Solving Nonlinear Equations by Adaptive Homotopy Continuation*

R. Kalaba

Department of Electrical Engineering
and Department of Biomedical Engineering
University of Southern California
Los Angeles, California 90089

and

L. Tesfatsion†

Department of Economics
and Department of Mathematics
Iowa State University
Ames, Iowa 50011

Transmitted by John Casti

ABSTRACT

Standard homotopy continuation methods for solving systems of nonlinear equations require the continuation parameter to move from 0 to 1 along the real line. Difficulties can occur, however, if a point of singularity is encountered during the course of the integration. To ameliorate these difficulties, this paper proposes extending the continuation parameter to complex values and adaptively computing a continuation path in the complex plane that avoids points giving rise to singularities. Specifically, it is proposed that the continuation parameter move from $0+0i$ to $1+0i$ along a spider-web grid centered at $1+0i$ in the complex plane. The actual path through the grid is determined step by step in accordance with two objectives: short path length, and avoidance of singular points. A two-phase homotopy continuation is used to study the implementation of this idea. Numerical examples are presented which indicate the effectiveness of the approach.

*This work was partially supported by NIH Grant DK 33729. The authors are grateful to A. Mas-Colell, J. Miller, J. Nicola, and L. Watson for helpful comments.

†Please address correspondence to the second author.

655 Avenue of the Americas, New York, NY 10010 0096-3003/91/$03.50

1. INTRODUCTION

Standard homotopy continuation methods involve the embedding of a function $F(x)$ into a parametrized family of functions $H(x,t)$ such that $H(x,0)$ has a simple known structure whereas $H(x,1)$ coincides with $F(x)$. Given certain regularity conditions, a solution for the system of nonlinear equations $\mathbf{O} = F(x)$ can in principle be found by following the curve of solutions $x(t)$ to $\mathbf{O} = H(x,t)$ as t varies from 0 to 1 along the real line. (See, e.g., References [1–3].) As is well known, this solution method can fail if there is a singularity of the embedding at some intermediate value of t, a situation which commonly arises when $H(x,0)$ differs significantly from $F(x)$.[1]

As a possible remedy for such singularities, this paper proposes extending the continuation parameter to complex values and adaptively computing a continuation path in the complex plane that avoids parameter values giving rise to singularities. More precisely, it is suggested that the continuation parameter be allowed to move in the complex plane form $0+0i$ to $1+0i$ through a spider-web grid centered at $1+0i$. The actual path through the grid is determined within the algorithm on a step-by-step basis in an attempt to satisfy two potentially conflicting objectives: short path length (minimal number of integration steps), and numerical stability (avoidance of singular points).

A two-phase homotopy continuation is used to study the implementation of this idea. An artificial continuation to obtain complete initial conditions at a starting point c for x is followed by a continuation which is a simple translation of the original system of equations, $\mathbf{O} = F(x)$. As will be clarified below, the Jacobian matrix in the second continuation phase coincides with the Jacobian matrix of $F(\cdot)$, which can ameliorate the problem of artificially induced singularities. In each phase of the continuation, the continuation parameter follows an adaptively computed path in the complex plane.

Section 2 describes in more detail the two-phase homotopy continuation. Section 3 takes up the sequential generation of continuation paths for the continuation parameters in the complex plane. Numerical examples are presented in Section 4, and concluding comments are given in Section 5. A technical remark is given in the appendix.

---

[1] For sufficiently smooth functions $F(\cdot)$, a properly constructed probability-one homotopy [4,5] is theoretically guaranteed to have no singular points for almost all starting points. Successful implementation of probability-one homotopy methods can require a mathematically sophisticated reformulation of the user's original problem.

2. A TWO-PHASE HOMOTOPY CONTINUATION

Let $F: D \subseteq R^n \to R^n$ be a continuously differentiable function for which the system of equations $\mathbf{O} = F(x)$ has at least one solution vector x^*. A standard homotopy continuation method for finding such a solution vector would be to solve a system of equations of the form

$$\mathbf{O} = H(x,t) \equiv t \cdot F(x) + [1-t] \cdot [x-c] \tag{2.1}$$

for x as a function of t as t varies from 0 to 1 along the real line. At $t = 0$, the system (2.1) takes the simple form

$$\mathbf{O} = H(x,0) \equiv x - c, \tag{2.2}$$

with solution vector $x(0) = c$. At $t = 1$, the system (2.1) takes the form

$$\mathbf{O} = H(x,1) \equiv F(x); \tag{2.3}$$

hence a solution vector $x(1)$ for (2.1) at $t = 1$ yields a solution vector for the original system of interest.

Unfortunately, the artificial component $[1-t] \cdot [x-c]$ of the homotopy (2.1) involves the vector x. In consequence, the Jacobian matrix

$$H_x(x(t),t) = t \cdot F_x(x(t)) + [1-t] \cdot I \tag{2.4}$$

is an artificial construct which changes in potentially complicated ways along the real continuation path from $t = 0$ to $t = 1$. In particular, the artificial component can induce singularities or regions of near-singularity in (2.4) even when the Jacobian matrix $F_x(x(t))$ for the original system is well behaved.

This difficulty with (2.1) suggests that it would be desirable to have the continuation path proceed through the original system function $F(\cdot)$ rather than through an artificial construct. First, in many applications the function $F(\cdot)$ represents a physical process. The singular points for such functions tend to be fairly well behaved (e.g., isolated), or at least fairly well understood. In contrast, as seen with (2.1), even the simplest artificially constructed continuation can have singularities or regions of near-singularity which are difficult to determine in advance. Second, having the continuation path proceed through $F(\cdot)$ rather than through an artificial construct has the

important advantage that potentially useful information about $F(\cdot)$ is obtained at each point along the path.

While surely not the only way to proceed, one continuation which essentially satisfies this requirement is the following simple translation of $F(\cdot)$:[2]

$$\mathbf{O} = H^*(x,\beta) \equiv [F(x) - F(c)] + \beta \cdot F(c). \tag{2.5}$$

As β varies from 0 to 1, the system of equations (2.5) varies from the translated form $\mathbf{O} = F(x) - F(c)$ to the system of interest, $\mathbf{O} = F(x)$. However, the Jacobian matrix for (2.5) is not an artificial construct. At each β-point, $H_x^*(x,\beta)$ coincides with $F_x(x)$.

Although singularity problems are potentially ameliorated by use of the β-continuation (2.5), they are not eliminated; the Jacobian matrix $F_x(x)$ could still become singular along the continuation path. Since locating singular points or regions of near-singularity prior to actual integration is generally not practical, the problem of determining a continuation path for β was therefore considered as a sequential multiobjective optimization problem with two objectives: short path length, and avoidance of singular points. Consideration of these two objectives resulted in the development of an algorithm for the step-by-step evolution of a continuation path for β from $0+0i$ to $1+0i$ in the complex plane. The exact determination of this path is taken up in Section 3.

The β-continuation (2.5) can be solved for x as a function of β as β varies from $0+0i$ and $1+0i$ in the complex plane by making use of the analytically complete system of ordinary differential equations developed in [7] for the solution of parametrized systems of nonlinear equations over possibly complex parameter intervals.[3] At each β-point one obtains a solution vector $x^*(\beta)$ together with evaluations $A^*(\beta)$ and $\delta^*(\beta)$ for the adjoint and

---

[2]The idea of using the embedding (2.5) with a *real*-valued continuation parameter β moving from 0 to 1 to solve the system of equations $\mathbf{O} = F(x)$ is by no means new; see, e.g., Reference [1, (3), p. 230] and Reference [6].

[3]More precisely, Reference [7] considers the problem of determining a solution vector $x(\lambda)$ for a *parametrized system of equations* $\mathbf{O} = H(x,\lambda)$. The well-known relation $dx(\lambda)/d\lambda = -(H_x)^{-1}H_\alpha$ is supplemented with ordinary differential equations for the adjoint $A(\lambda)$ and determinant $\delta(\lambda)$ of the Jacobian matrix $H_x(x(\lambda),\lambda)$. This analytically complete system of ordinary differential equations in principle permits *nonlocal sensitivity analysis*, i.e., the tracking of the solution vector $x(\lambda)$ and the sensitivity vector $dx(\lambda)/d\lambda$, together with the adjoint $A(\lambda)$ and determinant $\delta(\lambda)$, over any closed λ-interval where the determinant $\delta(\lambda)$ remains nonzero. For reference, the complete differential system is given in the appendix to the present paper; see Equations (A.4).

determinant of the Jacobian matrix

$$J^*(\beta) \equiv H_x^*(x^*(\beta), \beta) = F_x(x^*(\beta)). \tag{2.6}$$

In principle, the solution vector $x^*(1+0i)$ obtained for (2.5) at $\beta = 1+0i$ yields a solution vector for the original system of equations, $\mathbf{O} = F(x)$.

The initial conditions required by the complete differential system [7] to solve (2.5) at $\beta = 0+0i$ are the solution vector $x^*(0+0i) = c$ together with evaluations for the adjoint and the determinant of the Jacobian matrix $J^*(0+0i) = F_x(c)$. The vector c might be chosen to facilitate some standard algebraic method for obtaining these evaluations. Alternatively, these evaluations can be obtained differentially by solving the continuation

$$\mathbf{O} = \hat{H}(x, \theta) \equiv \theta \cdot [F(x) - F(c)] + [1+0i-\theta] \cdot J \cdot [x - c] \tag{2.7}$$

for x as a function of θ over a complex continuation path from $\theta = 0+0i$ to $\theta = 1+0i$, again by use of the complete differential system [7]. In (2.7), c denotes an initial guess for a solution vector for $\mathbf{O} = F(x)$ and J denotes an initial guess for the Jacobian matrix $F_x(c)$. The expression $J \cdot [x - c]$ thus constitutes a linear approximation for $F(x) - F(c)$, expanded around c.

The initial conditions required by the complete differential system [7] to solve (2.7) at $\theta = 0+0i$ are $\hat{x}(0+0i) = c$, $\hat{A}(0+0i) = \text{Adj}(J)$, and $\hat{\delta}(0+0i) = \text{Det}(J)$. At each subsequent θ-point, one obtains the (constant) solution vector $\hat{x}(\theta) = c$ for the system (2.7), together with evaluations for the adjoint $\hat{A}(\theta)$ and the determinant $\hat{\delta}(\theta)$ of the Jacobian matrix

$$\hat{J}(\theta) \equiv \hat{H}_x(x(\theta), \theta) = \theta \cdot F_x(c) + [1+0i-\theta] \cdot J. \tag{2.8}$$

The components of the Jacobian matrix $\hat{J}(\theta)$ have constant rates of change with respect to θ, i.e., $d\hat{J}(\theta)/d\theta = F_x(c) - J$, and these rates of change are reduced in magnitude to the extent that J is a good initial guess for $F_x(c)$.[4] At $\theta = 1+0i$, the system of equations (2.7) reduces to $\mathbf{O} = F(x) - F(c)$. Thus, the system (2.7) at $\theta = 1+0i$ coincides with the system (2.5) at $\beta = 0+0i$; and the solution for the system (2.7) at $\theta = 1+0i$ provides the needed initial conditions for the solution of the system (2.5) at $\beta = 0+0i$.

An important conceptual issue still needs to be addressed: How are the complex continuation paths for the continuation parameters β and θ in (2.5) and (2.7) to be determined? The following section takes up this question.

---

[4] As reported in Section 4 below, setting $J = I$ has in fact worked well in simulation experiments to date.

3. SEQUENTIAL DETERMINATION OF COMPLEX CONTINUATION PATHS

This section describes the algorithm used to generate continuation paths for the continuation parameters β and θ in (2.5) and (2.7). Each continuation path evolves sequentially in the complex plane in an attempt to keep the path as short as possible while avoiding points of singularity. Since the algorithm is similarly applied in both the β and θ continuation phases, the symbol λ is used below to denote either of the continuation parameters β or θ.

A basic assumption maintained throughout this section is that at least one path exists from $\lambda = 0+0i$ to $\lambda = 1+0i$ along which the absolute value of the system determinant $\delta(\lambda)$ is uniformly bounded away from zero.[5] However, no such path is known *a priori*. The problem is then to determine, on a step-by-step basis, an actual path of integration from $\lambda = 0+0i$ to $\lambda = 1+0i$ in approximate agreement with the shortness and stability objectives.

For simplicity, this problem is addressed in two stages. First, on what type of grid is λ going to be allowed to move? Second, how is the actual path taken by λ through the grid to be decided?

First consider the grid. If the continuation path is to be kept short, then it should be geometrically possible to proceed in a direct line to the desired endpoint $1+0i$ from any given current point on the grid. If the continuation path is to be numerically stable, singular points must of course be avoided; but the geometry of the grid should permit this avoidance to be carried out efficiently with respect to the shortness criterion. In particular, it should be geometrically possible to step away from a singular point without increasing the distance to the endpoint $1+0i$. This in turn suggests that the grid mesh should be denser in a neighborhood of the endpoint $1+0i$ in order to permit intricate paths to evolve in this neighborhood without increasing the distance from $1+0i$.

One simple grid specification which satisfies these geometric requirements is the spider-web grid depicted in Figure 1. This spider-web grid consists of a nested family of concentric circles ("rims") in the complex plane with common center $1+0i$, and with a number of equally spaced rays ("spokes") branching out from this common center. Points on the grid are defined by the intersections of spokes and rims. Starting from any current point on the grid, it is geometrically possible for the continuation parameter λ to proceed in a direct line to the endpoint $1+0i$ by stepping inward along the current spoke. On the other hand, a singular point along a current spoke can be avoided by taking a suitable number of rim steps before again attempting an inward spoke step. Rim steps do not increase the distance to

[5]The determinant $\delta(\lambda)$ denotes $\delta\hat{}(\theta)$ when $\lambda \equiv \theta$, and $\delta^*(\beta)$ when $\lambda \equiv \beta$.

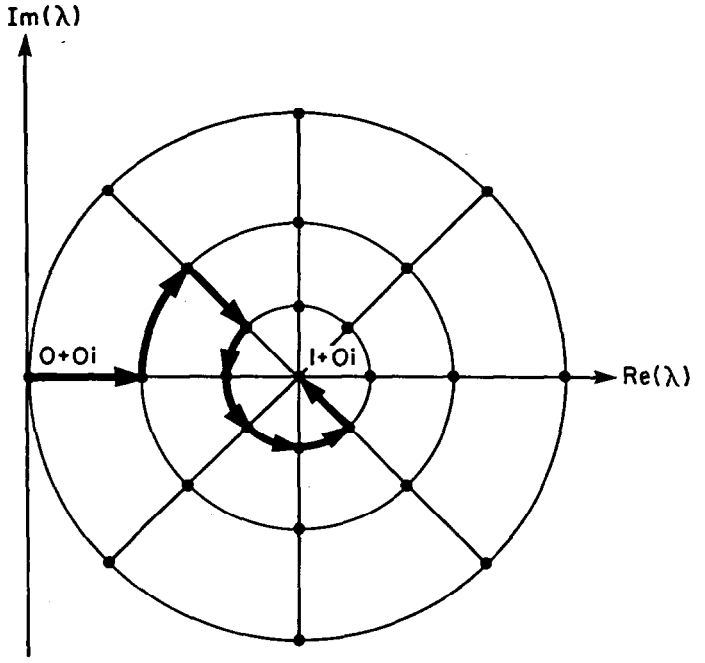

FIG. 3.1. Schematic illustration of a sequentially determined integration path for the continuation parameter λ through a complex spider-web grid.

the endpoint $1+0i$. Finally, the grid mesh along rims automatically becomes finer in a neighborhood of $1+0i$.

One possible path for the continuation parameter λ through the spider-web grid is depicted in Figure 1. How is the exact path taken by λ to be decided? The basic steps of the algorithm take the following form.

Suppose a minimum tolerance level TOL has been set for the absolute value $|\delta(\lambda)|$ of the determinant of the Jacobian matrix. Starting at any current point λ on the grid, an inward step $\Delta\lambda$ along the current spoke is considered. If this spoke step passes the tolerance test, i.e., if $|\delta(\lambda+\Delta\lambda)| \geqslant \text{TOL}$, then the spoke step is actually taken. Another inward step $\Delta\lambda$ along the current spoke is then considered. If this process continues without ever encountering a tolerance-test failure, then eventually the desired endpoint $\lambda = 1+0i$ is attained by successive inward steps along the current spoke.

On the other hand, if some considered spoke step fails the tolerance test, additional tolerance tests are performed to see if a rim step to a new spoke is possible at the current tolerance level. If so, the rim step is taken. An attempt is then made to have the continuation parameter attain the endpoint $1+0i$ by successive inward steps along the new spoke, in the manner described

above. If not, the minimum tolerance level TOL is relaxed (i.e., adjusted downward) until either an inward spoke step or a rim step away from the current point does pass the tolerance test. This step is then taken, and again an attempt is made to have the continuation parameter attain the endpoint $1+0i$ by successive inward steps along the new spoke. If a complete revolution around the current rim is made without finding a tolerable inward spoke step, then the minimum tolerance level TOL is relaxed until an inward spoke step from some point along the current rim does pass the tolerance test.[6] This spoke-step is then taken, and an attempt is made to continue stepping inward along this spoke until the endpoint $1+0i$ is attained.

In summary, this sequential procedure is designed to allow the continuation parameter λ to make its way from $0+0i$ to the desired endpoint $1+0i$ along a path which is both reasonably short and reasonably distant from singular points. The increasing fineness of the spider-web grid mesh along rims in a neighborhood of the endpoint $1+0i$ increases the chances that λ will reach the endpoint $1+0i$ even when the only tolerable path to $1+0i$ is a narrow curvy ridge. The possible reduction in the minimum tolerance level TOL along the integration path also enhances the possibility that λ will reach $1+0i$. For example, TOL may have to be substantially reduced over the final portion of the continuation path if the endpoint $1+0i$ is surrounded by a region in which the determinant $\delta(\lambda)$ is nearly zero. An example of this kind is given in the next section.

4. NUMERICAL EXAMPLES

This section reports on several numerical experiments conducted to test the ability of the two-phase complex continuation method to determine accurately a solution vector x^* for a system of equations $\mathbf{O} = F(x)$, together with evaluations A^* and δ^* for the adjoint and determinant of the Jacobian matrix $F_x(x^*)$. The experiments were carried out using a single-precision Fortran program *Nasa* (*N*onlocal *a*utomated *s*ensitivity *a*nalysis) developed in [8] for the sensitivity analysis of parametrized systems of nonlinear equations over parameter intervals.[7] The program incorporates a fourth-order Adams-Moulton integration method with a Runge-Kutta start, a recently developed method *Feed* for automatic derivative evaluation [9], and an

[6] Alternatively, for analytical functions $F(\cdot)$ one might use Cauchy residue formulas to obtain the desired evaluations at the center point $\lambda = 1+0i$ by appropriate integrations around the circular closed curve defined by the current rim.

[7] Specifically, *Nasa* numerically solves the complete differential system developed in [7]; see the appendix to this paper.

automatic initialization procedure based on the two-phase complex homotopy continuation method developed in Sections 2 and 3.[8]

In contrast to successive-approximation methods, the two-phase homotopy continuation method is a one-sweep procedure. That is, if the successive integrations along the closed θ and β continuation paths from $0+0i$ to $1+0i$ could be carried out in an exact manner, with all singular points successfully avoided, then in principle the evaluations $x^*(1+0i)$, $A^*(1+0i)$, and $\delta^*(1+0i)$ obtained at the endpoint $\beta = 1+0i$ should be solution values of the form x^*, A^*, and δ^*. In practice, however, roundoff and truncation errors degrade the accuracy of these evaluations, especially when the initial guess c for a solution vector is highly inaccurate. Specifying a smaller integration step size or an increased word length are two obvious ways one could attempt to increase numerical accuracy. Another possibility, however, is to turn the two-phase continuation method into a successive-approximation method by repeating the successive θ and β continuations in an iterative fashion. The approximate solution vector obtained at the end of one run of the successive θ and β continuations becomes the updated starting vector c for the next. The latter alternative has worked well in the numerical experiments conducted to date.

Specifically, in experiments run for a variety of functions $F(\cdot)$ having either one or two component functions, the evaluations obtained for x^*, A^*, and δ^* using at most two θ-β iterations (i.e., two repetitions of the successive θ and β continuations) were accurate to about four or five decimal places. This level of accuracy was obtained even for highly inaccurate initial guesses c, and despite the fact that no attempts were made to optimize the program specifications for the sequential determination of complex continuation paths for the continuation parameters. Typical CPU running times on an IBM 3090 were on the order of one to ten seconds.

For illustration, first consider the following variant of a single-equation problem investigated in Reference [10]:

$$\mathbf{O} = F(x) \equiv x - 1 + \log 1.5 + \log x. \tag{4.1}$$

The unique solution for (4.1) is $x^* = 0.807878\ldots$, with $\delta^* = 2.23781\ldots$.

---

[8] A natural consequence of this incorporation of the two-phase complex homotopy continuation method is that all variables in *Nasa* are dimensioned as complex variables. The use of complex-valued variables is potentially beneficial regardless of the method proposed for solving $\mathbf{O} = F(x)$. If the components of $F(\cdot)$ involve exponentials or logarithms, as is often the case, then difficulties can arise during the course of the solution procedure in the form of negative radicands or negative arguments for logarithms. The use of complex-valued variables eliminates these difficulties. Unfortunately, the software available to us at USC prohibited the use of double precision with complex-variable calculations.

TABLE 1

Numerical Solution of the Example (4.1)[a]

Starting value c	No. of θ-β iterations	Complex θ, β paths?	Numerical solution		
			x	δ	$F(x)$
$0.40+0i$	1	No	.80789E+00	.22377E+01	−.24795E−04
	2	No	.80788E+00	.22377E+01	−.37551E−05
$100+0i$	1	No	.80137E+00	.22483E+01	−.14694E−01
	2	No	.80787E+00	.22377E+01	−.11906E−04
$10+10i$	1	No	.80751E+00	.22382E+01	−.84686E−03
	2	No	.80788E+00	.22377E+01	−.84629E−05
$-1+0i$	1	θ, not β	(.53587E+01, .90648E+01)	(.47044E+01, −.90757E+01)	(−.35990E+01, .11170E+02)
	2	θ, not β	(.80788E+00, −.6109E−04)	(.22378E+01, .11628E−03)	(−.19074E−05, −.01478E−03)

[a]Analytical solution: $x^* = 0.807878\ldots$, $\delta^* = 2.23781\ldots$.

Various numerical experiments were run for the problem (4.1) with different starting values c for x, and with either one or two θ-β iterations.[9] As indicated in Table 1, at most two θ-β iterations resulted in convergence to approximate solution values for x^* and δ^* which were accurate to about four or five decimal places, even for highly inaccurate starting values c. For these values, $F(\cdot)$ itself was reduced to about 10^{-5}.

What kinds of continuation paths evolved for θ and β in each case? For each different starting value c, and for each iteration, the continuation parameter β moved from $0+0i$ to $1+0i$ along the real axis using the least possible number of integration steps for the given program specifications (i.e., 200 steps of size 0.005). Deviations into the complex plane to avoid singular points or regions of near-singularity did not turn out to be necessary. The same was true for the continuation paths for θ, with one exception; namely, when the starting value for x was chosen to be $c = -1.0+0i$.

[9]The following common program specifications were used for all of the numerical experiments reported in this section (see [8] for detailed explanations): $J = I$; VSS ≡ [integration step size along spokes] = 0.005; NSPS ≡ [total number of spoke steps to be taken, with VSS · NSPS = 1] = 200; MAXRS ≡ [maximum number of one-degree rim steps which can be taken along any one rim] = 360; TOL ≡ [initial minimum tolerance level for the absolute value of the determinant of the system Jacobian in the first θ-continuation phase] = 0.007; NR ≡ [number of one-degree rim steps to be attempted before another tolerance test after a spoke-step tolerance-test failure] = 1; and RED ≡ [reduction factor for reducing TOL when no tolerable move from the current point can be found at the current tolerance level] = 0.90.

For the latter case, the first θ-β iteration resulted in the evolution of an intricate path for the continuation parameter θ in a small neighborhood of the desired endpoint $\theta = 1 + 0i$. Specifically, θ first took 180 integration steps of size 0.005 along the real line to reach $\theta = 0.9 + 0i$, at which point a tolerance-test failure occurred. Ultimately, an additional 1238 one-degree rim steps and 20 spoke steps in the complex plane were needed to reach $\theta = 1 + 0i$. The minimum tolerance level TOL along this complex continuation path was sequentially reduced from $0.007\text{E} + 00$ at $\theta = 0.9 + 0i$ to $0.389\text{E} - 03$ at $\theta = 1 + 0i$. The succeeding β-path was entirely real, but the approximate solution values $(x^{\#}, \delta^{\#})$ obtained for x^* and δ^* at the end of the first θ-β iteration were far from satisfactory. Despite all this, starting from $c = x^{\#}$, the second θ-β iteration went quickly and smoothly to approximate solution values for x^* and δ^* which were accurate to five decimal places. Each of the continuation parameters θ and β followed an entirely real path, and took the least possible number of integration steps (200) to reach $1 + 0i$.

A more challenging two-equation system will now be considered. Consider the problem of numerically solving

$$\mathbf{O} = F(x), \tag{4.2a}$$

where the function $F = (F^1, F^2)$ taking R^2_{++} into R^2 is defined by

$$F^1(x_1, x_2) \equiv \tfrac{1}{2}(x_1)^{-1/2}(x_2)^{1/3} - 0.5; \tag{4.2b}$$

$$F^2(x_1, x_2) \equiv \tfrac{1}{3}(x_1)^{1/2}(x_2)^{-2/3} - \tfrac{1}{3}. \tag{4.2c}$$

The unique solution for (4.2) is $x^* = (1, 1)$, with $\delta^* = 0.02777\ldots$.

The problem (4.2) was considered in Reference [11], where it arose as the first-order necessary conditions for the maximization of firm profits with a "Cobb-Douglas" production function. Attempts to solve (4.2) by means of a simple t-continuation of the form (2.1) with the continuation parameter t following a real path from 0 to 1 failed repeatedly for different starting vectors c because the Jacobian matrix (2.4) became singular at some intermediate t-point. For example, with a starting vector $c = (1.2, 1.1)$, the Jacobian matrix (2.4) for the problem (4.2) has a singular point at approximately $t = 0.7$. Attempts to sidestep the singular points by having t take a prespecified U-shaped detour into the complex plane were only moderately successful. Regions of near-singularity were encountered along the path, which reduced integration accuracy, especially for starting vectors c which were an appreciable distance away from the exact solution vector $(1, 1)$.

When *Nasa* was used for the numerical solution of the problem (4.2) for a variety of starting vectors c, it was found that at most two θ-β iterations resulted in approximate solution values for x^* and δ^* which were accurate to about four or five decimal places. For these values, the real and imaginary parts of the component functions of $F(\cdot)$ were reduced to about 10^{-5} and 10^{-6}, respectively. Some of these numerical experiments are summarized in Table 2.

In each case depicted in Table 2, the continuation paths which evolved for β in the first and second θ-β iterations, and for θ in the second θ-β iteration, were entirely real and of minimum length for the given program specifications. Specifically, each path consisted of 200 steps of size 0.005 from $0+0i$ to $1+0i$ along the real axis. In contrast, in the first θ-β iteration for each case, the continuation path which evolved for θ became complex and intricate in a small neighborhood of the endpoint $1+0i$.

For example, in the first θ-β iteration of the experiment with starting vector $c=(15+0i,5+0i)$, the continuation parameter θ first took 180 integration steps of size 0.005 along the real axis at the minimum tolerance level TOL = 0.007E+00. A tolerance-test failure then occurred when a further inward step along the real-axis spoke was considered. The continuation parameter θ subsequently had to take 48 one-degree rim steps in the counterclockwise direction before it found another spoke along which it could continue stepping inward in the direction of the desired endpoint $1+0i$ at the current minimum tolerance level TOL = 0.007E+00. An additional 1925 integration steps, and a reduction in TOL from 0.007E+00 down to 0.247E−03, were ultimately needed to achieve $1+0i$ through the spider-web grid.

As is clear from the previous discussion, most of the computation for the numerical solution of the example (4.2) involved the θ-continuation used to obtain evaluations for the adjoint and determinant of the Jacobian matrix $F_x(c)$ at the starting vector c. As seen in Table 2, for each starting vector c the continuation parameter θ was forced to take on complex values in order to avoid regions where the absolute value of the determinant failed to exceed the minimum tolerance level TOL. On the other hand, since the function $F(\cdot)$ for this example has a nonsingular Jacobian matrix over the positive orthant, it is not surprising that the β-continuation parameter was never forced to veer into the complex plane. The question thus arises whether the use of an alternative method for solving the problem (4.2) would be more efficient.

John Miller at Texas Tech recently investigated five different methods for solving the example (4.2):[10] the predictor-corrector method [13], M. J. D. Powell's hybrid nonlinear solver, Newton's method, an IMSL subroutine,

[10] Private correspondence, 16 February and 26 March 1990.

TABLE 2

NUMERICAL SOLUTION OF THE EXAMPLE (4.2)[a]

No. θ-β iters.	c_1 c_2	Complex θ, β paths?	Numerical solution x_1 x_2	δ	$F_1(x)$ $F_2(x)$
1	$1.2+0i$	θ, not β	(.10E+01, +.79E−05)	(.28E−01, +.13E−05)	(.39E−05, −.75E−06)
	$1.1+0i$		(.10E+01, +.73E−05)		(.25E−05, −.32E−06)
1	$6.0+0i$	θ, not β	(.10E+01, −.12E−02)	(.27E−01, +.63E−04)	(−.15E−02, .91E−04)
	$5.0+0i$		(.10E+01, −.12E−02)		(−.12E−02, .68E−04)
2	$6.0+0i$	θ, not β	(.10E+01, −.51E−06)	(.28E−01, −.84E−06)	(.86E−05, +.34E−07)
	$5.0+0i$		(.10E+01, −.56E−06)		(.36E−05, +.40E−07)
1	$10+0i$	θ, not β	(.11E+01, −.52E−03)	(.23E−01, +.23E−04)	(−.58E−02, .37E−04)
	$9+0i$		(.11E+01, −.54E−03)		(−.51E−02, .30E−04)
2	$10+0i$	θ, not β	(.10E+01, −.28E−06)	(.28E−01, −.54E−07)	(.67E−05, .20E−07)
	$9+0i$		(.10E+01, −.30E−06)		(.44E−05, .20E−07)
1	$15+0i$	θ, not β	(.11E+01, +.58E−04)	(.22E−01, +.10E−06)	(−.12E−01, −.29E−05)
	$5+0i$		(.11E+01, +.66E−04)		(−.33E−02, −.46E−05)
2	$15+0i$	θ, not β	(.10E+01, −.27E−07)	(.28E−01, −.71E−08)	(.62E−05, .20E−08)
	$5+0i$		(.10E+01, −.29E−07)		(.50E−05, .19E−08)
1	$15+0i$	θ, not β	(.12E+01, −.32E−02)	(.17E−01, +.79E−04)	(−.15E−01, .16E−03)
	$15+0i$		(.13E+01, −.35E−02)		(−.15E−01, .19E−03)
2	$15+0i$	θ, not β	(.10E+01, +.46E−04)	(.28E−01, −.10E−03)	(.29E−05, −.99E−05)
	$15+0i$		(.10E+01, .+99E−05)		(.38E−05, +.55E−05)

[a]Analytical solution: $x^* = (1, 1)$, $\delta^* = 0.02777\ldots$.

and the ODE method proposed by Shampine and Gordon [12]. For the predictor-corrector method, which implements the β-continuation (2.5) with real-valued β, the example (4.2) was solved for 10,000 randomly generated starting vectors c with component values lying between $\frac{1}{10}$ and 10. According to Miller, the predictor-corrector program found the solution $(1, 1)$ quickly and smoothly, without apparent difficulty, in each of the 10,000 cases. Powell's method worked frequently, and when it did work, it worked as smoothly and rapidly as the predictor-corrector method. The ODE program did not work often, and even when it did work, it converged slowly and achieved results which were not very satisfactory. Newton's method and the IMSL subroutine did not work for any of the test cases attempted.

5. DISCUSSION

The basic proposal put forward in this paper is that paths for continuation parameters should be allowed to take on complex values and to evolve adaptively in the complex plane in order to avoid singular points. In this way an algorithm is achieved which adapts to whatever physical problem is at hand, with no required problem reformulations.

This proposal is investigated for the particular two-phase homotopy continuation described in Section 2, and for the particular spider-web algorithm described in Section 3 for the adaptive computation of the continuation path. Numerical examples presented in Section 4 suggest that allowing the continuation parameters to take on complex values, and to evolve adaptively in the complex plane, significantly enhances the ability of the two-phase homotopy continuation to generate useful approximate solutions for systems of nonlinear equations.

Further experimental and theoretical work is needed to determine more generally the power of adaptive homotopy continuation methods for solving nonlinear systems.

APPENDIX. A COMPLETE DIFFERENTIAL SYSTEM FOR HOMOTOPY CONTINUATION

Consider the problem of determining the response of a vector $x^* = (x_1^*, \ldots, x_n^*)$ to changes in a scalar λ^*, where x^* and λ^* are required to satisfy an n-dimensional system of nonlinear equations of the form

$$\mathbf{O} = H(x, \lambda) \equiv \begin{bmatrix} H^1(x, \lambda) \\ \vdots \\ H^n(x, \lambda) \end{bmatrix}. \tag{A.1}$$

Given standard regularity conditions, the implicit-function theorem guarantees the existence of a continuously differentiable function $x(\lambda)$ taking some open neighborhood $N(\lambda^*)$ of λ^* into R^n such that

$$\mathbf{O} = H(x(\lambda), \lambda), \qquad \lambda \in N(\lambda^*). \tag{A.2}$$

From (A.2) one obtains the fundamental equation of sensitivity analysis,

$$\frac{dx(\lambda)}{d\lambda} = -H_x(x(\lambda), \lambda)^{-1} H_\lambda(x(\lambda), \lambda), \qquad \lambda \in N(\lambda^*). \tag{A.3}$$

As it stands, (A.3) is an analytically incomplete system of ordinary differential equations. That is, a closed-form representation for the Jacobian inverse $J(\lambda)^{-1} \equiv H_x(x(\lambda), \lambda)^{-1}$ as a function of λ is often not obtainable for $n \geqslant 3$. Thus, the integration of (A.3) from initial conditions would typically require the supplementary algebraic determination of the Jacobian inverse $J(\lambda)^{-1}$ at each step in the integration process.

In [7] the differential system (A.3) is extended by the incorporation of ordinary differential equations for the Jacobian inverse. More precisely, letting $A(\lambda)$ and $\delta(\lambda)$ denote the adjoint and the determinant of the Jacobian matrix $J(\lambda)$, and recalling that the inverse of any nonsingular matrix can be represented as the ratio of its adjoint to its determinant, the following differential system is validated for $x(\lambda)$, $A(\lambda)$, and $\delta(\lambda)$:

$$\frac{dx(\lambda)}{d\lambda} = -\frac{A(\lambda) H_\lambda(x(\lambda), \lambda)}{\delta(\lambda)}, \tag{A.4a}$$

$$\frac{dA(\lambda)}{d\lambda} = \frac{A(\lambda)\,\mathrm{Trace}(A(\lambda)B(\lambda)) - A(\lambda)B(\lambda)A(\lambda)}{\delta(\lambda)}, \tag{A.4b}$$

$$\frac{d\delta(\lambda)}{d\lambda} = \mathrm{Trace}(A(\lambda)B(\lambda)), \tag{A.4c}$$

where $B(\lambda) \equiv dJ(\lambda)/d\lambda$ is a matrix whose ijth component is

$$\sum_{k=1}^{n} \left(H^i_{jk}(x(\lambda), \lambda) \cdot \frac{dx_k(\lambda)}{d\lambda} \right) + H^i_{j,n+1}(x(\lambda), \lambda). \tag{A.4d}$$

Given (A.4a), note that each of the components (A.4d) is expressible as a known function of $x(\lambda)$, $A(\lambda)$, $\delta(\lambda)$, and λ. Initial conditions for Equations

(A.4a) through (A.4c) must be provided at a parameter point λ^* by specifying values for $x(\lambda^*)$, $A(\lambda^*)$, and $\delta(\lambda^*)$ satisfying

$$H(x(\lambda^*), \lambda^*) = 0, \tag{A.4e}$$

$$A(\lambda^*) = \mathrm{Adj}(J(\lambda^*)), \tag{A.4f}$$

$$\delta(\lambda^*) = \mathrm{Det}(J(\lambda^*)) \neq 0. \tag{A.4g}$$

The system of equations (A.4) provides an analytically complete system of ordinary differential equations for tracking the solution vector $x(\lambda)$ and the sensitivity vector $dx(\lambda)/d\lambda$, together with the adjoint $A(\lambda)$ and determinant $\delta(\lambda)$ of the Jacobian matrix $J(\lambda)$, over any λ-interval $[\lambda^*, \lambda^{**}]$ where the determinant remains nonzero. The feasibility of carrying out nonlocal sensitivity analysis is thus enhanced.

To make the differential system (A.4) into a practical numerical tool, some method is needed for the automatic evaluation of derivatives. The components (A.4d) of the matrix $B(\lambda)$ appearing in (A.4b, c) involve the second-order partial derivatives of H. The Fortran program *Nasa* developed in [8] for solving the differential system (A.4) incorporates a fast and efficient algorithm *Feed* [9] for the automatic evaluation of higher-order partial derivatives.

REFERENCES

1 J. M. Ortega and W. C. Rheinboldt, *Iterative Solution of Nonlinear Equations in Several Variables*, Academic, New York, 1970.

2 E. Allgower and K. Georg, Simplicial and continuation methods for approximating fixed points and solutions to systems of equations, *SIAM Rev.* 22:28–85 (1980).

3 W. Zangwill and C. Garcia, *Pathways to Solutions, Fixed Points, and Equilibria*, Prentice-Hall, Englewood Cliffs, N.J., 1981.

4 S. N. Chow, J. Mallet-Paret, and J. A. Yorke, Finding zeros of maps: Homotopy methods that are constructive with probability one, *Math. Comp.* 32:887–899 (1978).

5 L. Watson, T. C. Billups, and A. P. Morgan, Algorithms G52:HOMPACK: A suite of codes for globally convergent homotopy algorithms, *ACM Trans. Math. Software* 13(3):281–310 (1987).

6 J. Miller, Finding the zeros of an analytical function, *Appl. Math. Comput.* 27:243–249 (1988).

7 R. Kalaba and L. Tesfatsion, Complete comparative static differential equations, *J. Nonlinear Anal. TMA* 5:821–833 (1981).

8 R. Kalaba and L. Tesfatsion, Nonlocal automated sensitivity analysis, *Comput. and Math. Appl.*, 20:53–65 (1990).
9 R. Kalaba, L. Tesfatsion, and J.-L. Wang, A finite algorithm for the exact evaluation of higher-order partial derivatives of functions of many variables, *J. Math. Anal. Appl.* 92:552–563 (1983).
10 A. Khilnani and E. Tse, A fixed point algorithm with economic applications, *J. Econom. Dynamics Control* 9:127–137 (1985).
11 J.-L. Wang, The Computation and the Sensitivity Analysis of Economic Equilibrium, Dissertation, Dept. of Economics, Univ. of Southern California, July 1984.
12 L. Shampine and M. Gordon, *Computer Solution of Ordinary Differential Equations: The Initial Value Problem*, Freeman, San Francisco, 1975.
13 C. Martin, J. Miller, and K. Pearce, Parameter identification by continuation methods, *Appl. Math. Comput.* 34:17–27 (1989).