A Simple Method for Tracking Turning Points in Parameter Space

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We describe a simple method for tracking solutions of nonlinear equations $f(u, \alpha) = 0$ through turning points (also known as limit or saddle-node bifurcation points). Our implementation makes use of symbolic software such as Mathematica to derive an exact system of nonlinear ODE equations to follow the solution path, using a parameterization closely related to arc length. We illustrate our method with examples taken from the engineering literature, including examples that involve nonlinear boundary value problems that have been discretized by finite difference methods. Since the code requirement to implement the method is modest, we believe the method is ideal for demonstrating continuation methods in the classroom.

Introduction

Mathematical models in chemical engineering transport phenomena (e.g., mass, heat and momentum transfer) can often be classified as lumped parameter models represented mathematically as system of ODEs in the form of Eq. (1), or as balance equations represented mathematically as systems of PDEs.

$$\frac{d\boldsymbol{u}}{dt} = \boldsymbol{f}(\boldsymbol{u}, \alpha) \tag{1}$$

A prototypical example of the latter is a reaction-diffusion system in the form of Eq. (2).

$$\frac{\partial \boldsymbol{u}}{\partial t} = \nabla^2 \boldsymbol{u} + \boldsymbol{R}(\boldsymbol{u}, \alpha) \tag{2}$$

Of interest in many applications are the equilibrium or steady state solutions. For lumped parameter models the steady state solutions are given by a system of nonlinear equations, as shown by Eq. (3).

$$\boldsymbol{f}(\boldsymbol{u}, \alpha) = 0 \tag{3}$$

Contrarily, in the case of balance equations, the steady state solutions, are given by a system of nonlinear boundary value problems (BVPs) as shown by Eq. (4), which are subjected to appropriate boundary conditions.

$$\nabla^2 \boldsymbol{u} + \boldsymbol{R}(\boldsymbol{u}, \alpha) = 0 \tag{4}$$

When the steady state solution space of either Eq.

(3) or (4) contains turning points (their locations are usually unknown *a priori*), special continuation methods are needed to track solutions in parameter space. The issue at hand is made plain by considering the following simple example of Eq. (5).

$$\frac{dy}{dt} = f(y, \alpha) \equiv [1 - \alpha + (y - 2)^2] \tag{5}$$

If y_s represents the steady state solution that satisfies $f(y, \alpha) = 0$, then by inspection, the steady state solution space is described by Eq. (6).

$$y_s = 2 \pm \sqrt{\alpha - 1} \tag{6}$$

These solutions are represented by the zero level set contour of $f(y_s, \alpha)$ as illustrated in **Figure 1**. The two solution families intersect at a turning point (also referred to as a limit point, or saddle-node bifurcation) located at $\alpha = 1$. If (y_s^*, α^*) denotes the intersection point, then mathematically the turning point is described by Eq. (7).

$$f(y_2^*, \alpha^*) = 0, \quad \left(\frac{\partial f}{\partial y}\right)_{y_s^*, \alpha^*} = 0, \quad \left(\frac{\partial f}{\partial \alpha}\right)_{y_s^*, \alpha^*} \neq 0 \tag{7}$$

Plainly, the tangent to the curve $dy\_s/d\alpha$ is not defined at the turning point. Without knowing much about our function $f(y, \alpha)$, one might attempt to find a point on the curve (y_0, α_0), and then integrate along the curve by solving the following initial value problem of Eq. (8).

$$\frac{dy\_s}{d\alpha} = -\frac{\partial f / \partial \alpha}{\partial f / \partial y_s} = \frac{1}{2(y_s - 2)}, \quad y_s(\alpha_0) = y_0 \tag{8}$$

Unfortunately, this naive approach of using α as the continuation parameter will fail at the turning point
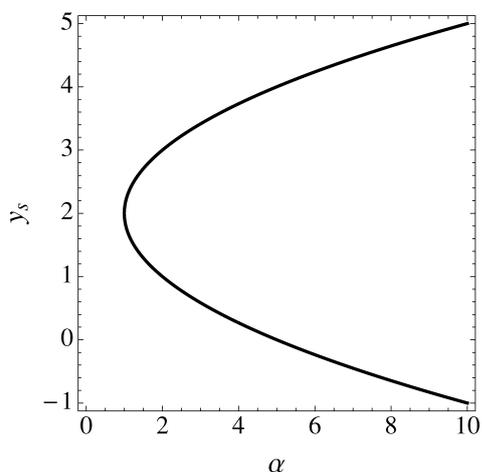
Fig. 1 Solution curve y versus α with a single turning point at $\alpha = 1$; see Eq. (5)

$y_s = 2$.

An accepted method to handle this type of singularity is to introduce a reparameterization of the problem in terms of arc length along the solution curve. Arc length and pseudo-arc length continuation methods are widely used in bifurcation theory (see Seydel (1988) for an overview of methods). Popular open source software packages such as AUTO (Doedel, 1981), and MATCONT (Dhooge *et al.*, 2003) are readily available for implementing continuation methods for many engineering related problems.

The goal of this paper is to introduce a variant of the arc length continuation method for handling saddle-node bifurcations called turning points. Although the method we propose builds on the standard approach used in the literature (Seydel, 1988; Nayfeh and Balachandran, 1995), we implement a result from the homotopy literature that does not appear to be widely known. We show that, with the capability of symbolic software such as Mathematica (Wolfram Research Inc.), it is possible to devise an arc length continuation method for handling turning points without the need to write complicated code. The underlying mathematics is covered in a typical undergraduate calculus course, and thus it is practical to introduce our method into the undergraduate engineering curriculum. Further, the simplicity of the method means that researchers who need unexpectedly to track steady state solutions with turning points, but whose main area of research is not nonlinear dynamics, have an alternative method that does not require learning new software tools such as AUTO (http://indy.cs.concordia.ca/auto/). All that is needed is access to symbolic software such as Mathematica or Maple (Waterloo Maple Inc.), both of which are widely available. In the next section we review the existing theory of arc length continuation and the proposed new method. We then show how the method can be used to track steady state solutions from lumped parameter mod-

els and boundary value problems that have been discretized by finite difference methods. We conclude with a brief discussion on the possible limitations of our method and suggestions for future work.

1. Arc Length Continuation

Consider a set of N nonlinear algebraic equations that depend on a parameter α. In vector notation these equations are represented as Eq. (9)

$$\boldsymbol{f}(\boldsymbol{u}, \alpha) = 0 \tag{9}$$

The components of the vectors $\boldsymbol{f}$ and $\boldsymbol{u}$ are given by Eq. (10).

$$\boldsymbol{f} = \{f_1, f_2, \ldots, f_N\}, \ \boldsymbol{u} = \{u_1, u_2, \ldots, u_N\} \tag{10}$$

Suppose we have found a solution pair $(\boldsymbol{u}_0, \alpha_0)$ to Eq. (9) by Newton's method. We represent the solution as Eq. (11).

$$\boldsymbol{f}(\boldsymbol{u}_0, \alpha_0) = 0 \tag{11}$$

Let us suppose that the solution $\boldsymbol{u}$ is an analytic function of α, i.e. $\boldsymbol{u} = \boldsymbol{u}(\alpha)$ is continuous and differentiable. Then, given a solution $\boldsymbol{u}_0 = \boldsymbol{u}(\alpha_0)$, we can find a neighboring solution $\boldsymbol{u} = \boldsymbol{u}(\alpha)$ on the solution curve by constructing a Taylor series expansion about $\boldsymbol{u}_0$. If the solution curve is a multi-value function of α, it is convenient to parameterize the solution in terms of a suitable parameter along the solution curve $\boldsymbol{u} = \boldsymbol{u}(\alpha)$. The preferred parameter in this study is the arc length s (or as we will see shortly, a suitable stand-in parameter for arc length) along the solution curve given by Eq. (12).

$$\boldsymbol{u} = \boldsymbol{u}(s), \ \alpha = \alpha(s) \tag{12}$$

This parameterization allows Eq. (9) to be written as Eq. (13).

$$\boldsymbol{f}(\boldsymbol{u}(s), \alpha(s)) = 0 \tag{13}$$

The total derivative of $\boldsymbol{f}$ along the solution curve is then given by Eq. (14).

$$\frac{\mathrm{d}\boldsymbol{f}}{\mathrm{d}s} = \boldsymbol{f}_{\boldsymbol{u}}(\boldsymbol{u}, \alpha)\frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}s} + \boldsymbol{f}_\alpha(\boldsymbol{u}, \alpha)\frac{\mathrm{d}\alpha}{\mathrm{d}s} = 0 \tag{14}$$

Equation (14) is a set of N equations in terms of $N + 1$ unknowns, where the unknowns are as shown in Eq. (15).

$$\left\{ \frac{\mathrm{d}u_1}{\mathrm{d}s}, \frac{\mathrm{d}u_2}{\mathrm{d}s}, \ldots, \frac{\mathrm{d}u_N}{\mathrm{d}s}, \frac{\mathrm{d}\alpha}{\mathrm{d}s} \right\} \tag{15}$$

Recall that $\boldsymbol{f}_{\boldsymbol{u}}(\boldsymbol{u}, \alpha) \equiv \boldsymbol{J}(\boldsymbol{u}, \alpha)$ is the familiar Jacobian used in Newton's method. It is convenient to write Eq. (14) in matrix notation as shown in Eq. (16).

$$(\boldsymbol{J} \mid \boldsymbol{f}_\alpha)\begin{pmatrix} \boldsymbol{u}' \\ \alpha' \end{pmatrix} = 0 \tag{16}$$

Here $\boldsymbol{u}' \equiv \mathrm{d}\boldsymbol{u}/\mathrm{d}s$ and $\alpha' \equiv \mathrm{d}\alpha/\mathrm{d}s$, while the notation $(\cdot | \cdot)$ denotes the block partition of a given matrix. Thus the vector given by Eq. (17) is tangent to the solution curve $\boldsymbol{u}(\alpha)$.

$$\boldsymbol{t} = \begin{pmatrix} \boldsymbol{u}' \\ \alpha' \end{pmatrix} \tag{17}$$

The homogeneous system of equations given by Eq. (16) is an under-determined system of equations, and will have a nontrivial solution if the rank r of $(\boldsymbol{J} | \boldsymbol{f}\_\alpha)$ has full row rank, namely $r = N$. This assumption holds at turning points, but breaks down if the solution curve has branch points (such as transcritical bifurcation points). We do not consider branch points in this analysis. The nontrivial solution is non-unique, however. In order to obtain a unique solution, we need to append to Eq. (16) an additional equation. The appropriate equation is given by the definition of arc length shown by Eq. (18).

$$\frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}s} \cdot \frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}s} + \left(\frac{\mathrm{d}\alpha}{\mathrm{d}s} \right)^2 = 1 \tag{18}$$

Equations (16) and (18) represent $N + 1$ equations in terms of the $N + 1$ unknowns. Although Eq. (16) is linear in the unknowns, Eq. (18) is not. Moreover, the coefficient matrix in Eq. (16) depends on $\boldsymbol{u}$ and α, usually in a nonlinear manner, which means that we need to solve Eqs. (16) and (18) using an appropriate ODE solver. However, although matters are complicated further by the fact that $\boldsymbol{J}(\boldsymbol{u}, \alpha)$ is singular at bifurcation points and turning points, the augmented matrix $(\boldsymbol{J} | \boldsymbol{f}_\alpha)$ has full rank at turning points, and it this feature that can be exploited to devise a numerical algorithm that can integrate through turning points. Generally one is not actually interested in how $\boldsymbol{u}$ and α depend on the arc length s, and thus Eq. (18) is not needed. The homogeneous system of equations defined by Eq. (16) can be solved using Cramer's rule. Thus, if we define $\boldsymbol{z} = \{u_1, u_2, \ldots, u_N, \alpha\}$, then the vector $\boldsymbol{z}$ is a solution to the system of equations given by Eq. (19).

$$\frac{\mathrm{d}z_i}{\mathrm{d}\xi} = (-1)^i \det(\boldsymbol{J} | \boldsymbol{f}_\alpha)_{-i}, \quad i = 1, 2, \ldots, N+1 \tag{19}$$

Herein, $\det(\boldsymbol{J} | \boldsymbol{f}_\alpha)_{-i}$ is the matrix with the i-th column removed (see Appendix for derivation). Though Eq. (19) follows from Eqs. (14) and (16), it does not imply that $\boldsymbol{f}(\boldsymbol{u}, \alpha) = 0$. The initial condition given by Eq. (11) ensures that the solution from Eq. (19) satisfies $\boldsymbol{f}(\boldsymbol{u}, \alpha) = 0$. In the homotopy literature, Garcia and Zangwill (1981) call Eq. (19) the basic differential equation. The advantage of using Eq. (19) instead of the full system Eqs. (16) and (18) is that Eq. (19) is linear in the derivatives. Note that the independent variable ξ is not the arc length along the solution curve, but is related to arc length by Eq. (20).

$$\frac{\mathrm{d}s}{\mathrm{d}\xi} = \sqrt{\left(\frac{\mathrm{d}z_1}{\mathrm{d}\xi} \right)^2 + \left(\frac{\mathrm{d}z_2}{\mathrm{d}\xi} \right)^2 + \cdots + \left(\frac{\mathrm{d}\alpha}{\mathrm{d}\xi} \right)^2} \tag{20}$$

Hence once the solution $z_i(\xi)$ has been found, a simple integration gives the dependence of s on ξ, if needed. The determinants on the RHS of Eq. (19) can be evaluated using symbolic software such as Mathematica or Maple. This means that we have an exact set of equations to track the solution as α is varied. Of course, these equations are nonlinear in terms of the dependent variables, which require that Eq. (19) be solved using a suitable ODE solver, but there is no need to implement separately corrector/predictor steps to ensure the integration maintains fidelity with the solution curve. It is this feature that vastly simplifies writing code. As is well known, the computation of determinants is an $O(N^2)$ operation, and the computational time for symbolic calculations can become prohibitive if N becomes large. Our experience shows that, if $N < 15$, symbolic computations are readily handled on desktop computers. For lager values of N, we modify the algorithm by computing the determinants numerically along the solution curve. We illustrate this alternative in one of the examples discussed below.

It has been pointed out that, if numerical stability is an issue, one could solve the following system.

$$(\boldsymbol{J} | \boldsymbol{f}_\alpha) \begin{pmatrix} \boldsymbol{u}' \\ \alpha' \end{pmatrix} = -k\boldsymbol{f}, \quad k > 0 \tag{21}$$

This system of equations is asymptotically stable, but the computational overhead to compute the corresponding determinants is raised.

In the next section, we show through examples how Eq. (19) can be used to implement a continuation method in parameter space. In our calculations, we used *Mathematica*. The relevant code can be obtained from the authors on request.

2. Examples

2.1 Heat generation in a CSTR

This example is related to heat generation in a CSTR, a topic that is discussed in most undergraduate text books on reactor design, e.g., Schmidt (1998). A lumped parameter model for the reactor temperature y as a function of the residence time α is given by Eq. (22)

$$\frac{\mathrm{d}y}{\mathrm{d}t} = y - \frac{19}{4} \alpha \frac{e^y}{(1 + \alpha e^y)} \tag{22}$$

Herein, the variables y, t, and α are expressed in suitable dimensionless form. The steady state reactor temperature is given by Eq. (23).

$$f(y, \alpha) = y - \frac{19}{4} \alpha \frac{e^y}{(1 + \alpha e^y)} = 0 \tag{23}$$
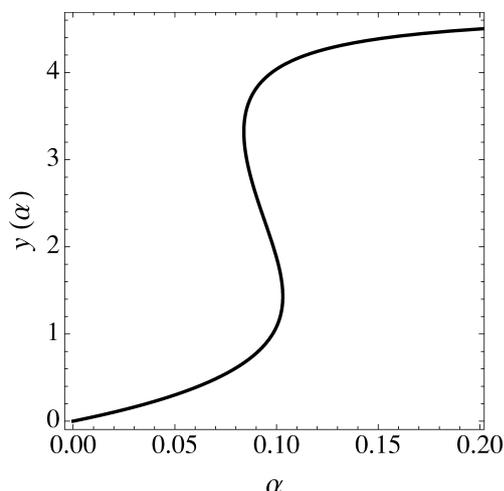
To determine the solution curve using our continuation

Fig. 2 Solution curve y versus α with two turning points; see Eq. (22)

Fig. 3 Dependence of arc length s on stand-in parameter ξ along solution curve in Figure 2

method we substitute Eq. (23) into Eq. (19) to obtain Eq. (24).

$$\frac{dy}{d\xi} = 19e^y, \quad \frac{d\alpha}{d\xi} = 4 - 11e^y\alpha + 4e^{2y}\alpha^2 \tag{24}$$

Here, ξ is related to arc length s as shown by Eq. (25).

$$\frac{ds}{d\xi} = \sqrt{\left(\frac{dy}{d\xi}\right)^2 + \left(\frac{d\alpha}{d\xi}\right)^2} \tag{25}$$

Equations (24) are solved subject to the initial conditions given by Eq. (26).

$$y(0) = 0, \; \alpha(0) = 0, \; \xi(0) = 0, \; s(0) = 0 \tag{26}$$

The solution curve as a function of the parameter α is shown in **Figure 2**.

It is evident from the plot that the solution curve exhibits two turning (limit) points where the solution curve locally turns back on itself. Thus for $\alpha \approx 0.09$ there are three steady-state reactor temperatures. A stability analysis (a separate topic) reveals that the middle temperature is unstable to small perturbations. The dependence of arc length on the stand-in coordinate ξ is displayed in **Figure 3**. In that plot, the range that ξ varies along the curve is limited to $0 \le \xi \le 0.05$. For values of ξ greater than 0.05, the arc length s increases rapidly with ξ, as is evident by the magnitude of the slope of $d\xi/ds$ near $\xi = 0.05$ (i.e. where $dy/d\alpha \approx 0$). The numerical range of ξ can be expanded by multiplying the RHS of Eq. (19) by a scaling factor. Recall the solution to Eq. (19) (see Appendix) is known up to an arbitrary multiplicative constant. Thus, for computational convenience, it is useful to scale the RHS of Eq. (19) so that it is of order unity at $\xi = 0$. Note that in this example, we are dealing with a single nonlinear equation, which obviously can be solved using routine contour plotting methods available in most software packages. However, this
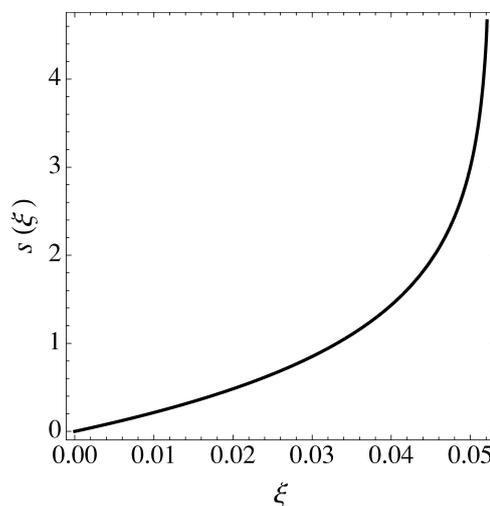
is not the case in most applications, as we illustrate with the next examples.

2.2 Heat generation in a two CSTRs in series

Next, we consider a far more complicated system of equations. We consider a cascade of two continuous stirred tank reactors in series with exothermic first order chemical reactions. The steady state is described by 4 nonlinear equations for the reaction conversions $\{\chi_1, \chi_2\}$ and dimensionless temperature $\{T_1, T_2\}$ and the parameter α (Damköhler number). The dimensionless equations describing the steady-state species and energy balances for each tank (Kubíček *et al.*, 1980; Kubíček and Marek, 1984) are Eqs. (27a) to (27d).

$$f_1 = \alpha e^{\frac{T_1}{1+0.001T_1}}(1-\chi_1) - \chi_1 \tag{27a}$$

$$f_2 = 22\alpha e^{\frac{T_1}{1+0.001T_1}}(1-3\chi_1) - 3T_1 \tag{27b}$$

$$f_3 = \chi_1 + \alpha e^{\frac{T_2}{1+0.001T_2}}(1-\chi_2) - \chi_2 \tag{27c}$$

$$f_4 = 22\alpha e^{\frac{T_2}{1+0.001T_2}}(1-\chi_2) + T_1 - 3T_2 \tag{27d}$$

A steady solution for $\alpha = 0.01$ is given by Eqs. (28a) to (28d).

$$\chi_1(0.01) = 0.0107005 \tag{28a}$$

$$\chi_2(0.01) = 0.0215779 \tag{28b}$$

$$T_1(0.01) = 0.0784704 \tag{28c}$$

$$T_2(0.01) = 0.105924 \tag{28d}$$

Figure 4 shows the dependence of T_2 on the parameter α. The solution path has 6 turning points, and for $\alpha \approx 0.039$, there are remarkably 7 steady-state solutions. Again, not all these steady-state solutions are stable to
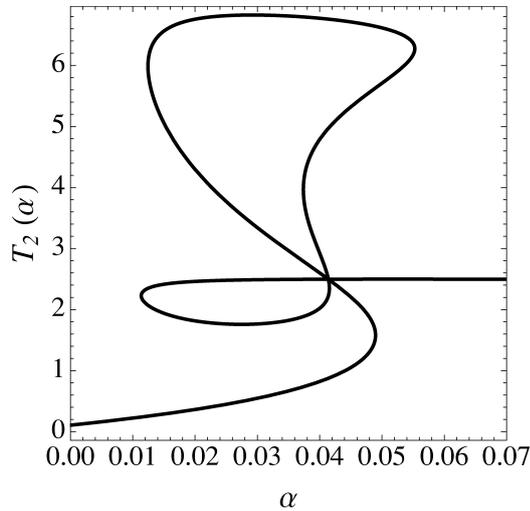
Fig. 4 Solution curve for T_2 as a function of α; see Eq. (27)

Fig. 5 Solution norm $\|u\|$ from finite difference grid versus α; see Eq. (29)

small perturbations. The stability of the steady states is determined by the sign of the real part of the eigenvalues of the Jacobian **J**. The algorithm based on Eq. (19) is readily coded in Mathematica and takes only a fraction of a second to compute the solution trajectory. Our results are in quantitative agreement with the results of Kubíček and Marek (1984) calculated using Eq. (16) coupled with the equation for arc length, Eq. (18). Though not shown, one can easily plot the dependence of the remaining variables χ_1, χ_2, and T_1 on α.

2.3 Self-heating of a reactive solid

The Frank–Kamenetskii problem relates to the self-heating of a reactive solid. When the heat generated by reaction is balanced by conduction in a one-dimensional slab of combustible material, the nonlinear boundary value problem (BVP) admits at least two steady solutions. The dimensionless form of the nonlinear boundary value problem is defined by Eqs. (29a) to (29c).

$$\frac{\mathrm{d}^2 u}{\mathrm{d}x^2} + \alpha e^u = 0, \quad 0 < x < 1 \tag{29a}$$

$$u = 0, \quad x = 0 \tag{29b}$$

$$\frac{\mathrm{d}u}{\mathrm{d}x} + hu, \quad x = 1 \tag{29c}$$

Here, u is a dimensionless temperature, α is a positive parameter related to the Frank–Kameneskii approximation of the Arrhenius reaction rate linearized about a reference temperature (Fowler, 1997), and h is a heat transfer coefficient. When $h \to \infty$, the above BVP can be solved analytically to give Eq. (30).

$$u(x) = u_{\mathrm{m}} - 2\ln\left(\cosh\left(\frac{1}{4}\sqrt{2\alpha}\, x e^{u_{\mathrm{m}}/2}\right)\right) \tag{30}$$

The variable $u_{\mathrm{m}} = u(1/2)$ denotes the maximum temperature in the slab. In this example, we use a finite differ-
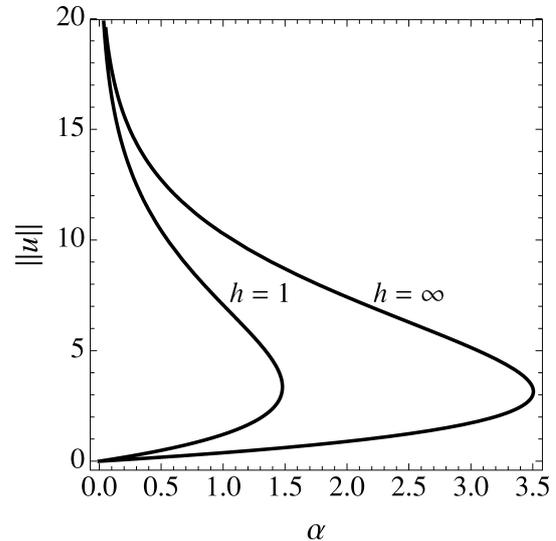
ence approximation to show how the steady-state solution evolves as the parameter α is varied for finite values of h. We discretized the domain $0 \leq x \leq 1$ into NP−1 intervals of uniform width Δx, giving NP nodes, and approximate Eq. (29a) with its finite difference form, using central differences for the spatial derivative. The value of $\mathrm{d}^2 u/\mathrm{d}x^2$ evaluated at the x_i internal node is given by Eq. (31).

$$\left(\frac{\mathrm{d}^2 u}{\mathrm{d}x^2}\right)_i \approx \frac{u(x_i + \Delta x) - 2u(x_i) + u(x_i - \Delta x)}{\Delta x^2} \tag{31}$$

Let $u[i] = u(x_i)$ represent the nodal value of u at the i-th node, then the finite difference representation of the ODE evaluated at the i-th node is given by Eq. (32).

$$f_i = u[i+1] - 2u[i] + u[i-1] + \Delta x^2 \alpha e^{u[i]} = 0 \tag{32}$$

The boundary condition at $x = 0$ and $x = 1$ are given by Eqs. (33a) and (33b).

$$u[1] = 0 \tag{33a}$$

$$u[\mathrm{NP}+1] = u[\mathrm{NP}-1] - 2\Delta x h u[\mathrm{NP}] \tag{33b}$$

Equation (32) is evaluated at nodes ($i = 2, \ldots, \mathrm{NP}$) to obtain $\mathrm{NP} - 1$ nonlinear algebraic equations in terms of $\mathrm{NP} + 1$ nodal unknowns $u[1], u[2], \ldots, u[\mathrm{NP}], u[\mathrm{NP}+1]$. Combined with the boundary conditions Eqs. (33a) and (33b), we have NP equations for NP nodal values for u. For our calculation, we selected $\mathrm{NP} = 15$ and determined the NP continuation equations for $\mathrm{d}u[i]/\mathrm{d}\xi$ by solving Eq. (19) symbolically. The system of ODEs are then integrated numerically with the initial conditions $u[i](0) = 0$, $\alpha(0) = 0$. In **Figure 5**, we plot the solution norm $\sqrt{\sum_{i=1}^{\mathrm{NP}} u[i]^2}$ as a function of the parameter α for
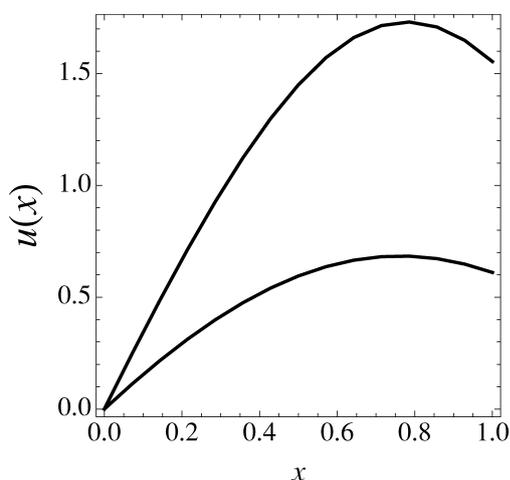
Fig. 6 Temperature profiles $u(x)$ at $\alpha = 1.33$ and $h = 1$; see Eq. (29)

two values of the heat transfer coefficient h. When $h = \infty$, the turning point is near $\alpha = 3.51$, which is in quantitative agreement with the analytical solution. As h decreases, the location of the turning point moves to smaller values of α. When α is less than its maximum value, the BVP has two steady state solutions. These solutions are displayed in **Figure 6** below for $\alpha = 1.33$, and $h = 1$. Again, a stability analysis reveals that the upper solution branch is unstable to small perturbations.

2.4 Flow in a tube with accelerating surface velocity

As our final example we consider a nonlinear BVP from fluid mechanics. Brady and Acrivos (1981) showed that the axisymmetric flow of a viscous fluid in a tube driven by an accelerating wall can be described by a similarity transformation that reduces the Navier–Stokes equations to a single third order nonlinear ordinary differential equation, as shown by Eq. (34).

$$\frac{1}{r}\frac{d}{dr}r\frac{d}{dr}\left(\frac{f'}{r}\right) =$$
$$\beta + Re\left\{\left(\frac{f'}{r}\right)^2 - \frac{f}{r}\left(\frac{f''}{r} - \frac{f'}{r^2}\right)\right\} \qquad (34)$$

The following boundary conditions are given by Eq. (35).

$$f(0) = f'(0) = 0, \ f(1) = 0, \ f'(1) = 1 \qquad (35)$$

The parameter β is given by

$$\beta = f'(1) - Re - f''(1) + f'''(1) \qquad (36)$$

where Re is the Reynolds number. The axial and radial components of velocity are related to the function $f(r)$ by

$$u = zf'(r)/r, \ v = -f(r)/r \qquad (37)$$

For low $Re < 100$, Brady and Acrivos (1981) showed that the solution space exhibits a turning point at $Re = 10.25$ in the plane of β versus Re. For $10.25 < Re < 147$, there are no steady axisymmetric solutions that satisfy

Eq. (34). For Reynolds numbers $Re > 147$, steady axisymmetric solutions reappear, but these solutions belong to a new solution family. In this study we focus on the solution family that exists for $Re < 10.25$.

When $Re = 0$, a simple integration of Eq. (34) gives the following analytically solution give by Eq. (38).

$$f_0(r) = \frac{1}{2}(r^4 - r^2), \ \beta = 8 \qquad (38)$$

We use f_0 to initiate the continuation problem. That is, we seek the function $f(r, Re)$ that satisfies Eq. (34) as Re is varied, starting with $Re = 0$. Once $f(r)$ is determined, we examine how β depends on Re by solving Eq. (36).

As in the previous example we use a finite difference method to solve Eq. (34). This problem is quite stiff and to ensure accuracy, we adopt the following finite difference scheme to minimize the number of nodal values in the finite difference grid:

(1) use central difference formulas $O(\Delta r^2)$ for all derivatives on the internal nodes $i = 3, \ldots, NP - 2$,
(2) use forward difference formulas $O(\Delta r^2)$ for all derivatives at the $i = 1$ node,
(3) use backward difference formula $O(\Delta r^2)$ for all derivatives at the $i = NP - 1$ node,
(4) set $f(0) = f(1) = 0$ at $i = 1$ and $i = NP$ nodes,
(5) use forward and backward differences formulas $O(\Delta r^2)$ at $i = 1$ and $i = NP$ to satisfy $f'(0) = 0$ and $f'(1) = 1$, and
(6) use backward difference formulas $O(\Delta r^3)$ to relate β to derivatives at $r = 1$.

The set of nonlinear equations for this example are substantially more complicated than those in the previous examples. Consequently, the calculation time to determine the determinants in Eq. (19) became excessive and unworkable, even when NP = 11. However, there is a simple remedy; instead of calculating the determinants symbolically, we calculate the determinants numerically at each step of the integration using our symbolic expression for the Jacobian. This required a minor change in the code, so the simplicity of the code was not compromised. The resulting continuation curve with NP = 16 is shown in **Figure 7**. The turning point occurs at $Re = 10.25$.

The resulting solution curve is in quantitative agreement with the work of Brady and Acrivos (1981). Not surprisingly, the computational time was about a factor of 3 faster than in those cases where we computed the determinants symbolically. Of course, additional numerical error is introduced when we use numerical values for the determinants, but this error can be managed by changing the working precision of the ODE solver and/or adding additional nodes to the finite difference grid.

Conclusions

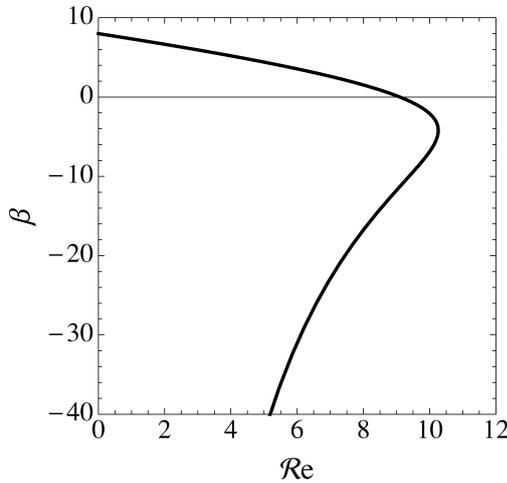We have shown through several examples a method

Fig. 7 Parameter β versus Re, with NP = 16; determinants computed numerically; see Eq. (34)

for computing the solution of a system of nonlinear equations as a function of a parameter when there are turning points present. The essential idea is that, for small systems of equations ($N < 15$), one can symbolically determine the differential equations required for solving the parameterized equations. For large N, we have the option to compute the determinants numerically along the integration path. Thus, the method is quite flexible. Moreover, we believe our approach is ideal for illustrating continuation methods in the classroom and is easily implemented in Mathematica, or equivalent software. Although we have not addressed the stability of the steady state solutions, this can be carried out in the context of infinitesimal perturbations to the steady state. The linear stability of the steady solutions is determined by the sign of the real part of the eigenvalues of the Jacobian in Eq. (16). Since the Jacobian is known analytically, it and its associated eigenvalues can be evaluated along the solution branch during the integration of Eq. (19).

In the examples used to illustrate our method there were no branch points along the solution curve. That is, the tangent vector t given by Eq. (17) was unique. At branch points (such as at transcritical bifurcation points) where the rank of $(J \mid f_\alpha)$ is less than N, the tangent vector t is no longer unique and continuation methods based on arc length will fail. Techniques using branch switching algorithms are then necessary, e.g., see Nayfeh and Balachandran (1995).

The simplicity of our method is that we do not use arc length along the curve explicitly as our parameterization, but instead use a stand-in variable we call ξ that is directly related to arc length by Eq. (20). Further, there is no need to implement explicitly a predictor–corrector strategy to maintain fidelity with the solution curve during the integration. At this point it is worth commenting on the pseudo-arc length method of Keller (1987) that is

used is the software package AUTO and other software packages. Keller's method is a predictor–corrector method in which the corrector method seeks a solution in a direction that is normal to the tangent vector t, i.e. it approximates the arc length in the tangent space of the curve rather than solve Eq. (20). In the MATCONT package, a predictor–corrector method is also used, but the corrector step implements Moore-Penrose corrections to advance along the solution curve. Both of these methods require a level of linear algebra sophistication not normally covered in an introductory undergraduate linear algebra course.

Finally, further study is needed to determine whether our strategy for computing the determinants numerically along the solution curve will be efficient for BVPs that involve multiple dimensions, such as those that arise from collocation on finite elements and other weighted residual methods. It will be interesting to see if a blending of Keller's method and our method can be implemented to solve large systems of nonlinear equations.

Appendix

In this section we show how to derive the basic differential equation given by Eq. (19). To compute a non-unique solution vector that lies in the null space of $F_z \equiv (J \mid f_\alpha)$ even at turning points, we need to impose a normalization on the tangent vector z'. We will use the normalization $\zeta \cdot z = \beta$, where ζ is the unit vector with all elements zero except $\zeta_r = 1$, and $r \neq N + 1$. Thus, our system of equations becomes Eq. (A1).

$$\begin{pmatrix} F_z \\ \cdots \\ \zeta \end{pmatrix}(z) = \begin{pmatrix} \mathbf{0} \\ \cdots \\ \beta \end{pmatrix} \tag{A1}$$

If $N = 2$, this system of equations in component form is Eq. (A2).

$$\begin{pmatrix} \dfrac{\partial F_1}{\partial z_1} & \dfrac{\partial F_1}{\partial z_2} & \dfrac{\partial F_1}{\partial z_3} \\[2mm] \dfrac{\partial F_2}{\partial z_1} & \dfrac{\partial F_2}{\partial z_2} & \dfrac{\partial F_2}{\partial z_3} \\[2mm] 0 & 1 & 0 \end{pmatrix}\begin{pmatrix} z_1 \\ z_2 \\ z_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \beta \end{pmatrix} \tag{A2}$$

We can solve this system using Cramer's rule. Let S be given by Eq. (A-3).

$$S = \left(\dfrac{\partial F_1}{\partial z_3} \right)\left(\dfrac{\partial F_2}{\partial z_1} \right) - \left(\dfrac{\partial F_1}{\partial z_1} \right)\left(\dfrac{\partial F_2}{\partial z_3} \right) \tag{A3}$$

Then the solution is given by Eqs. (A4a) to (A4c).

$$z_1 = \dfrac{1}{S}\det\begin{pmatrix} 0 & \dfrac{\partial F_1}{\partial z_2} & \dfrac{\partial F_1}{\partial z_3} \\[2mm] 0 & \dfrac{\partial F_2}{\partial z_2} & \dfrac{\partial F_2}{\partial z_3} \\[2mm] \beta & 1 & 0 \end{pmatrix} \tag{A4a}$$

$$z_2 = \dfrac{1}{S}\det\begin{pmatrix} \dfrac{\partial F_1}{\partial z_1} & 0 & \dfrac{\partial F_1}{\partial z_3} \\[2mm] \dfrac{\partial F_2}{\partial z_1} & 0 & \dfrac{\partial F_2}{\partial z_3} \\[2mm] 0 & \beta & 0 \end{pmatrix} \tag{A4b}$$

$$z_3 = \frac{1}{S} \det \begin{pmatrix} \dfrac{\partial F_1}{\partial z_1} & \dfrac{\partial F_1}{\partial z_2} & 0 \\[2mm] \dfrac{\partial F_2}{\partial z_1} & \dfrac{\partial F_2}{\partial z_2} & 0 \\[2mm] 0 & 1 & \beta \end{pmatrix} \tag{A4c}$$

Evaluating the determinants we have Eqs. (A5a) to (A5c).

$$z_1 = \frac{\beta}{S} \left\{ \left(\frac{\partial F_1}{\partial z_2} \right) \left(\frac{\partial F_2}{\partial z_2} \right) - \left(\frac{\partial F_1}{\partial z_3} \right) \left(\frac{\partial F_2}{\partial z_2} \right) \right\} \tag{A5a}$$

$$z_2 = \frac{\beta}{S} \left\{ \left(\frac{\partial F_1}{\partial z_3} \right) \left(\frac{\partial F_2}{\partial z_1} \right) - \left(\frac{\partial F_1}{\partial z_1} \right) \left(\frac{\partial F_2}{\partial z_1} \right) \right\} \tag{A5b}$$

$$z_3 = \frac{\beta}{S} \left\{ \left(\frac{\partial F_1}{\partial z_1} \right) \left(\frac{\partial F_2}{\partial z_2} \right) - \left(\frac{\partial F_1}{\partial z_2} \right) \left(\frac{\partial F_2}{\partial z_1} \right) \right\} \tag{A5c}$$

Recall the β is a normalizing constant that can be chosen for convenience. If we let β be given by Eq. (A6),

$$\beta = -\left\{ \left(\frac{\partial F_1}{\partial z_3} \right) \left(\frac{\partial F_2}{\partial z_1} \right) - \left(\frac{\partial F_1}{\partial z_1} \right) \left(\frac{\partial F_2}{\partial z_3} \right) \right\} \tag{A6}$$

then the solution is equivalent to Eq. (A7).

$$\frac{dz_i}{d\xi} = (-1)^i \det(\boldsymbol{F}_z)_{-i}, \tag{A7}$$

Here, $(\cdot)_{-i}\}$ means remove the i-th column of the matrix $\boldsymbol{F}_z$. There may be circumstances where the determinant of the matrix in Eq. (A2) is zero for certain values of the parameter α. This occurs when $\boldsymbol{u}$ versus α has an extremum, i.e. $du_i/d\alpha = 0$. However, since we compute the determinants symbolically, the extrema points are handled naturally during the integration of the solution curve.

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