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"Isolas" in Solution Diagrams

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Two computational algorithms for location of the point of formation of isolated branches of solutions of nonlinear algebraic equations in a solution diagram are proposed. The methods are tested on a problem from chemical kinetics. The convergence properties of the methods are evaluated and generalization to the problem of location of isolas in nonlinear boundary value problems for a set of ordinary differential equations is proposed.

1. INTRODUCTION

In a number of nonlinear problems described by a set of algebraic, ordinary, or partial differential equations we are usually seeking the solution of the problem in the form of a "solution diagram," i.e., in the form of the dependence of the chosen norm or the representative value of the solution on a parameter. Such solution diagrams are, for example, constructed in hydrodynamical problems (local velocity or temperature as a function of Reynold's or Rayleigh number), in ecology, reaction–diffusion problems (concentration of reaction component as a function of the magnitude of a transport coefficient), and in a number of other areas of physics and engineering. A bifurcation diagram, showing the dependence of bifurcation points on a parameter, is also often used to complete the solution diagram [1].

Isolas in solution diagrams appear as curves of solutions which close on themselves and are not connected to any other branch of solutions. The isolas create special problems in construction of solution diagrams. For example, in the techniques based on continuation algorithms [2, 3] we cannot determine the isolas unless we locate at least one point of the isola which could be used as a starting point for the application of the algorithm. Until now the results of simulation of the transient (nonstationary) problems or a random search away from known families of solutions usually pointed to the existence of isolated branches of solutions [4, 5]. When such a search for isolas is performed, however, the consumption of computer time is usually high.

Methods of qualitative approach to steady-state bifurcation theory, developed recently by Golubitsky and Schaeffer [6] ("singularity theory"), enable one, in certain cases, to determine whether universal unfolding of a given problem can contain a solution diagram with isolas. Even if we know that an isola should exist in

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a studied range of parameter values, however, we still have to locate it in the solution diagram. In [7] a description of the structure of a class of isolas is given. The isolas that shrink to a point as the characteristic parameter of the problem is varied (the point is called an isola center) are considered in the paper. The authors derive equations characterizing an isola center and construct approximate descriptions of isola solutions by a small parameter perturbation expansion in the neighbourhood of isola centers. The main problem in the application of the proposed methods is to determine the isola center by solving isola center equations. On the basis of the ideas of Reiss and coworkers [7], two numerical procedures for direct numerical evaluation of the point of formation of the isola (isola center) have been developed. The methods will be discussed for a well-known problem of complex chemical reaction in a continuously stirred tank reactor, described by a system of three nonlinear algebraic equations. Existence of isola solutions in this system is here reported for the first time. Generalization to a nonlinear boundary value problem for a set of ordinary differential equations will be described in the discussion section.

2. Numerical Algorithms

Let us assume that the stationary state of a dynamic system is described by a set of nonlinear algebraic equations depending at least on two parameters α and β

$$f_i(x_1, \ldots, x_n, \alpha, \beta) = 0, \qquad i = 1, 2, \ldots, n. \tag{1}$$

We shall seek such values of the parameter $\alpha = \alpha_0$, where a new isolated curve is formed depending on the parameter β, cf. Fig. 1.

The dependence of the solution x_1 on both parameters α and β is shown schematically in Fig. 2 (here $n = 1$). The isolas $x_1(\beta)$ are formed for $\alpha > \alpha_0$ at the point P. For $\alpha < \alpha_0$ the isolas disappear. The point P is called the isola center [7]. The authors of [7] have also considered other types of isolas in their analysis.

We shall now discuss the necessary conditions satisfied by the point P and suggest two procedures for their numerical realization.

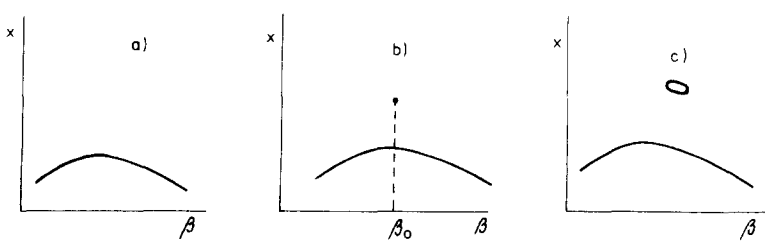

FIG. 1. Characteristic part of the solution diagram $x(\beta)$: (a) before $(\alpha = \alpha_0 - \varepsilon)$, (b) at $(\alpha = \alpha_0)$, and (c) after $(\alpha = \alpha_0 + \varepsilon)$ formation of isola.

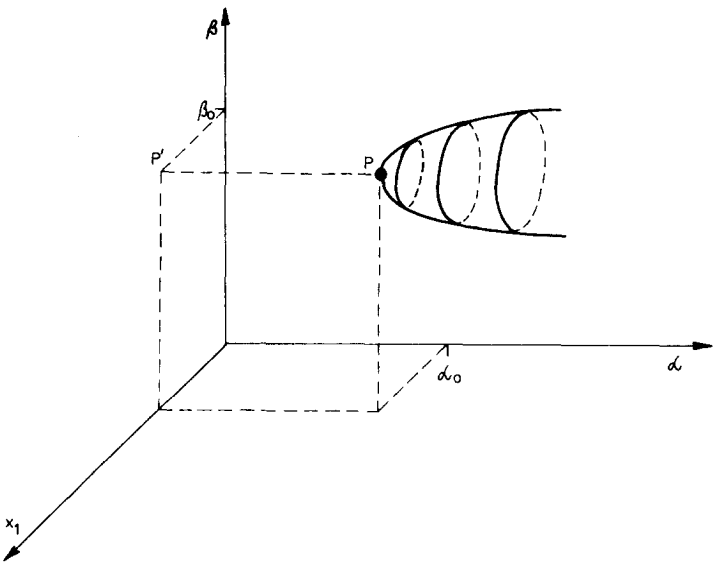

FIG. 2. Schematic picture of formation and occurrence of isolas.

A. *Algorithm* 1

In the neighbourhood of the point P the dependence

$$\alpha = \varphi(x_k, \beta) \tag{2}$$

is unique and has an extremum (a representative component x_k was chosen). When the values x_k and β are fixed, then $x_1,\ldots, x_{k-1}, x_{k+1},\ldots, x_n$, and α can be computed from (1) and φ can be evaluated. This will not be necessary, however, for the suggested computational algorithm.

For the extremum of φ to occur at the point P, we shall have

$$\partial\varphi/\partial x_k = 0, \qquad \partial\varphi/\partial\beta = 0. \tag{3}$$

Let us denote

$$J_k = \begin{bmatrix} \dfrac{\partial f_1}{\partial x_1} \cdots \dfrac{\partial f_1}{\partial x_{k-1}} & \dfrac{\partial f_1}{\partial \alpha} & \dfrac{\partial f_1}{\partial x_{k+1}} \cdots \dfrac{\partial f_1}{\partial x_n} \\ \dfrac{\partial f_2}{\partial x_1} \cdots & & \\ \vdots & & \\ \dfrac{\partial f_n}{\partial x_1} \cdots \dfrac{\partial f_n}{\partial x_{k-1}} & \dfrac{\partial f_n}{\partial \alpha} & \dfrac{\partial f_n}{\partial x_{k+1}} \cdots \dfrac{\partial f_n}{\partial x_n} \end{bmatrix}, \qquad \frac{\partial f}{\partial x_k} = \begin{bmatrix} \dfrac{\partial f_1}{\partial x_k} \\ \dfrac{\partial f_2}{\partial x_k} \\ \vdots \\ \dfrac{\partial f_n}{\partial x_k} \end{bmatrix} \tag{4}$$

and

$$r = (r_1,..., r_n)^T = \left(\frac{dx_1}{dx_k},..., \frac{dx_{k-1}}{dx_k}, \frac{d\alpha}{dx_k}, \frac{dx_{k+1}}{dx_k},..., \frac{dx_n}{dx_k}\right)^T. \tag{5}$$

Then on differentiating (1) with respect to x_k (taking into consideration that α depends on x_k) we obtain a system of linear algebraic equations (cf. the implicit function theorem)

$$J_k \cdot r = -\partial f/\partial x_k. \tag{6}$$

When system (6) is solved, the first equation in (3) is the same as

$$f_{n+1}(x_1, x_2,..., x_n, \alpha, \beta) = r_k(x_1, x_2,..., x_n, \alpha, \beta) = 0. \tag{7}$$

To obtain the second equation in (3) we denote

$$\begin{aligned} &\partial f/\partial\beta = (\partial f_1/\partial\beta, \partial f_2/\partial\beta,..., \partial f_n/\partial\beta)^T, \\ &s = (s_1, s_2,..., s_n)^T = \left(\frac{dx_1}{d\beta},..., \frac{dx_{k-1}}{d\beta}, \frac{d\alpha}{d\beta}, \frac{dx_{k+1}}{d\beta},..., \frac{dx_n}{d\beta}\right)^T. \end{aligned} \tag{8}$$

For fixed x_k we obtain a system of linear equations

$$J_k \cdot s = -\partial f/\partial\beta. \tag{9}$$

The kth component of the vector s is then used for the formulation of the second condition in (3)

$$f_{n+2}(x_1,..., x_n, \alpha, \beta) = s_k(x_1, x_2,..., x_n, \alpha, \beta) = 0. \tag{10}$$

Note that systems (6) and (9) have the same matrices, hence they can be solved by a single pass of the Gauss elimination procedure for two different right-hand sides.

Altogether, $n + 2$ nonlinear algebraic equations (1), (7), and (10) for $n + 2$ unknowns $X = (x_1,..., x_n, \alpha, \beta)^T$ result. The residua (left-hand sides) of this system can be calculated for chosen values of $x_1,..., x_n$, α, β. This is sufficient for any method of solution of the system of nonlinear equations without computation of derivatives or for Newton's method with the Jacobi matrix computed by means of finite differences. An analytical evaluation of the Jacobi matrix requires that for the last two rows we have second partial derivatives of f_i (requiring solution of a number of systems of linear algebraic equations). The method would be cumbersome. We can, however, combine the analytical evaluation of the first n rows of the Jacobi matrix (we have already computed these derivatives) with the use of difference approximations of the derivatives in the last two rows, i.e., the partial derivatives of Eqs. (7) and (10).

To determine whether isolas exist for $\alpha > \alpha_0$ or for $\alpha < \alpha_0$ (here α_0 together with β_0 and $x_1^0,\ldots, x_n^0$ result from the solution of the above system of $n+2$ nonlinear equations) we have three possibilities:

(1) Use some trial and error technique; here we choose the point $x_1^0,\ldots, x_n^0$ for $\beta = \beta_0$ and $\alpha = \alpha_0 \pm \varepsilon$ (or a slightly perturbed point) and solve equations (1), e.g., by Newton's method. The results indicate the direction of formation of isolas.

(2) Evaluate the second derivatives $\partial^2\varphi/\partial x_k^2$, $\partial^2\varphi/\partial\beta^2$ and $\partial^2\varphi/\partial x_k\partial\beta$ and use Sylvester conditions to differentiate between maxima and minima of φ (for determination of the direction of the formation of the isola).

(3) Use perturbation techniques as proposed in [7].

B. *Algorithm* 2

We have a limit point at the point of formation of an isola for fixed $\beta = \beta_0$ for $x(\alpha)$ (cf. point P in Fig. 2). A necessary condition for the existence of a limit point is [1, 8, 9],

$$f_{n+1}(x_1, x_2,\ldots, x_n, \alpha, \beta) = \det J(x_1,\ldots, x_n, \alpha, \beta) = 0, \tag{11}$$

where $J = \{\partial f_i/\partial x_j\}$ is the Jacobi matrix of system (1) with respect to the variables $x_1,\ldots, x_n$. We shall now choose an index k, $1 \leqslant k \leqslant n$, and fix the value of the coordinate x_k at the point of isola formation (in Fig. 2, $k = 1$ at the point P), hence $x_k = x_{k0}$. Then the dependence of $(x_1, x_2,\ldots, x_{k-1}, x_{k+1},\ldots, x_n, \beta)$ on α leads to a limit point at the point P determined by (cf. above)

$$f_{n+2}(x_1,\ldots, x_n, \alpha, \beta) = \det \bar{J}_k(x_1,\ldots, x_n, \alpha, \beta) = 0, \tag{12}$$

where

$$\bar{J}_k = \begin{bmatrix} \dfrac{\partial f_1}{\partial x_1} \cdots \dfrac{\partial f_1}{\partial x_{k-1}} & \dfrac{\partial f_1}{\partial \beta} & \dfrac{\partial f_1}{\partial x_{k+1}} \cdots \dfrac{\partial f_1}{\partial x_n} \\ \dfrac{\partial f_2}{\partial x_1} \cdots & & \\ \vdots & & \\ \dfrac{\partial f_n}{\partial x_1} \cdots \dfrac{\partial f_n}{\partial x_{k-1}} & \dfrac{\partial f_n}{\partial \beta} & \dfrac{\partial f_n}{\partial x_{k+1}} \cdots \dfrac{\partial f_n}{\partial x_n} \end{bmatrix}. \tag{13}$$

We have obtained a system of $n+2$ nonlinear equations (1), (11), and (12) for $n+2$ unknowns $x_1,\ldots, x_n$, α, β. We use Newton's method, as in Algorithm 1, combined with methods for evaluation of the Jacobi matrix (the first n rows are evaluated analytically and the last two rows, i.e., the partial derivatives of Eqs. (11) and (12), are obtained by means of a difference approximation). The testing of the direction of formation of isolas is also similar to the procedure described for Algorithm 1.

3. Example

The two algorithms described above were applied to a system of three nonlinear equations describing stationary states of flow through a continuously stirred tank reactor, where reactions of catalytic oxidation of malonic acid by acidic bromate occur (the well-known oscillatory Belousov–Zhabotinski reaction [10]). The mass balance equations are in the form

$$\begin{aligned} (\mu x_2 - x_1 x_2 + x_1 - x_1^2)/\varepsilon - \beta x_1 &= 0, \\ (-\mu x_2 - x_1 x_2 + f x_3)/\varepsilon' + \beta(\alpha - x_2) &= 0, \\ x_1 - x_2 - \beta x_3 &= 0. \end{aligned} \tag{14}$$

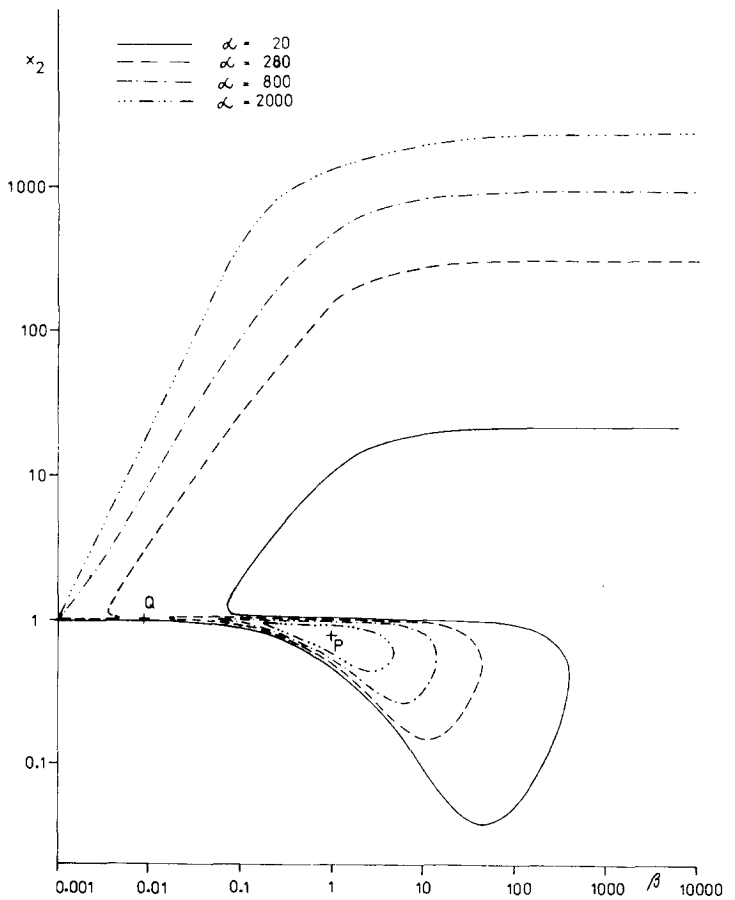

FIG. 3. Dependence $x_2(\beta)$, model (14) for various α. The point P denotes isola formation for $\alpha = 3508$.

TABLE I

The Course of Newton's Iteration Process for Algorithm 1.

Iteration	x_1	x_2	x_3	α	β
0	0.200	1.000	0.100	0.300	1.000
1	0.251	0.797	0.125	2022	1.018
2	0.251	0.748	0.125	3496	1.010
3	0.249	0.750	0.125	3508	0.997
4	0.249	0.750	0.125	3508	0.997
0	2.000	2.000	2.000	2.000	2.000
1	0.767	3.584	1.772	54260	0.726
2	0.443	3.650	1.143	43800	0.509
3	0.276	3.437	0.698	29715	0.389
4	0.186	3.053	0.417	18715	0.323
5	0.148	2.431	0.250	11154	0.321
6	0.193	1.117	0.171	6039	0.551
7	0.221	0.732	0.116	3180	0.790
8	0.246	0.758	0.127	3554	0.953
9	0.249	0.750	0.125	3509	0.993
10	0.249	0.750	0.125	3508	0.997

Note. $\mu = 8.4 \times 10^{-6}$, $f = 2$, $\varepsilon = 6.6667 \times 10^{-4}$, and $\varepsilon' = 1.7778 \times 10^{-5}$.

TABLE II

The Course of Newton's Iteration Process for Algorithm 2.

Iteration	x_1	x_2	x_3	α	β
0	0.200	1.000	0.100	0.300	1.000
1	0.156	0.889	0.106	1562	0.444
2	0.216	0.789	0.129	3737	0.704
3	0.257	0.741	0.127	3569	1.019
4	0.250	0.750	0.125	3511	0.998
5	0.249	0.750	0.125	3508	0.997
6	0.249	0.750	0.125	3508	0.997
0	2.000	2.000	2.000	2.000	2.000
1	1.197	1.006	0.660	−7117	1.609
2	0.758	0.683	0.407	−3152	1.146
3	0.485	0.674	0.291	709.6	0.806
4	0.314	0.742	0.205	2916	0.610
5	0.220	0.797	0.144	3611	0.549
6	0.217	0.783	0.120	3696	0.769
7	0.223	0.776	0.121	3671	0.807
8	0.232	0.767	0.123	3626	0.866
9	0.243	0.757	0.124	3563	0.940
10	0.250	0.750	0.125	3506	0.999
11	0.249	0.750	0.125	3508	0.997

Note. $\mu = 8.4 \times 10^{-6}$, $f = 2$, $\varepsilon = 6.6667 \times 10^{-4}$, and $\varepsilon' = 1.7778 \times 10^{-5}$.

Here, x_1, x_2, and x_3 are dimensionless concentrations of $[HBrO_2^+]$ radical, $[Br^-]$, and $[Ce^{4+}]$ ions, respectively (in Tyson's work [10] they are denoted x, y, z); μ, f, ε, and ε' are given model parameters, β is the dimensionless feed rate, and α is the dimensionless concentration of bromide ions in the feed (β and α are denoted k and y^0 in [10]).

Results obtained by using Newton's method for the solution of the system of five nonlinear equations (1), (7), and (10) (Algorithm 1) for example (14) are shown in Table I. The Jacobi matrix for Newton's method was evaluated by a combination of techniques, i.e., the first three rows were calculated analytically and the last two rows by means of a difference approximation. The convergence of the method is good. The dependence of the variable x_2 on the parameter β for different values of the parameter α is shown in Fig. 3, where the point P is the point of isola formation for $\alpha = 3508$.

The dependence of the solution on the parameter β was computed by using general continuation routine [3]. The starting points for the continuation were chosen randomly. The starting estimates for the continuation in the neighbourhood of isola centers can also be based on perturbation solutions as described in [7]. This could

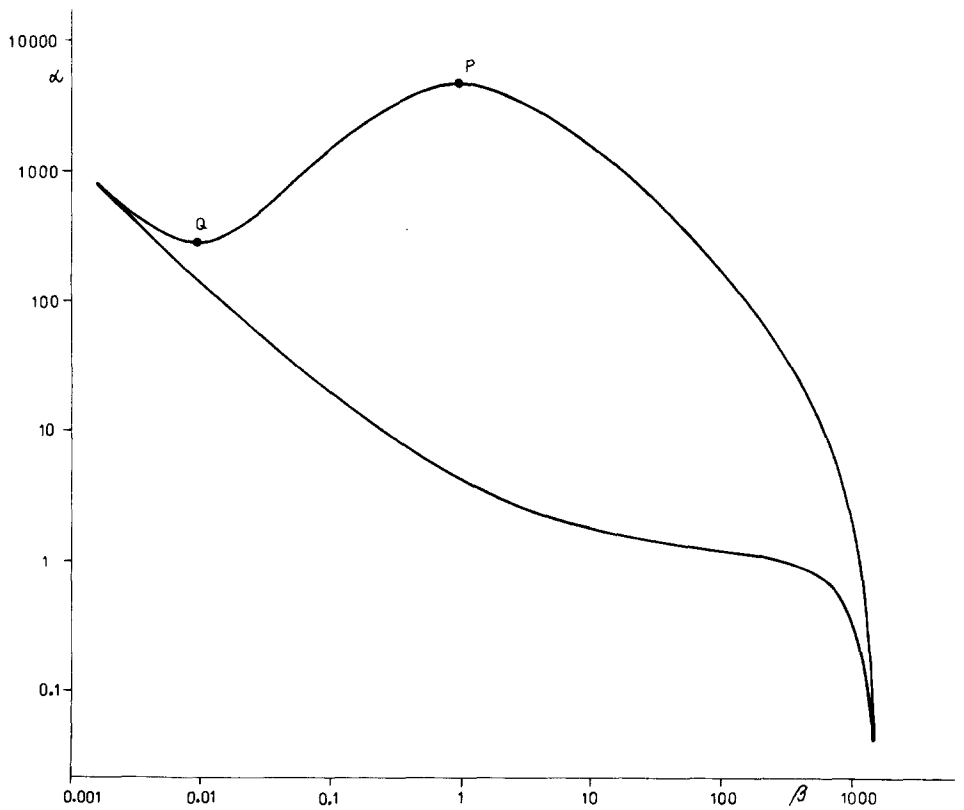

FIG. 4. Bifurcation diagram for system (14) in a parametric plane "$\beta - \alpha$."

bring significant computer time savings, particularly in the problems of higher dimensionality.

The examples of the use of Newton's method for the solution of Eqs. (1), (11), and (12) (Algorithm 2) are shown in Table II; the last two rows of the Jacobi matrix were again evaluated by means of a difference approximation. The convergence was again good. If the algorithms are compared, we can see that global convergence properties are somewhat better for Algorithm 1. An iteration according to both algorithms was used for a number of initial estimates. A comparison of the results obtained is summarized in Table III, confirming the effectiveness of both algorithms. When we solve the equations for necessary conditions we obtain not only the point of isola formation, but also the point of a saddle type, denoted Q in Fig. 3. The corresponding bifurcation diagram given in Fig. 4 clarifies the picture. Here the loci of limit points of $x(\beta)$ and $x(\alpha)$ are given depending on the values of the parameters α and β, respectively.

The points P and Q are also indicated, and correspond to the values of the parameter β where a minimum or a maximum is located. At the point P the limit points of $x(\beta)$ are approaching each other and for $\alpha < \alpha_P$ multiple solutions exist

TABLE III

Comparison of Efficiency of the Algorithms

Initial guess						
x_1	x_2	x_3	α	β	Algorithm 1	Algorithm 2
0.2	1	0.1	0.3	1	*P*–3	*P*–5
0.2	0.8	0.1	4000	1	*P*–5	div.
0.2	0.2	0.2	2	0.2	*Q*–13	div.
0.3	2	0.5	0.5	1	*P*–4	div.
0.1	1	0.1	0.3	1	div.	*Q*–12
0.2	2	0.1	0.3	1	*P*–4	*Q*–10
0.2	3	0.1	0.3	1	*P*–4	div.
0.5	0.5	0.25	5	0.5	*Q*–13	*P*–5
0.1	1	1	1	1	div.	div.
0.1	0.1	0.1	0.1	0.1	*Q*–11	div.
1	1	1	1	1	*Q*–14	*P*–7
2	2	2	2	2	*P*–10	*P*–11
3	3	3	3	3	div.	div.
10	10	10	10	10	div.	*P*–11
100	100	100	100	100	div.	*P*–16
1000	1000	1000	1000	1000	div.	*P*–21
10000	10000	10000	10000	10000	div.	div.

Note. Indicated in the last two columns is the number of iterations sufficient to reach an accuracy of three valid digits for all five components; div. denotes slow convergence or divergence; P or Q denotes that the iteration process reached the point P (0.249, 0.750, 0.125, 3508, 0.997) or Q (0.00413, 0.998, 0.00410, 229, 0.00836), respectively (cf. Figs. 3 and 4).

(isolas cease to exist for $\alpha \to \alpha_{P-}$). On the other hand, at the point Q the limit points with decreasing α separate and for β_Q multiplicities do not exist for the dependence $x(\beta)$ (the point Q corresponds to the point of contact of the limit points of the two different branches). Observe that the point of isola formation corresponds to the point of extremum on the convex part of the loci of the limit points (in their dependence on β), taken from the point of view of a set of multiplicities (multiple solutions of (1)).

4. Discussion

The algorithms described above can be effectively used in situations where we have found in some other way that isolas exist, or should exist, on the solution diagram. One of the possibilities already mentioned is a trial and error technique applied to the corresponding nonstationary problem. Another is to use singularity theory. Golubitsky and Schaeffer [6] have published a partial classification of bifurcation problems with one state variable x. In their classification an isola appears in the case where the normal form is $x^2 + \beta^2$, with a universal unfolding $x^2 + \beta^2 + \alpha$ (codimension 1 problem). Hence, if we can transform the given nonlinear algebraic problem into the above normal form and the corresponding universal unfolding will include that for an isola, we can start to locate the point of isola formation by the above techniques.

The procedure of location of isola centers described for algebraic equations can also be used for location of isola centers in solution diagrams of nonlinear boundary value problems (NBVP) for systems of ordinary differential equations. Let us describe such a procedure based on the transformation of the boundary value problem into an initial value problem by means of the shooting method.

Let us have a NBVP in the form ($' = d/dt$)

$$y_i' = g_i(y_1, \ldots, y_m, \alpha, \beta), \qquad i = 1, 2, \ldots, m, \tag{15}$$

with the two-point boundary conditions

$$y_i(0) = y_{i0}, \qquad i = 1, 2, \ldots, m - n, \tag{16}$$

$$y_{j_i}(1) = y_{j_i 1}, \qquad i = 1, 2, \ldots, n, \quad j_i \in [1, m]. \tag{17}$$

Boundary conditions (16) and (17) were chosen for simplicity; generalizations will be evident.

After choosing n missing initial conditions at $t = 0$,

$$y_{i+m-n}(0) = x_i, \qquad i = 1, 2, \ldots, n, \tag{18}$$

the initial problem of Eqs. (15), (16) and (18) can be integrated from $t = 0$ to $t = 1$ and n residua

$$f_i(x_1, \ldots, x_n, \alpha, \beta) = y_{j_i}(1) - y_{j_i 1} = 0, \qquad i = 1, \ldots, n, \tag{19}$$

are obtained (the value of the solution $y_{j_i}(1)$ is evidently dependent on the choice of $x_1, \ldots, x_n, \alpha, \beta$). The problem is thus transformed into form (1) and the procedures described in Section 2 can be used. The elements of Jacobi matrices (4) and (13) are obtained either by means of the introduction of variational differential equations for variables $\partial y_i/\partial x_j$, $\partial y_i/\partial \alpha$, and $\partial y_i/\partial \beta$ or by using difference formulas. In the first case, a total of $m(n+3)$ differential equations have to be integrated in one iteration; in the second case we have to integrate m differential equations (15) $(n+3)$ times.

The second possibility for the location of isola centers for NBVP is to apply the above described algorithms directly to difference approximations of Eqs. (15)–(17). The dimension of problem (1) will be high. In cases where the shooting method will fail, however, it seems that it will be easier to use this procedure than to construct multiple shooting procedures.

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