## A METHOD FOR THE NUMERICAL DETERMINATION OF BIFURCATION STATES OF NONLINEAR SYSTEMS OF EQUATIONS\*

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**Abstract.** A numerical technique is presented for determining a simple turning point in a branch of solutions of an algebraic system of equations depending on a scalar parameter. Results are given from testing the method on discrete versions of several mildly nonlinear boundary value problems to determine turning points in the positive solution branch.

1. Introduction. We wish to describe a numerical technique for analyzing a simple form of singular behavior in the solutions of nonlinear algebraic systems of equations. Consider such a system of N equations for an unknown N-vector, u, which depends on a scalar parameter,  $\lambda$ :

$$(1.1) A(u,\lambda) = 0.$$

A solution "curve,"  $u(\lambda)$ , which varies continuously with  $\lambda$  is called a branch of solutions. As a function of  $\lambda$ ,  $u(\lambda)$  will, in general, be multiple-valued and can exhibit complex behavior involving changing of its multiplicity (see [13] and its extensive bibliography). We shall treat a simple common case here, which we shall refer to as a turning point in the branch.

DEFINITION.  $\bar{\lambda}$  is a turning point of (1.1) if for every sufficiently small neighborhood of  $\lambda$ :

- (a) (1.1) has a continuous branch of solutions  $(\lambda, u(\lambda))$  through  $(\bar{\lambda}, u(\bar{\lambda}))$ ,
- (b) for  $(\lambda, u(\lambda))$  on the branch of (a),  $\lambda \leq \overline{\lambda}$  (turning to the left) or  $\lambda \geq \overline{\lambda}$  (turning to the right).

The problem that we wish to tackle, then, is the numerical determination of the turning points of a solution branch.

If the Jacobian matrix of A with respect to u is denoted by  $A_u(u, \lambda)$ , then the eigenvalues of  $A_u(w, \rho)$  can be designated by  $\mu_i(w, \rho)$ . It is well known [8] that if  $\bar{\lambda}$  is a turning point of (1.1), then

(1.2) 
$$\mu_k(u(\bar{\lambda}), \bar{\lambda}) = 0 \quad \text{for some } k.$$

Hence the problem of determining the turning points of branches of solutions of (1.1) can be viewed as a special case of solving (1.1) and (1.2) simultaneously. This is the basis of the method described here, and we assume throughout that  $A_u(u(\lambda), \lambda)$  is a symmetric matrix.

Such turning points occur in boundary value problems (with u being a function) for the equilibrium states of nonlinear systems (elasticity [1], [2], fluid mechanics [3], or nonlinear diffusion processes [4], [5]). They mark the loss (or gain) of dynamic stability of such states as the parameter  $\lambda$  varies [5]. We intend the method to be able to analyze discretized versions of such problems and have tested it on

<sup>\*</sup> Received by the editors February 13, 1974.

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problems with u being a function defined on a finite difference grid in the x-y plane and

(1.3) 
$$A(u,\lambda) = \Delta_h u + \lambda f(u).$$

Here  $\Delta_h$  represents a finite difference version of the Laplacian and f(y) is an increasing function of y. These problems are discrete versions of mildly nonlinear eigenvalue problems and the relation of their solution branches to the solution branches of their continuous counterparts has been studied by S. V. Parter in [6] and [7] and the author in [12] and [13].

Extensive numerical computations by a different approach to problems (1.3) have been reported by J. B. Rosen in [11]. The technique provides numerical solutions and error bounds for equations with a monotonicity property. This property holds for the minimal positive solution of a branch of positive solutions of (1.1) and is lost at  $\lambda = \bar{\lambda}$ . Hence upper bounds for  $\bar{\lambda}$  were obtained in [11] by observing the  $\lambda$  values for which the technique failed. The problem of computing a solution branch in the presence of a turning point has also been treated by Anselone and Moore in [1], and by Thurston in [15], from the point of view of getting past the turning point to the rest of the solution branch.

2. The method. In this section, we describe a numerical method for computing turning points of branches of nonlinear systems as discussed in the preceding section. This is done in three subsections after presenting the viewpoint and background assumptions: two sections on a mathematical description of the method and one on some details of its implementation for the experiments reported on.

We assume that rough quantitative knowledge of the turning point has been obtained, i.e., an estimate of  $\bar{\lambda}$  and whether the branch turns to the left  $(u(\lambda))$  is defined for  $\bar{\lambda} - \varepsilon \leq \lambda \leq \bar{\lambda}$  or the right. Some analytic techniques are available for this purpose [4], [5]. In the examples presented this was done by scanning the branch for a choice of  $\lambda$  values using Newton's method. We shall describe the method as applied to turning points turning to the left in this section.

It is based on an inverse interpolation technique for solving

$$\mu(u(\bar{\lambda}), \bar{\lambda}) = 0$$

(here we have suppressed the subscript of the eigenvalue  $\mu$ ) where  $\mu(u(\lambda), \lambda)$  is a "multivalued function" of  $\lambda$  as indicated by the solid line of Fig. 1 in § 3.

**2.1. Modified inverse interpolation.** For the *j*th step of the iterative procedure for solving (2.1), three current points on the graph of  $\mu(u(\lambda), \lambda)$  are retained  $(\lambda_j, \mu_j)$ ,  $(\lambda_{j+1}, \mu_{j+1}), (\lambda_{j+2}, \mu_{j+2})$ . The inverse data  $(\mu_i, \lambda_i)$  i = j, j+1, j+2 is interpolated by a quadratic,  $P_2(\mu)$ , and the next estimate of  $\bar{\lambda}$ ,  $\lambda_{j+3}$  is calculated as

$$\lambda_{j+3} = \alpha P_2(0) + (1-\alpha)\lambda_j$$

for some parameter value,  $\alpha$ ,  $0 < \alpha < 1$ .

One must ensure, of course, that  $\lambda_{j+3} < \bar{\lambda}$ , and this is the function of the parameter  $\alpha$ . In Lemma 1, it is stated that the  $\lambda_j$  converge monotonely to  $\bar{\lambda}$  under suitable conditions. Strictly speaking, to get monotonicity, a reassignment of indices j+1, j+2, j+3 may be necessary after each step. These conditions refer

to  $\lambda(\mu)$  as the inverse function to  $\mu(u(\lambda), \lambda)$  and require

(2.3a) 
$$\max \left| \frac{d^3 \lambda(\mu)}{d\mu^3} \right| \le K_3$$

and

where the maxima are taken for  $|\mu(\lambda_1)| \le |\mu| \le |\mu(\bar{\lambda})|$ .

LEMMA 1. Let  $k=K_3(2M_2)^{3/2}/6$  and  $\lambda_4$  be defined by (2.2) with  $\lambda_1 \le \lambda_2 \le \lambda_3 < \bar{\lambda}$ . If

$$(2.4) k(\bar{\lambda} - \lambda_1)^{1/2} = \rho < 1,$$

then for  $0 < \alpha < 1/(1 + \rho)$ ,

$$\lambda_1 < \lambda_4 < \bar{\lambda}.$$

The  $\lambda_j$  converge to  $\bar{\lambda}$  with linear asymptotic convergence rate  $= 1 - \alpha$ . (Proof is in Appendix A.) One could vary  $\alpha$  with j so that  $\alpha_j \to 1$  as  $j \to \infty$ ; however in the experiments tried a constant  $\alpha$  was used, in the range, .85 to .97 usually.

**2.2.** Evaluation of  $\mu(u(\lambda), \lambda)$ . The process just described requires the evaluation of  $\mu(u(\lambda), \lambda)$  for given  $\lambda$ . This involves solving

$$(2.6) A(u(\lambda), \lambda) = 0$$

for  $u(\lambda)$  and calculating the relevant eigenvalue  $\mu$  of  $A_u(u(\lambda), \lambda)$ . To accomplish this, we exploit some properties of Newton's method observed by Rall [10] generalizing the well-known behavior of Newton's method for multiple roots of a scalar equation.

The results pertinent to this discussion can be qualitatively summarized as follows. Suppose that  $A_u(w, \lambda)$  is symmetric; that  $\lambda$  is set to  $\bar{\lambda}$  and hence (2.6) has  $\bar{u}(\bar{\lambda})$  as a multiple solution; and suppose that Newton's method for (2.6) produces  $\{u_n(\bar{\lambda})\}$  which converges to  $\bar{u}(\bar{\lambda})$ .

If we let  $e_n$  be the error in  $u_n(\bar{\lambda})$ , i.e.,

$$(2.7) e_n = u_n(\bar{\lambda}) - \bar{u}(\bar{\lambda}),$$

then the components of  $e_n$  in the directions of the nullspace of  $A_u(\bar{u}, \bar{\lambda})$  are reduced at a linear rate, while those in the orthogonal complement are reduced at a quadratic rate.

If we are using  $\lambda$  near  $\bar{\lambda}$ , we could expect that similar behavior of the error in the Newton iterates would occur, i.e., that as the error  $e_n$  decreases, its direction is predominantly in the eigenspace of  $\mu(u(\lambda), \lambda)$ , (the eigenvalue of  $A_u(u(\lambda), \lambda)$  closest to zero). Although we would not know the error in the *n*th iterate  $e_n$ , we could expect that

$$(2.8) c_n = u_{n+1}(\lambda) - u_n(\lambda) \cong e_n,$$

i.e., that the correction to the *n*th iterate has predominantly the direction of the eigenspace referred to above. This vector is therefore put into the Rayliegh quotient for  $A_{\mu}(u(\lambda), \lambda)$  to give an approximate value for  $\mu(\lambda)$ . In practice, its direction could

be improved somewhat by several steps of the inverse power technique for calculating eigenvalues.

In principle, the *n*th step of Newton's method for calculating  $\mu(u(\lambda), \lambda)$  from a given  $\lambda \cong \bar{\lambda}$  could be described by (2.9). In (2.9) we are using square brackets [w, v] to denote the inner product of vectors w and v,

(2.9) 
$$A_{u}(u_{n}(\lambda), \lambda)c_{n} = -A(u_{n}(\lambda), \lambda) \equiv r_{n},$$

$$\mu_{n} = \frac{[c_{n}, A_{u}(u_{n}(\lambda), \lambda)c_{n}]}{[c_{n}, c_{n}]} = \frac{[c_{n}, r_{n}]}{[c_{n}, c_{n}]},$$

$$u_{n+1}(\lambda) = u_{n}(\lambda) + c_{n},$$

with  $u_n(\lambda)$  converging to  $u(\lambda)$  and  $\mu_n$  converging to  $\mu(u(\lambda), \lambda)$  for a successful implementation.

**2.3. Implementation details.** In implementing (2.9), one might anticipate that if Newton's method is continued until  $c_n$  is quite small, or effectively stops decreasing, then the direction of  $c_n$  would be heavily contaminated by roundoff effects, and in particular, might not be primarily in the eigenspace of  $\mu(u(\lambda), \lambda)$ . Hence (2.9) was terminated while  $c_n$  was still several orders of magnitude larger than the machine resolution of  $u_n$ .

When (2.9) was terminated, a couple of steps of the inverse power method using the fixed matrix  $A_u(u(\lambda), \lambda)$  for computing  $\mu$  were taken to improve the numerical value of  $\mu$  somewhat. Typically this resulted in about a 10% correction in the computed value of  $\mu$ . (See Table 1.)

In Newton's method, and the inverse power process, a linear system of equations must be solved with a sparse, symmetric matrix of coefficients which may not be positive definite. The system was solved using a Gaussian elimination program for band matrices which performed partial pivoting (GELB of the IBM Scientific Subroutine Package). In no runs did the program warning parameter signal the possible loss of significant digits.

Lemma 1 indicates that  $\lambda_1 < \lambda_4 < \bar{\lambda}$ , but does not give the relation between  $\lambda_2$ ,  $\lambda_3$  and  $\lambda_4$ . In this implementation, a three-vector  $(\lambda(1), \lambda(2), \lambda(3))$  is retained, but not in order. Instead, a variable, irepl, is maintained so that  $\lambda$ (irepl) is the least of the  $\lambda$  values at each stage (or the greatest for turning to the right). After  $\lambda_4$  is computed, it replaces  $\lambda$ (irepl) and, after  $\mu(u(\lambda_4), \lambda_4)$  is computed, irepl is recomputed.

In the discussion of Newton's method in the preceding section, the topic of starting values was omitted. One could retain  $u(\lambda_1)$ ,  $u(\lambda_2)$  and  $u(\lambda_3)$  and if, e.g.,  $\lambda_2$  were being replaced by  $\lambda_4$ , use  $u(\lambda_2)$  as the starting value for calculating  $u(\lambda_4)$ . Rather than retain  $u(\lambda_i)$ , i = 1, 2, 3, we made a least squares fit using two parameters

$$(2.10) A(\lambda_i)\phi_1 + B(\lambda_i)\phi_2$$

for each  $u(\lambda_i)$  and retained  $A(\lambda_i)$  and  $B(\lambda_i)$ . The shape functions  $\phi_1$  and  $\phi_2$  are discussed below.

The program was written to identify vectors u and c as mesh functions defined on a subset of a square mesh of spacing h on the unit square  $0 \le x \le 1, 0 \le y \le 1$ . This is a natural identification for boundary value problems in two independent variables; but, of course, other problems can be adapted to it. The submesh used is

described by two variables, RBOTM and RTOP indicating that the lines  $Y_{\text{bot}} = (\text{RBOTM} - 1)h$  and  $Y_{\text{top}} = (\text{RTOP} - 1)h$  are the bottom and top mesh boundary rows; and by two functions of y.  $f_l(y)$  and  $f_r(y)$ . The mesh subregion then is

$$\{(i-1)h, (j-1)h|i, j \text{ positive integers RBOTM} < j < \text{RTOP},$$
  
 $f((i-1)h) < (i-1)h < f((i-1)h)\}.$ 

The shape functions,  $\phi_1$  and  $\phi_2$ , used in the least squares fitting process then are the restrictions to the mesh of

(2.11) 
$$\phi_i(x, y) = (y - (RBOTM - 1)h)((RTOP - 1)h - y) \times (x - f_i(y))(f_r(y) - x)\cos(\pi\alpha_i x)\cos(\pi\alpha_i y)$$

where  $\alpha_i$ , i=1,2, are chosen to suit the symmetries of the problem at hand. The least squares parameters for the solutions are stored and used to generate initial guesses when required; they are printed out to provide a compact description of the solution branch (see Table 3, § 3), and they are used to generate initial guesses for subsequent runs. A schematic flow chart of the method with some comments on its implementation are given in Appendix B.

3. Some experiments. The method was tested on some finite difference versions of the mildly nonlinear boundary value problem for plane regions D,

(3.1) 
$$-\Delta u(x) = \lambda f(u(x)), \quad x \in D,$$
$$u(x) = 0, \qquad x \in \partial D,$$

The results reported on here are for:

- (A) D unit square  $(0 \le y \le 1; 0 = f_l(y) \le x \le f_r(y) = 1)$  and  $f(u) = e^u$ ,
- (B)  $D \text{six-sided region bounded by } y = 0; \ y = 1; \ x = f_l(y) \equiv \max(0, y \frac{1}{2}); \ x = f_r(y) = \min(y + \frac{1}{2}, 1); \ \text{and} \ f(u) = e^u,$
- (C) D unit square and  $f(u) = 1 + (u + u^2/2)/(1 + u^2/100)$ .

For problems (A) and (C) involving the unit square, an  $O(h^4)$  discretization was used ( $h \equiv$  the uniform mesh spacing). If  $\Box_h$  is used to denote the nine-point box form of the discrete Laplacian, and  $\Delta_h$  denotes the five-point discrete Laplacian, the algebraic system has the form

$$\Box_{h}U + \lambda \left( f(U) + \frac{h^{2}}{12} \Delta_{h} f(U) \right) = 0$$

for mesh function U. Alternative approaches to obtaining fourth and higher order accuracy for nonlinear boundary value problems are discussed in [9].

In Fig. 1 and Tables 1 and 2, we show some results from Problem A which are typical of the relation of  $\mu(u(\lambda), \lambda)$  to  $\lambda$  for these problems. The data used in Fig. 1 was obtained from two separate runs each using h = 1/16. In Table 1, part of the printout monitoring the progress of Newton's method and the inverse power method is shown. In Table 2, the later iterates of the modified inverse interpolation process for solving (2.1) are shown, (for this run  $\alpha$  was set = .9).

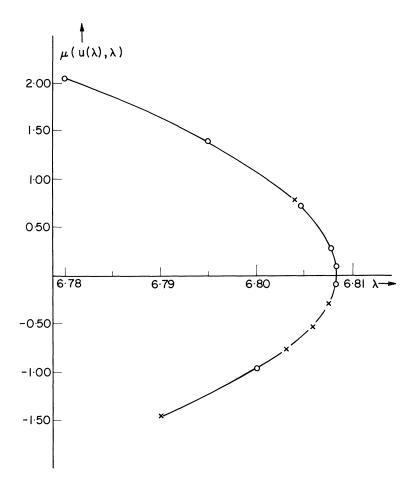


Fig. 1. Variation of the critical eigenvalue  $\mu(u(\lambda), \lambda)$  with  $\lambda$  for problem A.  $\times$ ,  $\bigcirc$  denote different runs.

The nonlinearity  $f(u) = e^u$  results in a unique turning point to the left in the branch of positive solutions to problems A and B. These two branches near their turning points are graphed in Fig. 2.

The nonlinearity in problem C is convex for small u, changing to concave for large u. The branch of positive solutions and the variation of the critical (=lowest) eigenvalue  $\mu(u(\lambda), \lambda)$ , with  $\lambda$  are graphed in Fig. 3.

The solution branch shows two turning points, the "lower" one to the left at  $\bar{\lambda}_1 = 7.957$  and the "upper" one to the right at  $\bar{\lambda}_2 = 6.423$ . As the branch turns to the left at  $\lambda = \bar{\lambda}_1$ , the critical eigenvalue becomes positive, indicating that the corresponding solutions have become dynamically unstable. As the branch turns to the right at  $\lambda = \bar{\lambda}_2$ , the critical eigenvalue becomes negative once more. Hence this boundary value problem is a model for a system which has two stable steady stables, a lower one existing for  $0 < \lambda < \bar{\lambda}_1$  and an upper one existing for  $\lambda > \bar{\lambda}_2$ .

Table 1

Reproduction of printout from monitoring method for two successive values of  $\lambda$  (problem A)

	Newton's Method for $\lambda =$	6.80814				
Iteration Number	Eigenvalue Estimate	Size of Newton Correction				
1	-158.2927	1.595E-01				
2	0.0481	2.421E-02				
3	0.1429 5.7431					
4	0.1349 5.554E-03					
	Inverse Iteration Phase for $\lambda$	= 6.80814				
Iteration Number	Eigenvalue Estimate					
1	0.1349					
2	0.1236					
3	0.1236					
$\lambda = 6.80814$	$u_{\text{max}} = 1.2742$					
	Newton's Method for $\lambda =$	6.80817				
Iteration Number	Eigenvalue Estimate	Size of Newton Correction				
1	-153.9710	1.560E-01				
2	0.1004	2.804E-02				
3	0.1438	1.862E-02				
	Inverse Iteration Phase for $\lambda$	= 6.80817				
Iteration Number	Eigenvalue Estimate					
1	0.1438					
2	0.1048					
3	0.1048					
$\lambda = 6.80817$	$u_{\rm max}=1.2732$					

The numerical estimates of the turning points discussed above are

Problem A 
$$\bar{\lambda}=6.8082$$
,  
Problem B  $\bar{\lambda}=9.64$ ,  
Problem C  $\bar{\lambda}_1=7.957$ ;  $\bar{\lambda}_2=6.423$ ,

The digits given are believed to be significant, based on running the problems with h=1/16 and h=1/21. The estimate for Problem A compares favorably with the upper bound for  $\bar{\lambda}$  of 6.81 obtained by J. B. Rosen [11].

As discussed in § 2.3, the program computes least square coefficients,  $A(\lambda)$ ,  $B(\lambda)$ , as brief summaries of  $u(\lambda)$ , the fitted forms being

$$u(x, y, \lambda) \cong \phi(x, y)(A(\lambda) + B(\lambda)\cos(a\pi x)\cos(a\pi y)),$$

with  $\phi(x, y) = (x - f_l(y))(f_r(y) - x)y(1 - y)$  and a = 3 for problems A and C and a = 2 for problem B. Some of these coefficients are given in Table 3 to provide a more quantitative description of the branches of positive solutions for these problems.

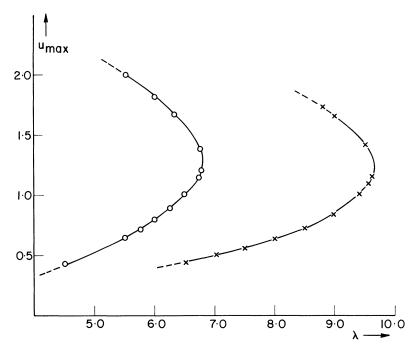


Fig. 2. Positive solution branches for  $f(u) = e^u$ . Problems A and B

## Appendix A.

*Proof of Lemma* 1, § 2.1. The inverse interpolation method is effectively an iterative scheme for evaluating  $\lambda(0) = \bar{\lambda}$ . In § 2.1, we let  $P_2(\mu)$  be the quadratic polynomial interpolating the function  $\lambda(\mu)$  at  $(\mu_i, \lambda_i)$ , i = 1, 2, 3. The improved estimate  $\lambda_4$  for  $\bar{\lambda}$  based on this data then is given by (2.2), i.e.,

(A.1) 
$$\lambda_4 = \alpha P_2(0) + (1 - \alpha)\lambda_1.$$

Here we wish to show that for  $\alpha$  chosen as in Lemma 1,

$$\lambda_1 < \lambda_4 < \bar{\lambda}.$$

Table 2
Summary of results from problem A

λ	$\mu$	$u_{\rm max}$	
6.80462	.7315	1.3065	
6.80659	.5001	1.2943	
6.80725	3128	1.2508	
6.80779	.2703	1.2821	
6.80802	.1869	1.2776	
6.80807	0919	1.2627	
6.80814	.1236	1.2742	
6.80817	.1048	1.2732	
6.80822—Nev	vton's method failed	to converge	

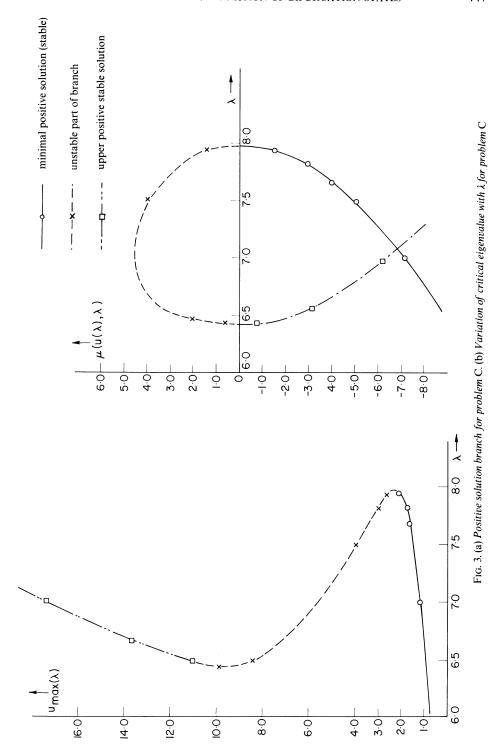


TABLE 3

Some least squares parameters for positive solution branches

			Problem A	A			
λ	Minimal positive Solution				Upper positive Solution		
		$A(\lambda)$	$B(\lambda)$		$A(\lambda)$	$B(\lambda)$	
5.50		10.6	04		34.1	6.45	
6.00		12.6	.11		30.2	4.81	
6.25		13.9	.24	29.1		3.99	
6.75		18.6	.91		23.2	1.98	
			Problem I	3			
λ	Minimal positive Solution			Upper positive Solution			
		$A(\lambda)$	$B(\lambda)$		$A(\lambda)$	$B(\lambda)$	
8.80		15.7	10.1		35.1		
9.00		16.7	10.6	33.6		11.6	
9.50		*	*		28.4	12.5	
			Problem (				
λ				able solution			
	$A(\lambda)$	$B(\lambda)$	$A(\lambda)$	$B(\lambda)$	$A(\lambda)$	$B(\lambda)$	
6.8	15.7	.25	90.9	12.2	240.	17.0	
7.0	16.9	.36	79.2	10.6	265.	16.0	
7.5	21.0	.81	57.8	70.8	*	*	

Since  $\mu = 0$  is a local maximum for  $\lambda(\mu)$ , we have (assuming  $\lambda(\mu)$  to be three times continuously differentiable) that

(A.3) 
$$\lambda_i = \lambda(\mu_i) = \bar{\lambda} + \frac{(d^2 \lambda(S_i)/d\mu^2)\mu_i^2}{2}$$

for some  $S_i$ ,  $\lambda_i < S_i < \bar{\lambda}$ . Using  $\bar{\lambda} - \lambda_1 \ge \bar{\lambda} - \lambda_j$ , j = 2, 3, and (2.3), i.e.,

$$\max_{\lambda_1 < S < \lambda} |d^2 \lambda(S)/d\mu^2|^{-1} \leq M_2,$$

we get

(A.4) 
$$\mu_i^2 = \frac{2(\lambda_i - \bar{\lambda})}{d^2 \lambda(S_i)/d\mu^2}$$

$$\leq 2(\bar{\lambda} - \lambda_1)M_2, \qquad i = 1, 2, 3.$$

Consequently, using the basic interpolation error formula and  $K_3$  from (2.3),

(A.5) 
$$\begin{split} |\bar{\lambda} - P_2(0)| &\leq K_3 |\mu_1 \mu_2 \mu_3|/6 \\ &\leq (K_3 (2M_2)^{3/2}/6) (\bar{\lambda} - \lambda_1)^{3/2}. \end{split}$$

Now

(A.6) 
$$\bar{\lambda} - \lambda_4 = (1 - \alpha)(\bar{\lambda} - \lambda_1) + \alpha(\bar{\lambda} - P_2(0))$$

so, using (A.5), and setting

$$k = K_3 (2M_2)^{3/2}/6$$

we get

(A.7) 
$$(1 - \alpha)(\bar{\lambda} - \lambda_1) - \alpha k(\bar{\lambda} - \lambda_1)^{3/2}$$

$$\leq \bar{\lambda} - \lambda_4 \leq (1 - \alpha)(\bar{\lambda} - \lambda_1) + \alpha k(\bar{\lambda} - \lambda_1)^{3/2}.$$

Hence, if  $\rho = k(\bar{\lambda} - \lambda)^{1/2} < 1$  and  $0 < \alpha < 1/(1 + \rho)$ , (A.7) shows that  $0 < \bar{\lambda} - \lambda_4$  and that as  $\bar{\lambda} - \lambda_1$  approaches zero,

(A.8) 
$$\bar{\lambda} - \lambda_4 = (1 - \alpha)(\bar{\lambda} - \lambda_1) + O((\bar{\lambda} - \lambda_1)^{3/2}).$$

**Appendix B.** The following are some comments on the schematic flow chart of Fig. 4.

All terminations result in printing out a summary of solution branch information obtained. The abnormal ones include a short diagnostic printout.

- (ii) The input data referred to are the parameters for the least squares form functions (see (2.9), (2.10)).
- (iii) The interpolation data, when complete, consists of three pairs  $(\lambda_i, \mu_i(u(\lambda_i), \lambda_i))$ , i = 1, 2, 3. (See § 2.1.)
  - (v) The convergence test for Newton's method is to check whether

$$||C||_2 \leq \text{CTOLER}$$

in less than, ITMAX1 iterations. Here C is the correction vector for updating the current Newton's iterate, and CTOLER and ITMAX1 are parameters. For the experiments described here, CTOLER = .001 and ITMAX1 varies from 10 to 15.

(viii) The convergence test for the inverse iteration scheme is to check whether

$$\frac{|\mu^{(n+1)} - \mu^{(n)}|}{|\mu^{(n+1)}| + .001} \le \text{FTOLER}$$

for n < ITMAX2. Here  $\mu^{(n)}$  denotes the *n*th iterate of the method, and parameters FTOLER and ITMAX2 were set to .005 and 10 respectively.

(xii) The inverse interpolation process terminates if at some stage

$$\frac{\max_{i} (\mu_{i}) - \min_{i} (\mu_{i})}{|\max_{i} (\mu_{i})| + .001} \le EPSF$$

or ILAMAX values of  $\lambda$  have been processed. For the experiments reported on here, EPSF = .01 and ILAMAX ranges from 10 to 20.

- (xiii) The inverse interpolation is performed using Newton's difference form of the quadratic interpolating polynomial. The sign of the second difference of the inverse data,  $(\mu_i, \lambda_i)$ , is checked against the expected turning direction (left is consistent with negative, see Fig. 2). Inconsistency produces an abnormal termination.
- (xv) The  $\lambda_i$  value in the interpolation data which is furthest from the expected turning point  $\lambda^*$  value is determined and replaced. The use of the phrase "abnormal termination" is perhaps misleading in that more runs ended in one of the abnormal

terminations, due to one of the iteration processes failing as  $\lambda^*$  is approached, than ended in the "normal" termination.

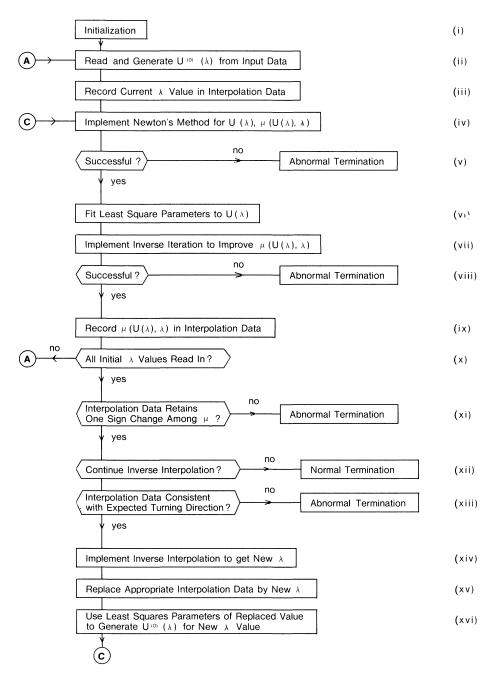


Fig. 4

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