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NUMERICAL BIFURCATION OF SEPARABLE PARAMETERIZED EQUATIONS*

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Dedicated to Víctor Pereyra on the occasion of his 70th birthday

Abstract. Many applications give rise to separable parameterized equations, which have the form $A(y,\mu)z + b(y,\mu) = 0$, where $z \in \mathbb{R}^N$, $y \in \mathbb{R}^n$, $\mu \in \mathbb{R}^s$, and the $(N+n)\times N$ matrix $A(y,\mu)$ and $(N+n)$ vector $b(y,\mu)$ are C^2-Lipschitzian in $(y,\mu) \in \Omega \subset \mathbb{R}^n \times \mathbb{R}^s$. We present a technique which reduces the original equation to the form $f(y,\mu) = 0$, where $f : \Omega \to \mathbb{R}^n$ is C^2-Lipschitzian in (y,μ). This reduces the dimension of the space within which the bifurcation relation occurs. We derive expressions required to implement methods to solve the reduced equation. Numerical examples illustrate the use of the technique.

Key words. separable parameterized equations, singular value decomposition, static bifurcation points, extended systems, Newton's method, LU factorization, curve switching and tracking.

AMS subject classifications. 65P30, 65H10, 37G10, 34C23

1. Introduction.

Separable parameterized equations have the form

$$A(y,\mu)z + b(y,\mu) = 0, \tag{1.1}$$

where the $(N+n)\times N$ matrix $A(y,\mu)$ and the $(N+n)$ vector $b(y,\mu)$ are C^2-Lipschitzian in $(y,\mu) \in \Omega \subset \mathbb{R}^n \times \mathbb{R}^s$, and $z \in \mathbb{R}^N$. Such equations arise in the analytical or numerical solution of differential equations and elsewhere. For example, the equilibrium solutions of the Lorenz equations

$$\frac{d}{dt}\begin{bmatrix} y \\ z_1 \\ z_2 \end{bmatrix} = \begin{bmatrix} \mu_2(z_1 - y) \\ \mu_1 y - z_1 - y z_2 \\ y z_1 - \mu_3 z_2 \end{bmatrix}$$

satisfy the separable equation

$$\begin{bmatrix} \mu_2 & 0 \\ -1 & -y \\ y & -\mu_3 \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} + \begin{bmatrix} -\mu_2 y \\ \mu_1 y \\ 0 \end{bmatrix} = 0. \tag{1.2}$$

As another example, consider the interface problem

$$\begin{aligned} \mu u(x) + F(u(x)) &= 0 \text{ on } x \in (0,\gamma), \\ u_{xx}(x) + \mu u(x) &= 0 \text{ on } x \in (\gamma, 1), \\ u(0) = u(1) &= 0, \\ u(\gamma+\epsilon) + \epsilon^2[\mu u(\gamma) + F(u(\gamma))] &= 0, \end{aligned}$$

for some small $\epsilon > 0$ and some nonlinear F. We discretize this problem with finite differences and write $y = [y_1, \ldots, y_n]^T$ for the node values of u on $(0,\gamma]$ and $z = [z_1, \ldots, z_N]^T$ for the node values on $(\gamma, 1)$. If we choose $h = \epsilon$, the discrete equations are

$$\begin{bmatrix} E_{n\times N} \\ [D(\mu)]_{N\times N} \end{bmatrix} z + \begin{bmatrix} [P(y,\mu)]_{n\times 1} \\ [Q(y,\mu)]_{N\times 1} \end{bmatrix} = 0, \tag{1.3}$$

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where

$$E = \begin{bmatrix} 0 & 0 & \cdots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & 0 \\ 1 & 0 & \cdots & 0 \end{bmatrix}, \quad D(\mu) = \begin{bmatrix} -2+h^2\mu & 1 & & \\ 1 & -2+h^2\mu & \ddots & \\ & \ddots & \ddots & 1 \\ & & 1 & -2+h^2\mu \end{bmatrix},$$

$$P(y,\mu) = \begin{bmatrix} h^2\mu y_1 + h^2F(y_1) \\ h^2\mu y_2 + h^2F(y_2) \\ \vdots \\ h^2\mu y_n + h^2F(y_n) \end{bmatrix}, \quad Q(y,\mu) = \begin{bmatrix} y_n \\ 0 \\ \vdots \\ 0 \end{bmatrix}.$$

Numerous applications that give rise to equations of the form (1.1), as well as a number of approaches to solving such problems, may be found in the review article [14].

This paper will focus on the most common situation, in which there is only one parameter μ, that is $s = 1$. When $s > 1$, there is generally one parameter that is of primary interest (for example, μ_1 in (1.2)) and we can treat this parameter as the only parameter.

We have previously presented techniques for solving

$$A(y)z + b(y) = 0 \tag{1.4}$$

by reducing the equation to a nonlinear system involving only the variable y [29, 37]. Alternatively, the standard projection method VARPRO [12, 13, 14] replaces (1.4) by the problem $\min_{y,z} \|A(y)z + b(y)\|_2$, which is equivalent to solving

$$\min_y \left\| \left(I - A(y)A^+(y)\right) b(y) \right\|_2 . \tag{1.5}$$

Iterative techniques for solving (1.5) usually require one SVD or QR factorization at each step [11, 13, 14, 21], whereas the method of [29, 37] requires only one LU factorization in every step [23, 29, 30, 33]. The latter method has recently been extended to rank-deficient matrices $A(y)$ [30, 33].

In this paper, we extend the method of [29, 37] to the parameterized form (1.1), solving instead a nonlinear equation of the form

$$f(y,\mu) = 0 \tag{1.6}$$

in y and μ only. We prove that our reduction preserves static bifurcations; we can thus locate the bifurcation in a smaller space and compute bifurcations more economically by solving (1.6) rather than solving (1.1) directly. Our general methods for computing bifurcation points [27, 28, 32] are here adapted to the particular form of (1.6) that arises from the separable form (1.1), which gives rise to distinctive analytical properties and expressions. Our specialized formulation is also applicable to curve tracking and switching [6].

There are numerous techniques for solving general bifurcation problems. The software packages AUTO [10] and MATCONT [8, 9] and their successors implement a variety of techniques for solving bifurcation problems in ordinary differential equations and algebraic systems. Our technique is restricted to the particular form (1.1), and in that context has the advantage of restricting the analysis and computations to a much smaller space. For background on bifurcation problems in general, see [2, 3, 16, 20, 26].

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2. Analysis. We assume throughout what follows that the matrix $A(y,\mu)$ has full rank throughout the region of interest. The techniques of [30, 33] can be extended to the case when $A(y,\mu)$ is rank deficient; for simplicity, we omit that generalization from this paper.

The following results form the basis for our method.

THEOREM 2.1. *Let the $(N+n)\times N$ matrix $A(y,\mu)$ have full rank N in a region $\Omega \in \mathbb{R}^n \times \mathbb{R}^s$. Let K be an $(N+n)\times n$ constant matrix such that the $(N+n)\times(N+n)$ matrix $\begin{bmatrix} A(y,\mu) & K\end{bmatrix}$ is nonsingular. Then (y,z,μ) is a solution of (1.1) if and only if (y,μ) satisfies*

$$f(y,\mu) \equiv \rho(y,\mu)^T b(y,\mu) = 0 \tag{2.1}$$

and

$$z = -A^+(y,\mu)b(y,\mu), \tag{2.2}$$

where

$$\rho(y,\mu)^T = -\begin{bmatrix} 0_{n\times N} & I_n\end{bmatrix}\begin{bmatrix} A(y,\mu) & K\end{bmatrix}^{-1}, \tag{2.3}$$

and A^+ is the pseudo-inverse of A.

Proof. $(\Longrightarrow)$ Clearly, (2.3) is equivalent to

$$\rho(y,\mu)^T\begin{bmatrix} A(y,\mu) & K\end{bmatrix} = -\begin{bmatrix} 0_{n\times N} & I_n\end{bmatrix}. \tag{2.4}$$

Assume (y,z,μ) satisfies (1.1). Multiplying both sides of (1.1) from the left by $\rho(y,\mu)^T$ and using (2.4), we have

$$\rho(y,\mu)^T[A(y,\mu)z + b(y,\mu)] = \rho(y,\mu)^T b(y,\mu) = 0,$$

which is (2.1). Since z is a solution of the linear system (1.1), z is also the unique least squares solution of the linear system, which implies (2.2).

$(\Longleftarrow)$ Assume (y,z,μ) satisfies (2.1) and (2.2). Then by (2.3)

$$0 = \rho(y,\mu)^T b(y,\mu) = -\begin{bmatrix} 0_{n\times N} & I_n\end{bmatrix}\begin{bmatrix} A(y,\mu) & K\end{bmatrix}^{-1} b(y,\mu),$$

which with (2.2) implies

$$\begin{aligned}
&A(y,\mu)z + b(y,\mu)\\
&= A(y,\mu)[-A^+(y,\mu)b(y,\mu)] + b(y,\mu)\\
&= [I_{N+n} - A(y,\mu)A^+(y,\mu)]\begin{bmatrix} A(y,\mu) & K\end{bmatrix}\begin{bmatrix} I_N & 0\\ 0 & I_n\end{bmatrix}\begin{bmatrix} A(y,\mu) & K\end{bmatrix}^{-1} b(y,\mu)\\
&= [I_{N+n} - A(y,\mu)A^+(y,\mu)]\begin{bmatrix} A(y,\mu) & K\end{bmatrix}\begin{bmatrix} \begin{bmatrix} I_N & 0\end{bmatrix}\begin{bmatrix} A(y,\mu) & K\end{bmatrix}^{-1} b(y,\mu)\\ 0\end{bmatrix}\\
&= [A(y,\mu) - A(y,\mu)A^+(y,\mu)A(y,\mu)]\begin{bmatrix} I_N & 0\end{bmatrix}\begin{bmatrix} A(y,\mu) & K\end{bmatrix}^{-1} b(y,\mu) = 0,
\end{aligned}$$

and thus (1.1) is satisfied. □

THEOREM 2.2. *Let the $(N+n)\times N$ matrix $A(y,\mu)$ have full rank N in a region $\Omega \in \mathbb{R}^n \times \mathbb{R}^s$. Let K be an $(N+n)\times n$ constant matrix such that the $(N+n)\times(N+n)$ matrix $\begin{bmatrix} A(y,\mu) & K\end{bmatrix}$ is nonsingular in Ω. Then $(y,\mu)\in\Omega$ and $(\tilde{y},\mu)\in\Omega$ are two distinct solutions of (2.1)–(2.3) if and only if (y,z,μ) and $(\tilde{y},\tilde{z},\mu)$ are two distinct solutions of (1.1).*

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Proof. ($\Longrightarrow$) This is trivial. ($\Longleftarrow$) Assume $(y,z,\mu)\neq(\tilde{y},\tilde{z},\mu)$. If $(y,\mu)=(\tilde{y},\mu)$, then $z=\tilde{z}$ by (2.2) contradicting the assumption. Therefore $(y,\mu)\neq(\tilde{y},\mu)$. ☐

From Theorem 2.2, for $(y^*,\mu^*)\in\Omega$ and a fixed μ near μ^*, the number of distinct solutions of (2.1) is the same as the number of distinct solutions of (1.1). Thus, we have the following corollary for static bifurcations:

COROLLARY 2.3. *Under the conditions of Theorem 2.2, the point $(y^*,\mu^*)\in\Omega$ is a bifurcation point of (2.1) if and only if (y^*,z^*,μ^*) is a bifurcation point of (1.1).*

These results imply that we only need to find bifurcation points of (2.1), which typically involves a much smaller space than the original problem (1.1).

3. Implementation. Henceforth, assume $s=1$. An appropriate matrix K to be used in conjunction with Theorem 2.1 may be found as follows. Let a QR factorization of $A(y_0,\mu_0)$ at some point $(y_0,\mu_0)\in\Omega$ near (y^*,μ^*) be

$$A(y_0,\mu_0)=Q_{(N+n)\times(N+n)}R_{(N+n)\times N}\equiv\begin{bmatrix}q_1 & \dots & q_{N+n}\end{bmatrix}\begin{bmatrix}r_{11} & \cdots & r_{1,N}\\ & \ddots & \vdots\\ & & r_{N,N}\\ & 0_{n\times N} & \end{bmatrix},$$

where $\{q_1,\dots,q_{N+n}\}$ is an orthonormal basis for $\mathbb{R}^{N+n}$ and all the diagonal entries $r_{11},\dots,r_{N,N}$ are nonzero because the rank of $A(y_0,\mu_0)$ is N. If

$$K=\begin{bmatrix}q_{N+1} & \dots & q_{N+n}\end{bmatrix} \tag{3.1}$$

then $\begin{bmatrix}A(y,\mu) & K\end{bmatrix}$ is nonsingular throughout a neighborhood of (y_0,μ_0), since it is nonsingular at (y_0,μ_0):

$$\begin{bmatrix}A(y_0,\mu_0) & K\end{bmatrix}=Q_{(N+n)\times(N+n)}\begin{bmatrix}R_{(N+n)\times N} & e_{N+1} & \dots & e_{N+n}\end{bmatrix}.$$

The next theorem describes the relation between the function $f(y,\mu)$ defined in (2.1), the derivatives of f, and the nonsingular matrix $\begin{bmatrix}A(y,\mu) & K\end{bmatrix}$. These expressions are required in our numerical algorithms. We use the following notation: for a matrix or a vector $B(y,\mu)$, denote by $(B(y,\mu))'_j$ and $(B(y,\mu))''_{jk}$ the matrix or vector having the same size with each entry replaced by its derivative with respect to y_j or by its second derivative with respect to y_j,y_k respectively. We identify $\mu\equiv y_{n+1}$. Thus,

$$(B(y,\mu))'_j\equiv\frac{\partial}{\partial y_j}B(y,\mu),\quad (B(y,\mu))''_{jk}\equiv\frac{\partial^2}{\partial y_k\partial y_j}B(y,\mu),\quad j,k=1,2,...,n+1.$$

THEOREM 3.1. *Let $\zeta(y,\mu)\in\mathbb{R}^N$, $\psi(y,\mu)\in\mathbb{R}^n$ satisfy*

$$\begin{bmatrix}A(y,\mu) & K\end{bmatrix}\begin{bmatrix}\zeta(y,\mu)\\ \psi(y,\mu)\end{bmatrix}=-b(y,\mu). \tag{3.2}$$

Then

$$\psi(y,\mu)=f(y,\mu); \tag{3.3}$$

$$(\psi'(y,\mu))_j=(f'(y,\mu))_j=\rho(y,\mu)^T\left([(A(y,\mu))'_j\zeta(y,\mu)]+(b'(y,\mu))_j\right); \tag{3.4}$$

$$\begin{aligned}(\psi(y,\mu))''_{jk}&=(f(y,\mu))''_{jk}\\ &=\rho(y,\mu)^T[(A(y,\mu))'_j(\zeta(y,\mu))'_k+(A(y,\mu))'_k(\zeta(y,\mu))'_j+\\ &\qquad (A(y,\mu))''_{jk}\zeta(y,\mu)+(b(y,\mu))''_{jk}].\end{aligned} \tag{3.5}$$

Proof. (a) By direct computation using (3.2), (2.3), and (2.1):

$$\psi(y,\mu) = -\begin{bmatrix} 0 & I_n \end{bmatrix} \begin{bmatrix} A(y,\mu) & K \end{bmatrix}^{-1} b(y,\mu) = f(y,\mu). \tag{3.6}$$

This proves (3.3).

(b) Differentiating both sides of (3.2) with respect to y_j or $\mu \equiv y_{n+1}$, we have

$$\begin{bmatrix} A(y,\mu) & K \end{bmatrix} \begin{bmatrix} (\zeta(y,\mu))'_j \\ (\psi(y,\mu))'_j \end{bmatrix} + \begin{bmatrix} (A(y,\mu))'_j & 0 \end{bmatrix} \begin{bmatrix} \zeta(y,\mu) \\ \psi(y,\mu) \end{bmatrix} = -(b(y,\mu))'_j. \tag{3.7}$$

Solving this equation for $(\psi(y,\mu))'_j$ gives

$$\begin{aligned} (\psi(y,\mu))'_j &= -\begin{bmatrix} 0 & I_n \end{bmatrix} \begin{bmatrix} A(y,\mu) & K \end{bmatrix}^{-1} [(A(y,\mu))'_j \zeta(y,\mu) + (b(y,\mu))'_j] \\ &= \rho(y,\mu)^T [(A(y,\mu))'_j \zeta(y,\mu) + (b(y,\mu))'_j], \end{aligned}$$

which proves (b).

(c) Differentiating both sides of (3.7) with respect to y_k or $\mu \equiv y_{n+1}$, we have

$$\begin{aligned} &\begin{bmatrix} A(y,\mu) & K \end{bmatrix} \begin{bmatrix} (\zeta(y,\mu))''_{jk} \\ (\psi(y,\mu))''_{jk} \end{bmatrix} + \begin{bmatrix} (A(y,\mu))'_j & 0 \end{bmatrix} \begin{bmatrix} (\zeta(y,\mu))'_k \\ (\psi(y,\mu))'_k \end{bmatrix} \\ &+ \begin{bmatrix} (A(y,\mu))'_k & 0 \end{bmatrix} \begin{bmatrix} (\zeta(y,\mu))'_j \\ (\psi(y,\mu))'_j \end{bmatrix} + \begin{bmatrix} (A(y,\mu))''_{jk} & 0 \end{bmatrix} \begin{bmatrix} \zeta(y,\mu) \\ \psi(y,\mu) \end{bmatrix} \\ = &-(b(y,\mu))''_{jk}. \end{aligned}$$

Solving this equation for $(\psi(y,\mu))''_{jk}$ gives

$$\begin{aligned} (\psi(y,\mu))''_{jk} &= -\begin{bmatrix} 0 & I_n \end{bmatrix} \begin{bmatrix} A(y,\mu) & K \end{bmatrix}^{-1} [(A(y,\mu))'_j (\zeta(y,\mu))'_k \\ &\quad + (A(y,\mu))'_k (\zeta(y,\mu))'_j + (A(y,\mu))''_{jk} \zeta(y,\mu) + (b(y,\mu))''_{jk}] \\ &= \rho(y,\mu)^T [(A(y,\mu))'_j (\zeta(y,\mu))'_k + (A(y,\mu))'_k (\zeta(y,\mu))'_j \\ &\quad + (A(y,\mu))''_{jk} \zeta(y,\mu) + (b(y,\mu))''_{jk}]. \end{aligned}$$

This proves (3.5). □

From (3.4), we see that the Jacobian matrix of $f(y,\mu)$ is given by

$$f'(y,\mu) = \rho(y,\mu)^T \left(\begin{bmatrix} (A(y,\mu))'_1 \zeta(y,\mu) & \ldots & (A(y,\mu))'_{n+1} \zeta(y,\mu) \end{bmatrix} + b'(y,\mu) \right). \tag{3.8}$$

The quantity $\rho(y,\mu)^T$ required in (3.5) and (3.8) may be computed from (2.3) by solving (2.4). The LU factorization of $\begin{bmatrix} A(y,\mu) & K \end{bmatrix}$ required also suffices to solve (3.2), thus producing both $\psi(y,\mu) = f(y,\mu)$ and the quantity $\zeta(y,\mu)$ required for (3.4). The quantity $(\zeta(y,\mu))'_j$ required for (3.5) can be obtained by solving (3.7) using the same factors. Thus one LU factorization suffices to compute all these quantities.

4. Computation. Let (y_0,μ_0) be a point in the solution set of (2.1). A nearby point (y^*,μ^*) that satisfies $f(y^*,\mu^*) = 0$ is to be located. We treat three separate cases: (y_0,μ_0) is (a) a regular point from which we seek another regular point (curve-tracking); (b) a point near a bifurcation from which we seek the bifurcation point; or (c) a bifurcation point from which we seek nearby regular points on different branches (curve-switching).

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Let the singular value decomposition (SVD) (see [15, 35, 36]) of the $n \times (n+1)$ matrix $f'(y_0, \mu_0)$ be

$$f'(y_0,\mu_0) = \begin{bmatrix} u_1 & \dots & u_n \end{bmatrix} \begin{bmatrix} \sigma_1 & \cdots & & 0 \\ & \ddots & & \vdots \\ & & \sigma_n & 0 \end{bmatrix} \begin{bmatrix} v_1 & \dots & v_{n+1} \end{bmatrix}^T, \tag{4.1}$$

where $\{u_1, ..., u_n\}$ and $\{v_1, ..., v_{n+1}\}$ form orthonormal bases for $\mathbb{R}^n$ and $\mathbb{R}^{n+1}$, respectively. The singular values satisfy $\sigma_1 \geq ... \geq \sigma_n \geq 0$. The point (y_0, μ_0) is a regular point of the solution set if the last singular value σ_n is nonzero, and it is a bifurcation point if $\sigma_n = 0$. The point is near a bifurcation point if σ_n is nonzero, but small [6]. We note that here and elsewhere, accurate determination of matrix rank is critical; relevant techniques may be found in [15, 18, 34, 36].

Case (a). For a regular point (y_0, μ_0) where the last singular value σ_n is not small, the tangent direction along the parameterized curve is given by v_{n+1} [6]. We choose $(y^{(0)}, \mu^{(0)})$ to be a point on that tangent line, then use Newton's method to solve $f(y, \mu) = 0$ in the affine space normal to the tangent vector to find the nearby point (y^*, μ^*), i.e., we select a starting point

$$\begin{bmatrix} y^{(0)} \\ \mu^{(0)} \end{bmatrix} = \begin{bmatrix} y_0 \\ \mu_0 \end{bmatrix} + \delta v_{n+1}, \tag{4.2}$$

for some $\delta > 0$ and then set

$$\begin{bmatrix} y^{(k+1)} \\ \mu^{(k+1)} \end{bmatrix} = \begin{bmatrix} y^{(k)} \\ \mu^{(k)} \end{bmatrix} - \begin{bmatrix} f'(y^{(k)}, \mu^{(k)}) \\ v_{n+1}^T \end{bmatrix}^{-1} \begin{bmatrix} f(y^{(k)}, \mu^{(k)}) \\ v_{n+1}^T \begin{bmatrix} y^{(k)} - y^{(0)} \\ \mu^{(k)} - \mu^{(0)} \end{bmatrix} \end{bmatrix}, \tag{4.3}$$

for $k = 0, 1, \ldots$. Note that the matrix involved in (4.3) is invertible for $(y^{(k)}, \mu^{(k)})$ sufficiently near (y_0, μ_0); see [22] for details. Under suitable conditions, this process converges to another regular point on the same parameterized curve. For Newton's method and convergence rates in more general contexts, see, for example, [7, 19, 24].

Case (b). We use the approach of [27, 28, 31, 32] to compute a bifurcation point (y^*, μ^*) from a nearby point (y_0, μ_0). When (y^*, μ^*) is a bifurcation point, $f'(y^*, \mu^*)$ is rank-deficient. Assume that its rank is r, $0 \leq r \leq n-1$. The rank-deficiency is assumed to be known, possibly detected by the existence of small singular values $\sigma_{r+1}, \ldots, \sigma_n$ at the nearby point (y_0, μ_0). The point (y_0, μ_0) near this bifurcation point (y^*, μ^*) is still a regular point, but the last singular value is small. The $(2n+1-r) \times (2n+1-r)$ bordered matrix

$$M(y,\mu) \equiv \begin{bmatrix} (f'(y,\mu))^T & L \\ R^T & 0 \end{bmatrix} \tag{4.4}$$

is nonsingular in a neighborhood of (y^*, μ^*) [28] if we select

$$R = \begin{bmatrix} u_{r+1} & \dots & u_n \end{bmatrix}, \quad L = \begin{bmatrix} v_{r+1} & \dots & v_{n+1} \end{bmatrix}, \tag{4.5}$$

where u_i and v_i are defined by the SVD (4.1). For alternative choices of auxiliary vectors to border a matrix, see, for example, [1, 16, 17, 25]. Following [27, 28], we embed $f(y, \mu)$ into an extended system

$$F(y,\mu,\lambda) \equiv \begin{bmatrix} f(y,\mu) + R\lambda \\ g(y,\mu) \end{bmatrix}, \tag{4.6}$$

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where $\lambda \in \mathbb{R}^{n-r}$ is a Lagrange-type vector and $g(y,\mu) \in \mathbb{R}^{n+1-r}$ is obtained by solving

$$M(y,\mu)\begin{bmatrix}\xi(y,\mu)\\ g(y,\mu)\end{bmatrix} = \begin{bmatrix}0_{(n+1)\times 1}\\ \alpha\end{bmatrix}, \tag{4.7}$$

with $\alpha \in \mathbb{R}^{n-r}$ being a random nonzero vector and $\xi(y,\mu) \in \mathbb{R}^n$. We use Newton's method to solve (4.6): starting from

$$\begin{bmatrix}y^{(0)}\\ \mu^{(0)}\\ \lambda^{(0)}\end{bmatrix} = \begin{bmatrix}y_0\\ \mu_0\\ 0\end{bmatrix},$$

we compute

$$\begin{bmatrix}y^{(k+1)}\\ \mu^{(k+1)}\\ \lambda^{(k+1)}\end{bmatrix} = \begin{bmatrix}y^{(k)}\\ \mu^{(k)}\\ \lambda^{(k)}\end{bmatrix} - \left[F'\left(y^{(k)},\mu^{(k)},\lambda^{(k)}\right)\right]^{-1} F\left(y^{(k)},\mu^{(k)},\lambda^{(k)}\right), \tag{4.8}$$

for $k = 0,1,2,\ldots$. The limit is $(y^*,\mu^*,0)$. As shown in [27, 28], the Jacobian matrix of $F(y,\mu,\lambda)$ is

$$F'(y,\mu,\lambda) = \begin{bmatrix} f'(y,\mu) & R\\ -\eta(y,\mu)^T[\xi(y,\mu)^T f''(y,\mu)] & 0\end{bmatrix}, \tag{4.9}$$

in which the matrix $\eta(y,\mu) \in \mathbb{R}^{(n+1)\times(n+1-r)}$ is obtained by solving

$$\begin{bmatrix}\eta(y,\mu)^T & h(y,\mu)^T\end{bmatrix} M(y,\mu) = \begin{bmatrix}0_{(n+1-r)\times n} & I_{(n+1-r)}\end{bmatrix}, \tag{4.10}$$

and $\xi(y,\mu)^T f''(y,\mu) \equiv \sum_{j=1}^n [\xi_j(y,\mu)\nabla^2 f_j(y,\mu)]$.

Case (c). Given a bifurcation point (y_0,μ_0), we can locate nearby regular points (y^*,μ^*) on several different branches. We adapt the method of [6] to find the relevant branch directions in the tangent space, then use the method (4.2)-(4.3) for computing a regular point to locate a point on any particular branch, using $(y^{(0)},\mu^{(0)})$ on a line given by the relevant direction vector w instead of the tangent vector v_{n+1}. To find the appropriate direction vectors

$$w = L\beta \equiv \begin{bmatrix}v_{r+1} & \ldots & v_{n+1}\end{bmatrix}\begin{bmatrix}\beta_1 & \ldots & \beta_{n+1-r}\end{bmatrix}^T,$$

we solve the numerical bifurcation equations

$$w^T[u_i^T f''(y_0,\mu_0)]w = 0, \quad i = r+1,\ldots,n;$$

that is, we find the vectors β that satisfy

$$\beta^T\left[L^T(\sum_{j=1}^n [u_{i,j}\nabla^2 f_j(y_0,\mu_0)]L\right]\beta = 0, \quad i = r+1,\ldots,n; \quad ||\beta||_2 = 1, \tag{4.11}$$

where $u_{i,j}$ is the jth component of the vector u_i obtained from (4.1). The unknown coefficients $\beta_1,\ldots,\beta_{n+1-r}$ in this system of quadratic equations can be found, for example, by a homotopy method [4, 5].

A summary of the three algorithms above for computing a nearby point (y^*,μ^*) from a given point (y_0,μ_0) in the solution set of (2.1) follows.

Procedure Summary. Given an equation of the form (1.1) with positive integers N, n, $s = 1$, and a point (y_0, μ_0) on the solution curve of (2.1), compute nearby point(s) (y^*, μ^*) in the solution set of (2.1) as follows:

Factor $A(y_0, \mu_0) = \mathrm{QR}$; set $K = [q_{n+1}, \dots, q_{n+N}]$ as in (3.1). Use (2.4) to find $\rho(y_0, \mu_0)^T$ and use (3.2) and (3.4) to find $f'(y_0, \mu_0)$. Do a singular value decomposition (4.1) of $f'(y_0, \mu_0)$ to find singular values $\sigma_1, \dots, \sigma_n$, and singular vectors $u_1, \dots, u_n$ and $v_1, \dots, v_{n+1}$. Identify the rank r of $f'(y_0, \mu_0)$. If σ_n is large, set $w = v_{n+1}$ and go to (a); if σ_n is small, go to (b); if $\sigma_n = 0$, go to (c).

(a) (Computing a regular point) Set $(y^{(0)}, \mu^{(0)}) = (y_0, \mu_0) + \delta w^T$ (4.2). Compute $(y^{(k+1)}, \mu^{(k+1)})$ by Newton's method (4.3) for $k = 0, 1, \dots$ until convergence.

(b) (Computing a bifurcation point) Form matrices R and L as in (4.5). Choose the random vector $\alpha \in \mathbb{R}^{n-r}$. Set $(y^{(0)}, \mu^{(0)}, \lambda^{(0)}) = (y_0, \mu_0, 0)$. For $k = 0, 1, \dots$ until convergence: compute $f(y^{(k)}, \mu^{(k)})$, $f'(y^{(k)}, \mu^{(k)})$, $f''(y^{(k)}, \mu^{(k)})$ as in (3.6), (3.4) and (3.5), form $F(y^{(k)}, \mu^{(k)}, \lambda^{(k)})$ and $F'(y^{(k)}, \mu^{(k)}, \lambda^{(k)})$ using (4.4)-(4.10), and use Newton's method (4.8).

(c) (Computing regular points near a bifurcation point) Form matrices R and L as in (4.5). Find direction vectors w by solving (4.11). For each w, use procedure (a).

By repeatedly using the above algorithm, we can track and switch between branches of a solution set of the reduced equation (2.1).

5. Numerical examples. We present three examples to illustrate our method. Our first example is the equilibrium solution of the Lorenz equation (1.2).

EXAMPLE 5.1.

$$\begin{bmatrix} \mu_2 & 0 \\ -1 & -y \\ y & -\mu_3 \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} + \begin{bmatrix} -\mu_2 y \\ \mu_1 y \\ 0 \end{bmatrix} = 0.$$

We fix the values of $\mu_2 = 2$ and $\mu_3 = 4$, and we denote μ_1 as μ. There is a bifurcation point at $(y^*, \mu^*) = (0, 1)$. With $(y_0, \mu_0) = (-0.1, 1.0025)$, a QR factorization gives

$$A(y_0, \mu_0) = \begin{bmatrix} -0.8935 & 0.0299 & 0.4480 \\ 0.4468 & -0.0400 & 0.8938 \\ 0.0447 & 0.9988 & 0.0223 \end{bmatrix} \begin{bmatrix} -2.2383 & -0.1340 \\ 0 & -3.9990 \\ 0 & 0 \end{bmatrix},$$

hence $K = \begin{bmatrix} 0.4480 & 0.8938 & 0.0223 \end{bmatrix}^T$. Using this K, (2.4), (3.2), and (3.8), we find $f'(y_0, \mu_0)$; an SVD factorization gives

$$f'(y_0, \mu_0) = \begin{bmatrix} 0.0045 & 0.0894 \end{bmatrix} = \begin{bmatrix} 1 \end{bmatrix} \begin{bmatrix} 0.0895 & 0 \end{bmatrix} \begin{bmatrix} 0.0499 & 0.9988 \\ -0.9988 & 0.0499 \end{bmatrix},$$

which suggests that a bifurcation point (y^*, μ^*) is nearby, since the only singular value $\sigma_1 = 0.0895$ is small. We extend the equation (2.1) to (4.6) by introducing a Lagrange-type vector $\lambda \in \mathbb{R}$, selecting $\alpha = 0.6319$ at random, and defining the nonsingular bounded matrix

$$M(y, \mu) = \begin{bmatrix} (f'(y, \mu))^T & L \\ R^T & 0 \end{bmatrix} \quad \text{with} \quad R = 1, \quad L = \begin{bmatrix} 0.0499 & -0.9988 \\ 0.9988 & 0.0499 \end{bmatrix}.$$

Applying Newton's method (4.8) to the extended system (4.6) using (b) in the Procedure Summary, we approximate the bifurcation point $(y^*, \mu^*, \lambda^*) = (0, 1, 0)$. Table 5.1 shows quadratic convergence of Newton's method for this extended system, with $d^{(k)}(y, \mu, \lambda) = \|(y^{(k+1)}, \mu^{(k+1)}, \lambda^{(k+1)}) - (y^{(k)}, \mu^{(k)}, \lambda^{(k)})\|_2$.

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TABLE 5.1
Newton iterations for computing a bifurcation point in Example 5.1.

k	$y^{(k)}$	$\mu^{(k)}$	$\lambda^{(k)}$	$d^{(k)}(y,\mu,\lambda)$
0	-1.0000e-01	1.0025e+00	0.0000e+00	—
1	1.5025e-04	9.9248e-01	4.4822e-04	1.0065e-01
2	1.1248e-10	1.0000e+00	1.0112e-06	7.5373e-03
3	6.2814e-23	1.0000e+00	2.8357e-18	1.0116e-06
4	0.0000e+00	1.0000e+00	0.0000e+00	2.8357e-18

At the bifurcation point $(y,\mu)=(0,1)$, the SVD gives $\sigma_1=0$ and $L=I_2$. We find β by solving (4.11):

$$\beta^T \begin{bmatrix} 0 & -0.8944 \\ -0.8944 & 0 \end{bmatrix} \beta = 0, \quad \beta^T\beta = 1.$$

We obtain $\beta=[\pm 1,0]^T, [0,\pm 1]^T$. Hence, the direction vectors are $w=L\beta=I_2\beta=\beta$ at this bifurcation point. The direction $[-1,0]^T$ points to the solution $(y_0,\mu_0)=(-0.1,1.0025)$ which is on the previously computed branch. So we only need to compute solutions on the other three branches. With $\delta=0.1$, we obtain three points $(0.1,1.0025)$, $(0,1.1)$, $(0,0.9)$ on these three branches respectively by using (c) of the Procedure Summary, as shown in Table 5.2, with

$$d^{(k)}(y,\mu) = \|(y^{(k+1)},\mu^{(k+1)}) - (y^{(k)},\mu^{(k)})\|_2.$$

TABLE 5.2
Newton iterations for computing branch points in Example 5.1.

k	$y^{(k)}$	$\mu^{(k)}$	$d^{(k)}(y,\mu)$
0	1.0000e-01	1.0000e+00	—
1	1.0000e-01	1.0025e+00	2.5000e-03
2	1.0000e-01	1.0025e+00	1.6263e-18
0	0.0000e+00	1.1000e+00	—
1	0.0000e+00	1.1000e+00	8.3267e-017
0	0.0000e+00	9.0000e-01	—
1	0.0000e+00	9.0000e-01	2.7756e-017

EXAMPLE 5.2. This example is (1.3) with $h=0.1$, $\gamma=0.3$, $n=3$, $N=6$, and $F(u)=u^2-u^3$:

$$\begin{bmatrix} 0 & & & \\ 0 & & & \\ 1 & & & \\ -2+0.01\mu & 1 & & \\ 1 & \ddots & \ddots & \\ & \ddots & \ddots & 1 \\ & & 1 & -2+0.01\mu \end{bmatrix} z + \begin{bmatrix} 0.01(\mu y_1 + y_1^2 - y_1^3) \\ 0.01(\mu y_2 + y_2^2 - y_2^3) \\ 0.01(\mu y_3 + y_3^2 - y_3^3) \\ y_3 \\ 0 \\ \vdots \\ 0 \end{bmatrix} = 0,$$

where $z\in\mathbb{R}^6$. There is a bifurcation point at $(y^*,\mu^*)=(0,0,0,0)$. We begin with a point

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$(y_0, \mu_0) = (0, 0, 0, -0.1)$. A QR factorization of $A(y_0, \mu_0)$ gives

$$K^T = \begin{bmatrix} 0.523 & 0.324 & 0.468 & 0.400 & 0.333 & 0.266 & 0.199 & 0.133 & 0.066 \\ -0.805 & -0.118 & 0.345 & 0.295 & 0.246 & 0.196 & 0.147 & 0.098 & 0.049 \\ 0.282 & -0.939 & 0.118 & 0.101 & 0.084 & 0.067 & 0.050 & 0.033 & 0.017 \end{bmatrix}.$$

With this K, (2.4), (3.2), and (3.8) give $f'(y_0, \mu_0)$. An SVD decomposition gives $\sigma_1 = 0.5067$, $\sigma_2 = 0.0010$ and $\sigma_3 = 0.0010$. Since two of these singular values are much smaller than the first, the rank of $f'(y^*, \mu^*)$ is taken to be $r = 1$; that is, a bifurcation point (y^*, μ^*) is assumed to be nearby. The SVD also gives L and R for use in (4.4). We extend the equation (2.1) to (4.6) by introducing a Lagrange-type vector $\lambda \in \mathbb{R}^2$, selecting $\alpha = [0.2722, 0.4590]^T$ at random, and defining the nonsingular bordered matrix $M(y, \mu)$ by (4.4). Applying Newton's method (4.8) to the extended system (4.6) using (b) in the Procedure Summary with $\lambda^{(0)} = [0, 0]^T$, we approximate the bifurcation point $(y^*, \mu^*, \lambda^*) = (0, 0, 0, 0, 0, 0)$. Table 5.3 shows quadratic convergence of Newton's method for this extended system, with $d^{(k)}(y, \mu, \lambda) = \|(y^{(k+1)}, \mu^{(k+1)}, \lambda^{(k)}) - (y^{(k)}, \mu^{(k)}, \lambda^{(k)})\|_2$.

TABLE 5.3
Newton iterations for computing a bifurcation point in Example 5.2.

k	$y_1^{(k)}$	$\mu^{(k)}$	$\lambda_1^{(k)}$	$d^{(k)}(y, \mu, \lambda)$
0	0.0000e+00	-1.0000e-01	0.000e+00	—
1	-5.6807e-18	4.1633e-17	-8.2888e-21	1.0000e-01
2	3.8519e-33	-1.8489e-32	-1.5046e-36	4.2531e-17
3	-6.8423e-49	2.7369e-48	0.0000e+00	1.9641e-32

At the bifurcation point $(y_0, \mu_0) = (0, 0, 0, 0)$ the SVD gives $\sigma_1 = 0.5071$, $\sigma_2 = \sigma_3 = 0$ and

$$L = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad R = \begin{bmatrix} -0.5816 & -0.1984 \\ 0.8109 & -0.0645 \\ -0.0645 & 0.9780 \end{bmatrix}.$$

We solve for β from (4.11) for $i = 2, 3$: $\beta^T \beta = 1$ and

$$\beta^T \begin{bmatrix} 0.0045 & 0 & 0.0022 \\ 0 & 0.0195 & 0.0097 \\ 0.0022 & 0.0097 & 0 \end{bmatrix} \beta = 0,$$

$$\beta^T \begin{bmatrix} 0.0195 & 0 & 0.0097 \\ 0 & -0.0045 & -0.0022 \\ 0.0097 & -0.0022 & 0 \end{bmatrix} \beta = 0.$$

We obtain eight β values:

$$\begin{bmatrix} 0 \\ 0 \\ \pm 1 \end{bmatrix}, \begin{bmatrix} 0 \\ \pm 0.7071 \\ \mp 0.7071 \end{bmatrix}, \begin{bmatrix} \pm 0.7071 \\ 0 \\ \mp 0.7071 \end{bmatrix}, \begin{bmatrix} \pm 0.5774 \\ \pm 0.5774 \\ \mp 0.5774 \end{bmatrix},$$

which with $w = L\beta$ gives eight direction vectors w:

$$\begin{bmatrix} 0 \\ 0 \\ 0 \\ \pm 1 \end{bmatrix}, \begin{bmatrix} \pm 0.7071 \\ 0 \\ 0 \\ \mp 0.7071 \end{bmatrix}, \begin{bmatrix} 0 \\ \pm 0.7071 \\ 0 \\ \mp 0.7071 \end{bmatrix}, \begin{bmatrix} \pm 0.5774 \\ \pm 0.5774 \\ 0 \\ \mp 0.5774 \end{bmatrix}.$$

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Besides the known solution point on the incoming branch, we obtain seven other solutions $(y^*, \mu^*)^T$, each on a different branch:

$$\begin{bmatrix} 0 \\ 0 \\ 0 \\ 0.1 \end{bmatrix}, \begin{bmatrix} 0.073404 \\ 0 \\ 0 \\ -0.068016 \end{bmatrix}, \begin{bmatrix} -0.068373 \\ 0 \\ 0 \\ 0.073047 \end{bmatrix}, \begin{bmatrix} 0 \\ 0.073404 \\ 0 \\ -0.068016 \end{bmatrix},$$

$$\begin{bmatrix} 0 \\ -0.068373 \\ 0 \\ 0.073047 \end{bmatrix}, \begin{bmatrix} 0.058896 \\ 0.058896 \\ 0 \\ -0.055427 \end{bmatrix}, \begin{bmatrix} -0.056670 \\ -0.056670 \\ 0 \\ 0.059881 \end{bmatrix}.$$

We list in Table 5.4 the Newton iterations for the last point, with

$$d^{(k)}(y, \mu) = \|(y^{(k+1)}, \mu^{(k+1)}) - (y^{(k)}, \mu^{(k)})\|_2.$$

TABLE 5.4
Newton iterations for computing branch points in Example 5.2.

k	$y_1^{(k)}$	$y_2^{(k)}$	$y_3^{(k)}$	$\mu^{(k)}$	$d^{(k)}(y,\mu)$
0	-5.7740e-02	-5.7740e-02	0.0000e+00	5.7740e-02	—
1	-5.6689e-02	-5.6689e-02	0.0000e+00	5.9841e-02	2.5735e-03
2	-5.6670e-02	-5.6670e-02	-1.7241e-23	5.9881e-02	4.8580e-05
3	-5.6670e-02	-5.6670e-02	-4.9661e-30	5.9881e-02	1.7311e-08
4	-5.6670e-02	-5.6670e-02	-5.9353e-34	5.9881e-02	2.1932e-15

EXAMPLE 5.3. We apply our method to a single species problem from mathematical biology. Suppose the species grows exponentially with time and disperses by diffusion across a thin region, which we treat as an open interval. At the right end of this interval the species exhibits logistic growth with rate-dependent carrying capacity and migration. This gives rise to a parameterized linear parabolic equation with nonlinear boundary conditions. Let $u(t, x)$ denote the population of the species, and let the population at the right end point of the interval be $v(t)$. We have the following equations:

$$u_t = \mu u + u_{xx}, \quad x \in (0,1) \quad \text{with} \quad u(t,0) = 0, \quad u(t,1) = v(t) \quad \text{and}$$
$$v_t = \mu v[1 - (\beta/\mu)v] + u(t, 1-\epsilon) + (-2 + \mu\epsilon^2)v - c$$

for some small $\epsilon > 0$, where the parameter μ and the constants β, c are all positive.

Now consider the state solutions of the differential equations. Discretize u in x using $h = 1/(N+1)$, $u_{xx}(x) \approx (u(x+h) + u(x-h) - 2u(x))/h^2$. Denoting

$$z = [u(h), u(2h), ..., u(Nh)]^T, \quad y = v$$

and choosing $\epsilon = h$, we obtain the state solutions z, y in the form of (1.1) with $n = 1$:

$$A(y, \mu)z + b(y, \mu) = 0,$$

where

$$A(y,\mu) \equiv \begin{bmatrix} -2+h^2\mu & 1 & & \\ 1 & -2+h^2\mu & \ddots & \\ & \ddots & \ddots & 1 \\ & & 1 & -2+h^2\mu \\ 0 & \dots & 0 & 1 \end{bmatrix}_{(N+1)\times N}$$

and

$$b(y,\mu) \equiv \begin{bmatrix} ye_N \\ (-2+h^2\mu)y + \mu y - \beta y^2 - c \end{bmatrix},$$

with e_N the Nth standard basis element in $\mathbb{R}^N$.

For certain values of the constants β, c, there is a turning point on the solution curve. To illustrate this numerically, we choose $h = 0.1$, so $N = 9$, and we set $\beta = 0.2$, $c = 82.0409593298$. Table 5.5 lists eight successive regular points for (y, μ) along this curve, computed using (4.2)–(4.3) repeatedly. The only singular value σ_1 of the derivative $f'(y,\mu)$ of the reduced function at each point has the value $\sigma_1(y^{(k)}) > 3$. Our method traverses the turning point without difficulty, treating it as any regular point. The turning point, which is near $(y^{(4)}, \mu^{(4)})$, can be located exactly using the methods of [32].

TABLE 5.5
Branch of regular points passing through a turning point in Example 5.3.

k	$y^{(k)}$	$\mu^{(k)}$	k	$y^{(k)}$	$\mu^{(k)}$
1	1.725427e+01	8.162099e+00	5	2.125353e+01	8.106957e+00
2	1.825369e+01	8.127131e+00	6	2.225342e+01	8.122532e+00
3	1.925353e+01	8.107532e+00	7	2.325313e+01	8.146625e+00
4	2.025353e+01	8.101405e+00	8	2.425265e+01	8.177871e+00

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