOR STEPS
C      IF (KN.LE.1) THETA=8.0
C      IF (KN.EQ.4) THETA=1.0
C      IF (THETA.NE.0.0) GO TO 290
C      IF (KN.GT.4) GO TO 240
C      LK=4*KN-7
C      THETA=1.0
C      IF (OMEGA.GE.WRGE(LK)) GOTO 290
C      LST=LK
C      IF (OMEGA.GE.WRGE(LK+1)) GOTO 250
C      LST=LK+2
C      IF (OMEGA.GE.WRGE(LK+2)) GOTO 250
C      THETA=8.0
C      GOTO 290
240 THETA=0.125
C      IF (KN.GE.7) GOTO 290
C      LK=4*KN-14
C      IF (OMEGA.LE.WRGE(LK)) GOTO 290
C      LST=2*KN-1
250 THETA=ACOF(LST)+ACOF(LST+1)*ALOG(OMEGA)
C      GOTO 290
C C C MODIFIED NEWTON METHOD FOR CORRECTOR STEPS
260 IF (KN.LE.1) THETA=8.0
C      IF (KN.EQ.10) THETA=1.0
C      IF (THETA.NE.0.0) GO TO 290
C      EXPON=FLOAT(KN-1)/FLOAT(KN-10)
C C C AVOID OVERFLOW OR UNDERFLOW BY ANTICIPATING
C C C CUTOFF VALUES OF THETA
C      IF (KN.GT.10) GO TO 270
C      IF (8.0**EXPON.GT.OMEGA) THETA=8.0
C      IF (.125**EXPON.LT.OMEGA) THETA=.125
C      IF (THETA.NE.0.0) GO TO 290
C      GO TO 280
270 IF (8.0**EXPON.LT.OMEGA) THETA=8.0
C      IF (.125**EXPON.GT.OMEGA) THETA=.125
C      IF (THETA.NE.0.0) GO TO 290
280 EXPON=1.0/EXPON
C      THETA=OMEGA**EXPON
C      THETA=AMAX1(THETA,0.125)
C      THETA=AMIN1(THETA,8.0)
C C C SET THE MODIFIED VALUE OF CORDIS
290 CORDIS=THETA*CORDIS
C      IF (IWRITE.GE.2) WRITE(6,400) OMEGA, THETA, CORDIS
300 CALL SCOPY(NVAR,RWORK(IXF),1,RWORK(IXC),1)
C      CALL SCOPY(NVAR,RWORK(IXR),1,RWORK(IXF),1)
C      GO TO 340
C C C *****
C C C RETURNS. SET VALUE OF IRET. IF AN ERROR OCCURRED, PRINT
C C C A MESSAGE AS WELL.
C C C *****
C C C RETURN LIMIT POINT
310 IRET=2
C      RETURN
C C RETURN WITH TARGET POINT

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PTCN1191
PTCN1192
PTCN1193
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PTCN1196
PTCN1197
PTCN1198
PTCN1199
PTCN1200
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PTCN1260

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C	320 IRET=1	PTCN1261
	RETURN	PTCN1262
C	RETURN WITH CONTINUATION POINT	PTCN1263
C		PTCN1264
C	330 CALL SCOPY(NVAR,RWORK(IXF),1,RWORK(IXR),1)	PTCN1265
	340 IRET=0	PTCN1266
	H=HTANCF	PTCN1267
	RETURN	PTCN1268
C	ERROR RETURNS	PTCN1269
C		PTCN1270
C		PTCN1271
C		PTCN1272
	350 IRET=-1	PTCN1273
	IF(IWRITE,GE,1)WRITE(6,450)	PTCN1274
	RETURN	PTCN1275
	360 IRET=-2	PTCN1274
	IF(IWRITE,GE,1)WRITE(6,460)	PTCN1277
	RETURN	PTCN1278
	370 IRET=-3	PTCN1279
	IF(IWRITE,GE,1)WRITE(6,470)	PTCN1280
	RETURN	PTCN1281
	380 IRET=-4	PTCN1282
	IF(IWRITE,GE,1)WRITE(6,480)	PTCN1283
	RETURN	PTCN1284
	390 IRET=-5	PTCN1285
	IF(IWRITE,GE,1)WRITE(6,490)HTANCF,HMIN	PTCN1286
	RETURN	PTCN1287
	400 IRET=-6	PTCN1288
	IF(IWRITE,GE,1)WRITE(6,500)	PTCN1289
	RETURN	PTCN1290
	410 IRET=-7	PTCN1291
	IF(IWRITE,GE,1)WRITE(6,510)	PTCN1292
	RETURN	PTCN1293
	420 IRET=-8	PTCN1294
	IF(IWRITE,GE,1)WRITE(6,520)	PTCN1295
	RETURN	PTCN1296
	430 IRET=-9	PTCN1297
	IF(IWRITE,GE,1)WRITE(6,530)	PTCN1298
	RETURN	PTCN1299
	440 IRET=-10	PTCN1300
	IF(IWRITE,GE,1)WRITE(6,540)NVAR,ISIZE	PTCN1301
	RETURN	PTCN1302
	450 FORMAT(26HOLIMIT POINT FINDER FAILED)	PTCN1303
	460 FORMAT(50HOCORECT, SEEKING TARGET POINT, TOOK TOO MANY STEPS)	PTCN1304
	470 FORMAT(50HOCORECT, SEEKING TARGET, CALLED SOLVE WHICH FAILED)	PTCN1305
	480 FORMAT(45HOCORECT, SEEKING TARGET, FAILED WITH RAD STEP)	PTCN1306
	490 FORMAT(10H0STEP SIZE ,F12.7,15H LESS THAN HMIN,F12.7)	PTCN1307
	500 FORMAT(42HONORM OF F(X) IS TOO LARGE ON INITIAL CALL)	PTCN1308
	510 FORMAT(33H0SOLVE FAILED IN CALL FROM TANGNT)	PTCN1309
	520 FORMAT(33H0SOLVE FAILED IN CALL FROM CORECT)	PTCN1310
	530 FORMAT(23H0TANGENT VECTOR IS ZERO)	PTCN1311
	540 FORMAT(26H0UNACCEPTABLE INPUT NVAR=,I10,7H ISIZE=,I10)	PTCN1312
	550 FORMAT(36H ANGLE BETWEEN OLD AND NEW TANGENTS=,F12.5)	PTCN1313
	560 FORMAT(9H CURVCF =,E14.6,9H CURVXF =,E14.6)	PTCN1314
	570 FORMAT(16H USING STEP SIZE=,F12.5)	PTCN1315
	580 FORMAT(12H PREDICTED X/1X,5F12.5)	PTCN1316
	590 FORMAT(1H ,I2,16H STEP REDUCTIONS)	PTCN1317
	600 FORMAT(7H OMEGA=,F12.5,7H THETA=,F12.5,9H NEW RAD=,F12.5)	PTCN1318
	610 FORMAT(31H TANGNT ANTICIPATES LIMIT POINT)	PTCN1319
C		PTCN1320
C	*****	PTCN1321
C		PTCN1322
	END	PTCN1323
		PTCN1324


```

C
C ITERATION LOOP
C
C      DO 20 I=1, KNMAX
C          KN=I
C          CALL SOLVE(NVAR,X,WORK,IMHOLD,DETA,IEXP,IERR,ICALL,IMOD,FPRYM,
1          IPVT)
C          ICRSL=ICRSL+1
C          IF(IMOD.EQ.1)ICALL=0
C          ISOLVE=ISOLVE+1
C          IF(IERR.NE.0) GO TO 50
C          FNRML=FNRM
C          XSTEPL=XSTEP
C          CALL SAXPY(NVAR,-1.0,WORK,1,X,1)
C          IMAX=ISAMAX(NVAR,WORK,1)
C          XSTEP=ABS(WORK(IMAX))
C          IMAX=ISAMAX(NVAR,X,1)
C          XNRM=ABS(X(IMAX))
C          CALL FCTN(NVAR,X,WORK)
C          IFEVAL=IFEVAL+1
C          IMAX=ISAMAX(NVAR,WORK,1)
C          FNRM=ABS(WORK(IMAX))
C          WORK(NVAR)=0.0
C
C ACCEPTANCE TEST
C
C          IF (FNRM.IE.EPSATE) GO TO 60
C          IF (FNRM.GT.ABSERR) GO TO 10
C          IF (XSTEP.LE.(ABSERR+RELERR*XNRM)) GO TO 60
C
C REJECTION TEST
C
C      10      IF (KN.GT.1.AND.XSTEP.GT.(FMP*XSTEPL)) GO TO 30
C          IF (FNRM.GT.(FMP*FNRML)) GO TO 30
C      20      FMP=1.05
C          GO TO 40
C
C UNSUCCESSFUL STEP
C
C      30 IERR=-3
C          IF(IWRITE.EQ.2)WRITE(6,120)
C          GO TO 70
C
C MAXIMUM NUMBER OF CORRECTOR STEPS REACHED
C
C      40 IERR=-2
C          IF(IWRITE.EQ.2)WRITE(6,110)
C          GO TO 70
C
C ERROR RETURN IN SOLVE
C
C      50 IERR=-1
C          IF(IWRITE.EQ.2)WRITE(6,100)
C          GO TO 70
C
C SUCCESSFUL STEP
C
C      60 IERR=0
C      70 KNSUM=KNSUM+KN
C          IF(IWRITE.EQ.2)WRITE(6,80) KN,XSTEP
C          IF(IWRITE.EQ.2)WRITE(6,90)IMHOLD
C          RETURN
C      80 FORMAT(13H CORECT TOOK ,I2,21H STEPS, LAST ONE WAS ,E12.5)
C      90 FORMAT(14H CORECT IMHOLD=,I3)
C     100 FORMAT(31HOSOLVE FAILED, CALLED BY CORECT)
C     110 FORMAT(25HOTOO MANY CORRECTOR STEPS)
C     120 FORMAT(24HOCORRECTOR STEP REJECTED)
C
C *****
C
C      END

```

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CRCT0071
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CRCT0141

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SUBROUTINE TANGNT(NVAR,X,IP,TAN,IRET,ICALL,FPRYM,IPUT,NEQN,DETA,  TNGN0001
1 IEXP)  TNGN0002
C*****  TNGN0003
C*****  TNGN0004
C*****  TNGN0005
C SURROUTINE TANGNT COMPUTES THE UNIT TANGENT VECTOR TO THE SOLUTION  TNGN0006
C CURVE OF THE UNDERDETERMINED NONLINEAR SYSTEM  $FX = 0$ . THE  TNGN0007
C TANGENT VECTOR TAN IS THE SOLUTION OF THE LINEAR SYSTEM  TNGN0008
C  TNGN0009
C      DFA(X,IPL)*TAN = E(NVAR)  TNGN0010
C  TNGN0011
C WHERE DFA(X,IPL) IS THE NVAR BY NVAR MATRIX WHOSE FIRST NVAR-1 ROWS  TNGN0012
C ARE DFX/DX (X), THE DERIVATIVE OF FX EVALUATED AT X, AND WHOSE LAST  TNGN0013
C ROW IS (E(IPL)) TRANSPOSE, THE NVAR COMPONENT EUCLIDEAN COORDINATE  TNGN0014
C VECTOR WITH 1 IN THE IPL-TH POSITION AND ZEROS ELSEWHERE. E(NVAR) IS  TNGN0015
C THE NVAR COMPONENT EUCLIDEAN COORDINATE VECTOR WITH ONE IN THE  TNGN0016
C LAST COMPONENT.  TNGN0017
C THE TANGENT VECTOR IS THEN NORMALIZED AND ITS SIGN ADJUSTED.  TNGN0018
C  TNGN0019
C INPUT  TNGN0020
C NVAR = THE NUMBER OF VARIABLES  TNGN0021
C X = THE CURRENT CONTINUATION POINT  TNGN0022
C IP = CONTINUATION COMPONENT SET ON LAST STEP  TNGN0023
C  TNGN0024
C OUTPUT  TNGN0025
C TAN = THE UNIT TANGENT VECTOR IN CONTINUATION DIRECTION AT X  TNGN0026
C DETA = BINARY MANTISSA OF DETERMINANT OF JACOBIAN DFA(X,IPL)  TNGN0027
C IEXP = BINARY EXPONENT OF THE DETERMINANT OF JACOBIAN DFA(X,IPL)  TNGN0028
C IP = LOCATION OF LARGEST COMPONENT OF TANGENT VECTOR TAN  TNGN0029
C CANDIDATE FOR NEW CONTINUATION COMPONENT  TNGN0030
C  TNGN0031
C THIS SUBROUTINE IS CALLED BY  TNGN0032
C PITCON  TNGN0033
C AND CALLS  TNGN0034
C SOLVE  TNGN0035
C LINPAK ISAMAX  TNGN0036
C LINPAK SNRM2  TNGN0037
C LINPAK SSCAL  TNGN0038
C  TNGN0039
C*****  TNGN0040
C  TNGN0041
C REAL X(NVAR),TAN(NVAR),FPRYM(NVAR,NVAR)  TNGN0042
C INTEGER IPUT(NVAR)  TNGN0043
C COMMON /COUNT1/ ICRSL,ITNSL,NSTCR,NCMCR,NTRCR,NLMCR,NLMRT  TNGN0044
C COMMON /COUNT2/ IFEVAL,IPEVAL,ISOLVE,NRED,NRDSUM,KN,KNSUM  TNGN0045
C COMMON /OUTPUT/ IWRITE  TNGN0046
C  TNGN0047
C COMPUTE TANGENT VECTOR  TNGN0048
C  TNGN0049
C DO 10 I=1,NEQN  TNGN0050
C 10 TAN(I)=0.0  TNGN0051
C TAN(NVAR)=1.0  TNGN0052
C IERR=0  TNGN0053
C CALL SOLVE(NVAR,X,TAN,IP,DETA,IEXP,IERR,ICALL,IMOD,FPRYM,  TNGN0054
C 1 IPUT)  TNGN0055
C ITNSL=ITNSL+1  TNGN0056
C ISOLVE=ISOLVE+1  TNGN0057
C IF (IERR.NE.0) IRET=-1  TNGN0058
C IF (IRET.LT.0) RETURN  TNGN0059
C  TNGN0060
C OBTAIN EUCLIDEAN NORM OF TANGENT VECTOR  TNGN0061
C  TNGN0062
C IP=ISAMAX(NVAR,TAN,1)  TNGN0063
C TNORM=SNRM2(NVAR,TAN,1)  TNGN0064
C IF (TNORM.EQ.0.0) IRET=-2  TNGN0065
C IF (IRET.LT.0) RETURN  TNGN0066
C  TNGN0067
C NORMALIZE THE VECTOR  TNGN0068
C  TNGN0069
C .SCALER=1.0/TNORM  TNGN0070
C CALL SSCAL(NVAR,SCALER,TAN,1)  TNGN0071
C RETURN  TNGN0072
C  TNGN0073
C*****  TNGN0074
C  TNGN0075
C END  TNGN0076

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SUBROUTINE ROOT(A,FA,B,FR,C,FC,KOUNT,IFLAG)
C
C*****
C
C SUBROUTINE ROOT SEEKS A ROOT OF THE EQUATION F(X)=0.0,
C GIVEN A STARTING INTERVAL (A,C) ON WHICH F CHANGES SIGN.
C ON FIRST CALL TO ROOT, THE INTERVAL AND FUNCTION VALUES
C FA AND FC ARE FED IN AND AN APPROXIMATION B FOR THE ROOT IS RETURNED.
C BEFORE EACH SUBSEQUENT CALL, THE USER EVALUATES FR=F(B), AND THE
C PROGRAM TRIES TO RETURN A BETTER APPROXIMATION B.
C
C THIS PROGRAM IS BASED ON THE FORTRAN FUNCTION ZERO
C GIVEN IN THE BOOK:
C 'ALGORITHMS FOR MINIMIZATION WITHOUT DERIVATIVES'
C BY RICHARD P. BRENT, PRENTICE HALL, INC, 1973
C
C THE MODIFICATIONS WERE DONE BY JOHN BURKARDT.
C
C ON INPUT:
C
C A - IS ONE ENDPOINT OF AN INTERVAL IN WHICH F CHANGES SIGN.
C FA - THE VALUE OF F(A). THE USER MUST EVALUATE F(A) BEFORE FIRST
C CALL ONLY. THEREAFTER THE PROGRAM SETS FA.
C B - ON FIRST CALL, B SHOULD NOT BE SET BY THE USER.
C ON SUBSEQUENT CALLS, B SHOULD NOT BE CHANGED
C FROM ITS OUTPUT VALUE, THE CURRENT APPROXIMANT
C TO THE ROOT.
C FB - ON FIRST CALL, FB SHOULD NOT BE SET BY THE USER.
C THEREAFTER, THE USER SHOULD EVALUATE THE FUNCTION
C AT THE OUTPUT VALUE B, AND RETURN FR=F(B).
C C - IS THE OTHER ENDPOINT OF THE INTERVAL IN WHICH
C F CHANGES SIGN. NOTE THAT THE PROGRAM WILL RETURN
C IMMEDIATELY WITH AN ERROR FLAG IF FC*FA.GT.0.0.
C FC - THE VALUE OF F(C). THE USER MUST EVALUATE F(C) BEFORE FIRST
C CALL ONLY. THEREAFTER THE PROGRAM SETS FC.
C KOUNT - A COUNTER FOR THE NUMBER OF CALLS TO ROOT. KOUNT
C SHOULD BE SET TO ZERO ON THE FIRST CALL FOR A GIVEN
C ROOT PROBLEM.
C IFLAG - AN ERROR RETURN FLAG WHOSE INPUT VALUE IS IMMATERIAL.
C
C ON RETURN FROM A CALL TO ROOT
C
C A - ONE ENDPOINT OF CHANGE OF SIGN INTERVAL.
C FA - THE VALUE OF F(A).
C B - CURRENT APPROXIMATION TO THE ROOT. BEFORE ANOTHER
C CALL TO ROOT, EVALUATE F(B).
C FB - FB WILL BE OVERWRITTEN BY THE USER BEFORE ANOTHER
C CALL. ITS VALUE ON RETURN IS ONE OF FA, FR OR FC.
C C - OTHER ENDPOINT OF CHANGE IN SIGN INTERVAL.
C FC - THE VALUE OF F(C).
C KOUNT - CURRENT NUMBER OF CALLS TO ROOT.
C IFLAG - PROGRAM RETURN FLAG:
C IFLAG=-2 MEANS THAT ON FIRST CALL, FA*FC.GT.0.0.
C THIS IS AN ERROR RETURN, SINCE A BRACKETING
C INTERVAL SHOULD BE SUPPLIED ON FIRST CALL.
C IFLAG=-1 MEANS THAT THE CURRENT BRACKETING INTERVAL
C WHOSE ENDPOINTS ARE STORED IN A AND C
C IS SO SMALL (LESS THAN 4*EPMACH*ABS(B)+EPMACH)
C THAT B SHOULD BE ACCEPTED AS THE ROOT.
C THE FUNCTION VALUE F(B) IS STORED IN FB.
C IFLAG= 0 MEANS THAT THE INPUT VALUE FB IS EXACTLY
C ZERO, AND B SHOULD BE ACCEPTED AS THE ROOT.
C
C IFLAG.GT.0 MEANS THAT THE CURRENT APPROXIMATION TO
C THE ROOT IS CONTAINED IN B. IF A BETTER
C APPROXIMATION IS DESIRED, SET FR=F(B)
C AND CALL ROOT AGAIN. THE VALUE OF IFLAG INDICATES
C THE METHOD THAT WAS USED TO PRODUCE B.
C
C IFLAG= 1 BISECTION WAS USED.

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C          IFLAG= 2 LINEAR INTERPOLATION (SECANT METHOD).
C          IFLAG= 3 INVERSE QUADRATIC INTERPOLATION.
C
C LOCAL VARIABLES INCLUDE:
C
C EPMACH- SMALLEST POSITIVE NUMBER SUCH THAT 1.0+EPMACH.GT.1.0
C          .5*BETA**(1-TAU) FOR ROUNDED, TAU-DIGIT ARITHMETIC
C          BASE BETA. TWICE THAT VALUE FOR TRUNCATED ARITHMETIC.
C          THIS IS THE RELATIVE MACHINE PRECISION.
C HALFBC- SIGNED HALFWIDTH OF INTERVAL. DURING SEGMENT 3, THE
C          CHANGE OF SIGN INTERVAL IS (B,C) OR (C,R). THE MIDPOINT
C          OF THAT INTERVAL IS XMID=B+HALFBC, REGARDLESS OF ORIENTATION.
C SDEL1 - SIZE OF CHANGE IN SIGN INTERVAL.
C SDEL2 - PREVIOUS VALUE OF SDEL1.
C SDEL3 - PREVIOUS VALUE OF SDEL2.
C SDEL4 - PREVIOUS VALUE OF SDEL3.
C STEP - THE NEW ROOT IS COMPUTED AS A CORRECTION TO B OF THE
C          FORM B(NEW)=B(OLD)+STEP.
C TOLER - A NUMBER WE ACCEPT AS 'SMALL' WHEN EXAMINING INTERVAL
C          SIZE OR STEP SIZE. TOLER=2.0*EPMACH*ABS(B) + EPMACH IS
C          A MINIMUM BELOW WHICH WE WILL NOT ALLOW SUCH VALUES TO FALL.
C THIS SUBROUTINE IS CALLED BY
C PITCON
C AND CALLS
C FORTRAN ABS
C FORTRAN SIGN
C
C *****
C REAL A,B,C,FA,FR,FC,STEP,TOLER,P,Q,R,S
C COMMON /TOL/ EPMACH,EPSATE,EPSQRT
C
C SEGMENT 1: FIRST CALL HANDLED SPECIALLY. DO BOOKKEEPING.
C
C SET CERTAIN VALUES ONLY FOR INITIAL CALL WITH KOUNT=0
C
C IF (KOUNT.GT.0) GO TO 10
C IF (FA.GT.0.0.AND.FC.GT.0.0) GO TO 110
C IF (FA.LT.0.0.AND.FC.LT.0.0) GO TO 110
C KOUNT=1
C SDEL1=2.0*ABS(C-A)
C SDEL2=2.0*SDEL1
C SDEL3=2.0*SDEL2
C B=C
C FB=FC
C GO TO 20
C
C ON EVERY CALL, INCREMENT COUNTER
C
C 10 KOUNT=KOUNT+1
C
C RETURN IF HIT MACHINE ZERO FOR F(B)
C
C IF(FB.EQ.0.0) GO TO 90
C
C SEGMENT 2: REARRANGE POINTS AND FUNCTION VALUES IF
C NECESSARY SO THAT FB*FC.LT.0.0, AND SO THAT
C ABS(FB).LT.ABS(FC)
C
C IF((FB.LE.0.0).AND.(FC.GT.0.0)) GO TO 30
C IF((FB.GT.0.0).AND.(FC.LE.0.0)) GO TO 30
C
C FB AND FC ARE OF SAME SIGN.
C (ROOT CHANGED SIGN)
C OVERWRITE C WITH VALUE OF A
C
C 20 C=A
C FC=FA

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C
C IF NECESSARY, SET A:=B, B:=C, C:=B
C TO ENSURE THAT ABS(FB).LE.ABS(FC)
C
30 IF(ABS(FC).GE.ABS(FB)) GO TO 40
   A=B
   B=C
   C=A
   FA=FB
   FB=FC
   FC=FA
C
C SEGMENT 3: CHECK FOR ACCEPTANCE BECAUSE OF SMALL INTERVAL.
C CURRENT CHANGE IN SIGN INTERVAL IS (C,B) OR (B,C).
C
40 TOLER=2.0*EPMACH*ABS(B)+EPMACH
   HALFRC=0.5*(C-B)
   SDEL4=SDEL3
   SDEL3=SDEL2
   SDEL2=SDEL1
   SDEL1=ABS(C-B)
   IF(ABS(HALFRC).LE.TOLER) GO TO 100
C
C SEGMENT 4: COMPUTE NEW APPROXIMANT TO ROOT OF THE FORM
C B(NEW)=B(OLD)+STEP.
C METHODS AVAILABLE ARE LINEAR INTERPOLATION
C INVERSE QUADRATIC INTERPOLATION
C AND BISECTION.
C
   IF(ABS(FB).GE.ABS(FA))GO TO 70
   IF(A.NE.C) GO TO 50
C
C ATTEMPT LINEAR INTERPOLATION IF ONLY TWO POINTS AVAILABLE
C COMPUTE P AND Q FOR APPROXIMATION B(NEW)=B(OLD)+P/Q
C
   IFLAG=2
   S=FB/FA
   P=2.0*HALFRC*S
   Q=1.0-S
   GO TO 60
C
C ATTEMPT INVERSE QUADRATIC INTERPOLATION IF THREE POINTS AVAILABLE
C COMPUTE P AND Q FOR APPROXIMATION B(NEW)=B(OLD)+P/Q
C
50 IFLAG=3
   S=FB/FA
   Q=FA/FC
   R=FB/FC
   P=S*(2.0*HALFRC*Q*(R-R)-(B-A)*(R-1.0))
   Q=(Q-1.0)*(R-1.0)*(S-1.0)
C
C CORRECT THE SIGNS OF P AND Q
C
60 IF(P.GT.0.0)Q=-Q
   P=ABS(P)
C
C IF P/Q IS TOO LARGE, GO BACK TO BISECTION
C
   IF(8.0*SDEL1.GT.SDEL4) GO TO 70
   IF (P.GE.1.5*ABS(HALFRC*Q)-ABS(TOLER*Q)) GO TO 70
   STEP=P/Q
   GO TO 80
C
C PERFORM BISECTION:
C IF ABS(FB).GE.ABS(FA)
C OR INTERPOLATION IS UNSAFE (P/Q IS LARGE)
C OR IF THREE CONSECUTIVE STEPS H/VE NOT DECREASED
C THE SIZE OF THE INTERVAL BY A FACTOR OF 8.0
C
70 IFLAG=1
   STEP=HALFRC
   GO TO 80

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ROOT0139
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ROOT0199
ROOT0200
ROOT0201
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ROOT0203
ROOT0204
ROOT0205
ROOT0206
ROOT0207
ROOT0208
ROOT0209
ROOT0210

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C		ROOT0211
C	SEGMENT 5: VALUE OF STEP HAS BEEN COMPUTED.	ROOT0212
C	UPDATE INFORMATION: A:=B, FA:=FB, B:=B+STEP.	ROOT0213
C	CHANGE IN SIGN INTERVAL IS NOW (A,C) OR (C,A).	ROOT0214
C		ROOT0215
	80 A=B	ROOT0216
	FA=FB	ROOT0217
	IF(ABS(STEP).LE.TOLER) STEP=SIGN(TOLER,HALFRC)	ROOT0218
	B=B+STEP	ROOT0219
	RETURN	ROOT0220
C		ROOT0221
C	SPECIAL RETURNS	ROOT0222
C		ROOT0223
C	INPUT POINT B IS EXACT ROOT	ROOT0224
C		ROOT0225
	90 IFLAG=0	ROOT0226
	RETURN	ROOT0227
C		ROOT0228
C	CHANGE IN SIGN INTERVAL IS OF SIZE LESS THAN 4*EPMACH*ABS(B)+EPMACH	ROOT0229
C	INTERVAL RETURNED AS (B,C) OR (C,B).	ROOT0230
C	ACCEPT B AS ROOT WITH RESIDUAL F(B) STORED IN FB.	ROOT0231
C		ROOT0232
	100 IFLAG=-1	ROOT0233
	A=B	ROOT0234
	FA=FB	ROOT0235
	RETURN	ROOT0236
C		ROOT0237
C	CHANGE OF SIGN CONDITION VIOLATED	ROOT0238
C		ROOT0239
	110 IFLAG=-2	ROOT0240
	KOUNT=0	ROOT0241
	RETURN	ROOT0242
C		ROOT0243
C	*****	ROOT0244
C		ROOT0245
	END	ROOT0246

```

SUBROUTINE SOLVE(NVAR,X,Y,IP,DETA,IEXP,IERR,ICALL,IMOD,FPRYM,
1 IPVT)
C*****
C THIS SUBROUTINE IS CALLED BY
C CORECT
C TANGNT
C AND CALLS
C FORTRAN ABS
C LINPAK SGEFA
C LINPAK SGEFL
C USER FPRIME
C THIS SUBROUTINE SOLVES THE LINEAR SYSTEM DFA(X,IP)*YOUT = YIN
C WHERE DFA(X,IP) IS THE (NVAR)*X(NVAR) MATRIX WHOSE FIRST NVAR - 1
C ROWS ARE THE JACOBIAN COMPUTED BY FPRIME, AND WHOSE LAST
C ROW IS ALL 0 EXCEPT FOR A 1 IN THE IP-TH COMPONENT.
C YIN IS THE NVAR COMPONENT VECTOR Y ON INPUT, AND THE SOLUTION
C VECTOR YOUT IS RETURNED IN Y ON OUTPUT AFTER A SUCCESSFUL
C SETUP AND SOLUTION.
C **NOTE** SUBROUTINE SOLVE USES FULL MATRIX STORAGE TO SOLVE THE
C LINEAR SYSTEM. THE USER MAY WISH TO REPLACE THIS ROUTINE WITH
C ONE MORE SUITED TO HIS PROBLEM.
C DETA BINARY MANTISSA OF THE DETERMINANT OF JACOBIAN DFA(X,IP)
C IEXP BINARY EXPONENT OF THE DETERMINANT OF JACOBIAN DFA(X,IP)
C IMOD NEWTON METHOD FLAG.
C IMOD=0, JACOBIAN IS TO BE EVALUATED FOR EVERY CORRECTOR STEP
C AND EVERY TANGENT CALCULATION
C IMOD=1, JACOBIAN IS TO BE EVALUATED ONLY FOR FIRST CORRECTOR
C STEP, AND EVERY TANGENT CALCULATION
C ICALL SET UP FLAG.
C IF (ICALL.EQ.0.AND.IMOD.NE.0) DON'T RE-EVALUATED JACOBIAN
C INFO OUTPUT FROM SGEFA. IF INFO.NE.0, SGEFA FOUND A ZERO
C PIVOT WHEN ELIMINATING INFO-TH VARIABLE.
C IERR RETURN FLAG, 0 MEANS SUCCESSFUL SOLUTION, 1 MEANS FAILURE
C NVAR THE NUMBER OF VARIABLES IN THE NONLINEAR SYSTEM
C X THE POINT AT WHICH TO EVALUATE FPRYM
C Y THE RIGHT HAND SIDE ON INPUT, THE SOLUTION
C ON OUTPUT
C FPRYM ARRAY WHERE DFA(X,IP) IS TO BE STORED.
C IPVT INTEGER WORK SPACE FOR PIVOT ROW SWITCHES DEMANDED BY SGEFA
C IP THE VARIABLE USED IN THE AUGMENTING EQUATION THAT IS OF THE
C FORM X(IP)=B. HENCE THE LAST ROW OF DFA(X,IP) IS ALL
C ZERO EXCEPT FOR A 1.0 IN THE IP-TH COLUMN.
C*****
C REAL X(NVAR),Y(NVAR),FPRYM(NVAR,NVAR)
C INTEGER IPVT(NVAR)
C COMMON /COUNT2/ IFEVAL,IPEVAL,ISOLVE,NRED,NRDSUM,KN,KNSUM
C DEPENDING ON VALUES OF ICALL AND IMOD, EITHER SET UP
C AUGMENTED JACOBIAN, DECOMPOSE INTO L-U FACTORS, AND GET DETERMINANT,
C OR USE CURRENT FACTORED JACOBIAN WITH NEW RIGHT-HAND SIDE.
C IF (ICALL.EQ.0.AND.IMOD.NE.0) GO TO 50
C CALL FPRIME(NVAR,X,FPRYM)
C IPEVAL=IPEVAL+1
C DO 10 I=1,NVAR
C 10 FPRYM(NVAR,I)=0.0
C FPRYM(NVAR,IP)=1.0
C CARRY OUT IN CORE LU DECOMPOSITION OF NVAR BY NVAR MATRIX
C AND USE PIVOT INFORMATION TO COMPUTE DETERMINANT

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SLVE0001
SLVE0002
SLVE0003
SLVE0004
SLVE0005
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SLVE0060
SLVE0061
SLVE0062
SLVE0063
SLVE0064
SLVE0065
SLVE0066
SLVE0067
SLVE0068

```

C	CALL SGEFA(FPRYM,NVAR,NVAR,IPUT,INFO)	SLVE0069
	DETA=1.0	SLVE0070
	IEXP=0	SLVE0071
	TWO=2.0	SLVE0072
	DO 40 I=1,NVAR	SLVE0073
	IF (IPUT(I).NE.I) DETA=-DETA	SLVE0074
	DETA=FPRYM(I,I)*DETA	SLVE0075
	IF (DETA.EQ.0.0) GO TO 60	SLVE0076
20	IF (ABS(DETA).GE.1.0) GO TO 30	SLVE0077
	DETA=DETA*TWO	SLVE0078
	IEXP=IEXP-1	SLVE0079
	GO TO 20	SLVE0080
30	IF (ABS(DETA).LT.TWO) GO TO 40	SLVE0081
	DETA=DETA/TWO	SLVE0082
	IEXP=IEXP+1	SLVE0083
	GO TO 30	SLVE0084
40	CONTINUE	SLVE0085
	IF (INFO.NE.0) GO TO 60	SLVE0086
C		SLVE0087
C	USING L-U FACTORED MATRIX, SOLVE SYSTEM USING FORWARD-BACKWARD	SLVE0088
C	ELIMINATION, AND OVERWRITE RIGHT HAND SIDE WITH SOLUTION	SLVE0089
C		SLVE0090
	50 CALL SGESL(FPRYM,NVAR,NVAR,IPUT,Y,0)	SLVE0091
	IERR=0	SLVE0092
	RETURN	SLVE0093
60	IERR=1	SLVE0094
	INFO=0	SLVE0095
	RETURN	SLVE0096
C		SLVE0097
C	*****	SLVE0098
		SLVE0099
		SLVE0100
	END	SLVE0101

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