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A Robust Homotopy Continuation Method for Seeking All Real Roots of Unconstrained Systems of Nonlinear Algebraic and Transcendental Equations

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S Supporting Information

ABSTRACT: A new homotopy developed for finding all real roots to a single nonlinear equation is extended to a system of nonlinear algebraic and transcendental equations written as $f\{x\} = 0$ to find all real roots, including those on isolas. To reach roots that may lie on isolas, the functions are squared. This causes all roots to be bifurcation points that are connected to each other through stemming branches. As a result, a new system of homotopy functions, including numerous bifurcation points, is formed as $H\{x,t\} = (x - x^0)(1 + f^2 - t)$, where x^0 is the starting point. Because the functions are squared, many systems of equations must be solved to find a starting point on a reduced system of homotopy functions written as $H\{x,t\} = 1 + f^2 - t$. Therefore, robustness is achieved at the expense of increased computation time. To improve the efficiency of the algorithm, the Levenberg−Marquardt method is used to find the starting point for the reduced homotopy system by solving a system of nonlinear equations with the degree of freedom equal to one. Then, a continuation method is used to track the paths from the resulting starting point to seek at least one root. Because all roots are bifurcation points, tracking the stemming branches from each subsequent root is the final step. The new algorithm was able to find successfully all the reported roots for 20 test problems that included a variety of algebraic and transcendental terms. In some cases additional roots were obtained.

1. INTRODUCTION

Many of the equations used by chemical engineers to solve problems contain nonlinear algebraic or transcendental terms. In Stuart W. Churchill's 1974 unified treatment of rate processes, "The Interpretation and Use of Rate Date: The Rate Concept",[1] nonlinear equations abound in almost all of the 19 chapters.

With the advent of digital computers in the 1950s, interest in numerical methods for solving nonlinear equations began to gain momentum among engineers. This momentum was accelerated in 1969 by the widely used textbook, "Applied Numerical Methods" by Carnahan, Luther, and Wilkes,[2] written expressly for engineers and scientists. For nonlinear systems of equations, the authors developed and illustrated two methods: successive substitution and Newton−Raphson, which became the methods of choice in early process simulation programs. The former method was used to converge the overall process, while the latter method was used to converge nonlinear models of operations within the process.

Despite the popularity of the Newton−Raphson method, which is straightforward to implement and efficient, it is well-known that the method has two deficiencies: lack of robustness, often requiring a good initial guess to achieve convergence; and inability to automatically seek multiple solutions, which have been found to be more common than expected in chemical engineering applications. Significant improvement in 2002 of the Newton−Raphson method by Lucia and Feng,[3] referred to as global terrain methods, shows an ability to surmount the two deficiencies and is expected to gain prominence in the near future.

Another alternative to the Newton−Raphson method is the homotopy continuation method, which, since 1983 as discussed below, has found wide application to engineering problems. An extension of this method is the subject of this paper.

2. BACKGROUND

The basic concept of homotopy continuation is credited to Lahaye,[4] whose method is sometimes referred to as classical homotopy continuation and is discussed and illustrated by Wayburn and Seader[5] and presented in a numerical methods textbook by Conte and de Boor.[6] The method involves following a homotopy path from a system of equations whose solution is known or easily obtained to the target system of equations whose solution is difficult to obtain by the Newton−Raphson method.

When the path is difficult to follow because of steep gradients and/or turning points, it is preferred to convert the nonlinear homotopy equations to an initial-value problem in ordinary differential equations (ODEs), as first proposed by Davidenko[7]

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in 1953. A further, and very important refinement, was introduced by Kloppenstein[8] in 1961, who parametrized the system of ODEs with respect to the arclength of the path to handle branching points. The resulting method is sometimes referred to as differential arclength homotopy continuation. An early computer program for applying the method was published by Kubicek[9] in 1976, and an extensive treatment of the method was presented by Keller[10] in 1977.

Early applications of the arclength method sought just one solution of the system of equations. However, as the incidence of multiple roots, particularly in many chemical engineering and electrical engineering applications became evident, interest mounted in developing ways to extend the method to find all solutions. At first, it was conjectured that all roots would lie on the homotopy path. Thus, it was only necessary to continue following the path from one solution to the next until the path approached infinity in the homotopy parameter. This technique proved to be successful for solving single nonlinear equations, e.g., Khaleghi Rahimian et al.[11] and some systems of nonlinear equations, e.g., Seader et al.[12] However, Choi and Book[13] showed that all solutions could not be found with such a global homotopy method when one or more roots occurred on an unreachable isola. Thus, a further extension of the arclength method was needed that would include any and all isolas on the homotopy path so that all roots could be found. Such an extension is the subject of this paper.

3. THEORETICAL DEVELOPMENT

The extension makes use of a new homotopy (FPN), developed and discussed in detail by Khaleghi Rahimian et al.,[11] but applied by them only to single nonlinear equations, whose homotopy paths can never contain an isola. The FPN homotopy is extended to a system of equations, where isolas may exist on homotopy paths, as follows:

The system of N nonlinear equations to be solved is written in zero form as

$$\begin{cases} f_1(\underline{x}) = 0 \\ f_2(\underline{x}) = 0 \\ \cdots \\ f_n(\underline{x}) = 0 \end{cases} \tag{1}$$

A new system of equations is formulated that can easily generate useful bifurcation points—as will be illustrated shortly—and can reach isolas from these bifurcations points if each function is squared, followed by multiplication of the squared function by $(x_i - x_i^0)$, where the 0 superscript indicates a starting value.

This property is based on the Kuznetsov[14] criterion, which proves that squaring the functions makes all roots bifurcation points as shown in Appendix A, including any roots on isolas, which now become reachable.

Thus, the new system of equations is

$$\begin{cases} F_1(\underline{x}) = (x_1 - x_1^0)f_1^{\,2}(\underline{x}) \\ F_2(\underline{x}) = (x_2 - x_2^0)f_2^{\,2}(\underline{x}) \\ \qquad \cdots \\ F_n(\underline{x}) = (x_n - x_n^0)f_n^{\,2}(\underline{x}) \end{cases} \tag{2}$$

Studies show that it matters not which equation is multiplied by which $(x_i - x_i^0)$.

The FPN homotopy is now formulated using the new system of equations.

For a single nonlinear equation, a linear homotopy is

$$H(x,t) = tF(x) + (1-t)G(x) = 0 \tag{3}$$

The $G(x)$ function is taken as a linear combination of the fixed point and Newton functions, giving the following homotopy:

$$H(x,t) = tF(x) + (1-t)\{(x - x^0) + [F(x) - F(x^0)]\} = 0 \tag{4}$$

Although eq 4 appears to be considerably more complicated than the commonly used fixed-point, Newton, and affine homotopies, the following simplification results by noting that $F(x^0) = 0$ and by replacing $F(x)$ with $f^2(x)(x - x^0)$ from the single equation form of eq 2:

$$H(x,t) = (x - x^0)[1 + f^2(x) - t] = 0 \tag{5}$$

For a system of nonlinear equations, the FPN homotopy equations become

$$\begin{cases} H_1 = (x_1 - x_1^0)(1 + f_1^{\,2} - t) = 0 \\ H_2 = (x_2 - x_2^0)(1 + f_2^{\,2} - t) = 0 \\ \cdots \\ H_n = (x_n - x_n^0)(1 + f_n^{\,2} - t) = 0 \end{cases} \tag{6}$$

Equation 6 contains the following bifurcation points:

- Maximum N initial bifurcation points (BP^0):

$$BP_k^{\,0} = \begin{cases} x_i = x_i^0, i = 1 \cdots N \\ t_{BP}^{\,k} = 1 + f_j^2(x^0), j = 1 \cdots N \end{cases} \quad k = 1 \cdots N$$

- First bifurcation points (BP^1):

$$BP^1 = \begin{cases} x_j \neq x_j^0, j = \begin{pmatrix} N \\ 1 \end{pmatrix} \text{ of } 1 \ldots N \\ x_i = x_i^0, i = 1 \ldots N, i \neq j \end{cases}$$

- Second bifurcation points (BP^2):

$$BP^2 = \begin{cases} x_j \neq x_j^0, j = \begin{pmatrix} N \\ 2 \end{pmatrix} \text{ of } 1 \ldots N \\ x_i = x_i^0, i = 1 \ldots N, i \neq j \end{cases}$$

- and finally, $(N-1)^{\text{th}}$ bifurcation points (BP^{N-1}):

$$BP^{N-1} = \begin{cases} x_j \neq x_j^0, j = \begin{pmatrix} N \\ N-1 \end{pmatrix} \text{ of } 1 \ldots N \\ x_i = x_i^0, i = 1 \ldots N, i \neq j \end{cases}$$

where $\begin{pmatrix} p \\ q \end{pmatrix}$ means q numbers of 1,2,..,p. For example $\begin{pmatrix} 3 \\ 2 \end{pmatrix}$ are (1,2), (1,3), and (2,3).

To find the BP^1, it is necessary to trace the following N homotopy systems, including the paths which stem from BP^0.

$$\begin{cases} H_j = 1 + f_j^2 - t = 0, \; j = \begin{pmatrix} N \\ 1 \end{pmatrix} \text{ of } 1 \cdots N \\ H_i = x_i - x_i^0 = 0, i = 1 \cdots N, i \neq j \end{cases}$$

The points at which two of $f_i^2, i = 1 \cdots N$ coincide are the BP^1 that are saved for further stemming to find BP^2. By continuing the procedure, the BP^{N-1}, where all the squared functions are the same and only one element of the variables is the same as the initial guess, are obtained that are considered as the starting points of the previous homotopy system:

$$\begin{cases} H_1 = 1+f_1{}^2 - t = 0 \\ H_2 = 1+f_2{}^2 - t = 0 \\ \cdots \\ H_n = 1+f_n - t = 0 \end{cases} \tag{7}$$

As an example, consider the following FPN homotopy for a system of two nonlinear equations:

$$\begin{cases} H_1 = (x_1 - x_1{}^0)(1+f_1{}^2 - t) = 0 \\ H_2 = (x_2 - x_2{}^0)(1+f_2{}^2 - t) = 0 \end{cases}$$

The BP^0 are

$$BP_1{}^0 = \begin{cases} x_1 = x_1{}^0 \\ x_2 = x_2{}^0 \\ t = 1+f_1{}^2(x^0) \end{cases}, \quad BP_2{}^0 = \begin{cases} x_1 = x_1{}^0 \\ x_2 = x_2{}^0 \\ t = 1+f_2{}^2(x^0) \end{cases}$$

The following homotopy functions 1 and 2 are traced from $BP_1{}^0$and $BP_2{}^0$, respectively:

$$(1) \begin{cases} H_1 = 1+f_1{}^2 - t \\ H_2 = x_2 - x_2{}^0 \end{cases} \qquad (2) \begin{cases} H_1 = x_1 - x_1{}^0 \\ H_2 = 1+f_2{}^2 - t \end{cases}$$

The points where $f_1{}^2{=}f_2{}^2(x_1{=}x_1{}^0$ or $x_2{=}x_2{}^0)$ are the BP^1, which are considered to be the starting points of the following homotopy functions:

$$\begin{cases} H_1 = (1+f_1{}^2 - t) = 0 \\ H_2 = (1+f_2{}^2 - t) = 0 \end{cases}$$

Instead of solving numerous sets of equations to find BP^{N-1}, a much faster procedure is applied to solve the following system of $(N-1)$ equations by the Levenberg−Marquardt method, discussed by Edgar et al.,[15] for an optimal root that minimizes the functions. This root lies on the homotopy path and becomes the starting point to obtain all bifurcation points and all roots including any that lie on isolas. The equations are

$$\begin{cases} f_1{}^2 = f_2{}^2 \\ f_1{}^2 = f_3{}^2 \\ \cdots \\ f_1{}^2 = f_n{}^2 \end{cases} \tag{8}$$

Because the degree of freedom of eq 8 is one, the probability of finding a solution is very high. However, if the Levenberg−Marquardt method fails to converge to a solution, the most efficient remedy is to try another initial guess (discussed later in Step 3 of the Example section). Alternatively, other continuation methods, such as the fixed point or Newton homotopy, could be applied, but they are less efficient.

An initial guess, e.g., all $x^0 = 0$, is made and the Levenberg−Marquardt method is applied, e.g., with the MATLAB fsolve function in the Optimization Toolbox with the following NLE_DOF1.m file:

```
function F = NLE_DOF1(x, fun)
f = feval(fun, x)
F = f(1)^2 - f(2:end).^2
```

where "fun" is the function containing the system of equations.

With the Levenberg−Marquardt solution as a starting point, an efficient continuation algorithm, discussed below, is used to find at least one root, which is also a bifurcation point. Because all homotopy paths and isolas containing at least one root are now connected, all roots can be found by tracking all homotopy paths from all bifurcation points. This new method is referred to as the "efficient f^2 method". No mathematical proof is offered here that all bifurcation points, including roots, are connected. However, in all of the problems that have been solved with the method−20 of which are included here−all roots, including those on isolas, were found to be connected. Also, it is important to note that the homotopy functions in eq 7 are independent of the starting point. Thus, all starting points find the same set of roots.

4. PATH-TRACKING METHOD FOR CONTINUATION

As discussed by Khaleghi Rahimian et al.,[11] a number of methods have been used to track continuation paths. In this development, CL_MATCONT of Dhooge et al.,[16,17] a convenient and widely available toolbox in MATLAB was used. MATLAB facilitates data exchange, visualization of computed results in the form of plots and tables, and implements many efficient and robust core numerical computing methods.

CL_MATCONT finds limit points and bifurcation points for algebraic systems of equations. The tangent vector at the bifurcation (branching) point is also computed to obtain the direction of the secondary branch. Consider the following cubic polynomial solved by Jalali,[30] using the fixed-point homotopy in the complex domain:

$$f(z) = -z(z-1)(z+1) \tag{9}$$

The equation can be split in two equations by replacing z with $x + iy$ and equating the real and complex parts to zero:

$$\begin{aligned} f_1(x,y) &= x(-x^2 + 3y^2 + 1) = 0 \\ f_2(x,y) &= y(y^2 - 3x^2 + 1) = 0 \end{aligned} \tag{10}$$

Applying the fixed-point homotopy, the following two simultaneous nonlinear algebraic equations are generated and tracked by CL_MATCONT:

$$H_1 = tf_1 + (1-t)(x - x_0) \qquad H_2 = tf_2 + (1-t)(y - y_0)$$

where (x^0, y^0) is the starting point. CL_MATCONT readily solves for the values of x and y as a function of the homotopy parameter, t, by continuation from the starting point, which may be taken at $(x, y, t) = (2, 0, 0)$. CL_MATCONT detects all limit and branching points. For this example, a branching point (BP) is found at (2.879385, 0.0, 0.040205). By stemming, another bifurcation point and one limit point (LP) on the homotopy path are found at (0.652704, 0.0, 0.782432) and (−0.532089, 0.0, 1.177363), respectively.

As with most continuation algorithms, CL_MATCONT uses a predictor-corrector method to track the branches. As is common, a new point is predicted using the tangent to the curve and a step-size. However, a Newton iteration based on an efficient Moore−Penrose pseudoinverse [Penrose[18]] is used, rather than an iteration based on a pseudoarclength. A reliable convergence-dependent method is applied to control step-size. An example of the CL_MATCONT algorithm when applied to a single nonlinear equation is given by Khaleghi Rahimian, et al.[11]

5. EXAMPLE

Consider the application of the efficient f^2 method to the following three-equation problem of Kuno and Seader,[19] who added a third equation to Example 2 (The Four-Cluster problem) of Brown and Gearhart.[20]

Step 1:

Write the system of equations in zero form:

$$f_1(\underline{x}) = (x_1 - x_2^2)(x_1 - \sin x_2) = 0$$
$$f_2(\underline{x}) = (\cos x_2 - x_1)(x_2 - \cos x_1) = 0$$
$$f_3(\underline{x}) = x_2(x_2 - 1) + x_3^2 = 0$$

Step 2:

Write the equations to be solved by the Levenberg–Marquardt method:

$$f_1^2 = f_2^2$$
$$f_1^2 = f_3^2$$

Step 3:

Select a set of initial guesses for the Levenberg–Marquardt method from the general equation

$$x_i^0 = xU_i - Coef(xU_i - xL_i)$$

where, xU and xL are arbitrary upper and lower limits, and $Coef$ is an arbitrary set of values. In this study, values of xU were often selected between 1 and 0, while xL was most often selected between 0 and −1. The set of $Coef$ values used was [0, 0.05, 0.40, 0.50, 0.60, 0.95, 1.00].

If the first set of initial values produces a result, no further sets are needed.

For this example, the following arbitrary values were successful: xU = [1, 1, 1], xL = [0, 0, 0], and $Coef$ = 0.4, giving an initial guess of

x^0 = [0.6, 0.6, 0.6]

Step 4:

Use the Levenberg–Marquardt method in the Optimization Toolbox of MATLAB with the second set of equations in Step 2 with the initial guess of Step 3 to find an optimal starting point, *xopt*, for the homotopy continuation calculations.

The result was

$$xopt = [0.66609, 0.61346, 0.51314]$$

corresponding to $f_1^2 = f_2^2 = f_3^2 = 6.8591 \times 10^{-4}$

Because the functions are not zero, *xopt* is not a solution of the equations in Step 1, but it is a bifurcation point on the homotopy path, from which all roots can be found by tracking in the subsequent steps. If *xopt* lies on an isola containing no real roots, another initial guess is required. However, this condition is very rare and most isolas contain at least one real root.

Step 5:

Write the homotopy equations from eq 6, noting that as discussed by Khaleghi Rahimian et al.,[11] the only part of the homotopy that needs to be tracked is the far-right factor. Therefore, for this example, the homotopy equations to tracked are:

$$H_1 = (1 + f_1^2 - t) = 0$$
$$H_2 = (1 + f_2^2 - t) = 0$$
$$H_3 = (1 + f_3^2 - t) = 0$$

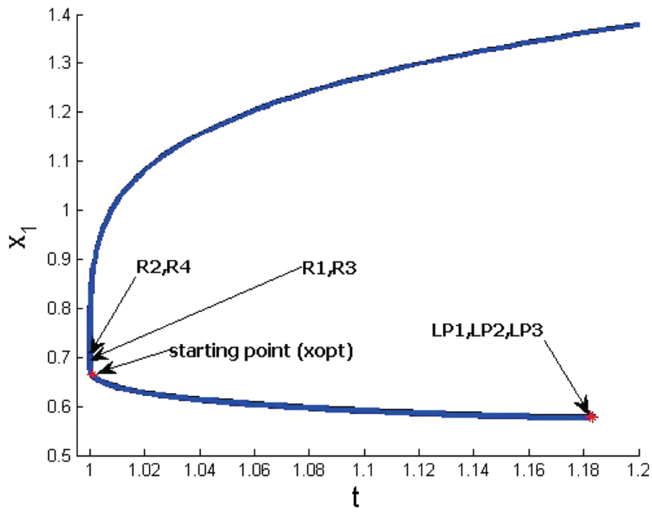

Figure 1. Homotopy Path in Step 6 of the Example for x_1.

It is important to note that because the functions are squared, the homotopy parameter is bounded to $t \geq 1$, which makes all roots limit points. Unlike other homotopy methods, tracking does not begin from $t = 0$, but from the value of t corresponding to *xopt* found in Step 4, which now becomes the starting point for tracking. Thus, for this example, the initial value is:

$$t = 1 + 6.8591 \times 10^{-4} = 1.00068591.$$

Step 6:

The homotopy path is tracked using the CL_MATCONT toolbox in MATLAB, first for the backward branch by increasing t from its initial value and then for the forward branch by decreasing t from the its initial value. If the two branches meet, the path is an isola. For this example, the homotopy paths for x_1, x_2, and x_3, starting from *xopt*, are shown in Figures 1, 2, and 3, respectively. It can be seen that the forward and backward branches have the following four roots (R) and three limit points (LP):

$$\mathrm{R1}: x_1 = 0.69482,\ x_2 = 0.76817,\ x_3 = 0.42200$$
$$\mathrm{R2}: x_1 = 0.70711,\ x_2 = 0.7854,\ x_3 = 0.41055$$
$$\mathrm{R3}: x_1 = 0.69482,\ x_2 = 0.76817,\ x_3 = -0.42200$$
$$\mathrm{R4}: x_1 = 0.70711,\ x_2 = 0.7854,\ x_3 = -0.41055$$
$$\mathrm{LP1}: x_1 = 0.578972,\ x_2 = -0.296503,\ x_3 = 0.20825$$
$$\mathrm{LP2}: x_1 = 0.580041,\ x_2 = -0.322775,\ x_3 = 0$$
$$\mathrm{LP3}: x_1 = 0.578972,\ x_2 = -0.296503,\ x_3 = -0.20825$$

Note that all roots are both bifurcation points and limit points, and the homotopy parameter, t, is always $\geq$1.0, with the roots being located at $t = 1$.

Step 7:

Because the roots found in Step 6 are bifurcation points, it is necessary to track the branches stemming from these points to seek other roots. To do this, the tangent vectors must be calculated. However, because all roots are also limit points, the

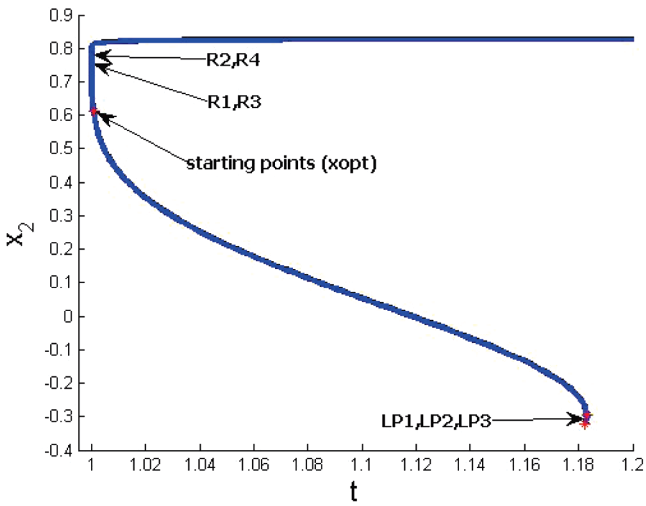

Figure 2. Homotopy Path in Step 6 of the Example for x_2.

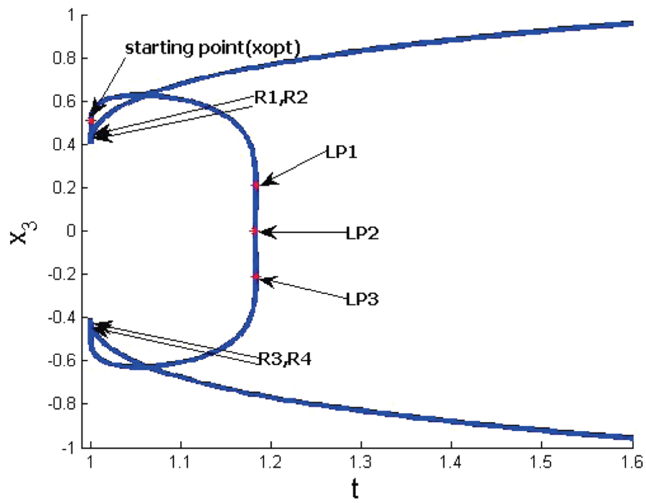

Figure 3. Homotopy Path in Step 6 of the Example for x_3.

tangent vector, v_t, with respect to the homotopy parameter, t, might equal exactly to zero. Consequently it is not possible to find the different tangent vectors on the stemming branches. To make sure that v_t is different from zero, the MATLAB fsolve is first applied with the following Root_V.m file using the root found in Step 6 as an initial guess to find a point close to the root:

$$\text{function F} = \text{Root\_V}(\text{x, a, fun})$$

$$\text{F} = \text{feval}(\text{fun, x})\text{-a}$$

where "a" is a small value close to zero such as 1e-17. Next, the tangent vector on the new point is calculated. If v_t differs from zero, the new tangent vector is used to obtain the tangent vectors on the stemming branches; otherwise "a" is multiplied by a factor 1.1 and the above procedure is repeated. The resulting tangent vectors for the four roots found in Step 6 were

$$\text{v1R1}: v_1 = 0.6942 \quad v_2 = 0.62199 \quad v_3 = -0.36225 \quad v_t = 1.0824\text{e-}017$$

$$\text{v1R2}: v_1 = 0.53072 \quad v_2 = 0.69444 \quad v_3 = -0.4859 \quad v_t = 1.4354\text{e-}019$$

$$v\text{1R3}: v1 = 0.69499 \quad v_2 = 0.61933 \quad v_3 = 0.36526 \quad v_t = 1.459\text{e-}017$$

$$v\text{1R4}: v_1 = 0.30506 \quad v_2 = 0.7691 \quad v_3 = 0.56162 \quad v_t = -1.5981\text{e-}017$$

Step 8:

With the tangent vectors found in Step 7, for the four roots found in Step 6, the tangent vectors for the stemming branches can be calculated. CL_MATCONT is able to find the two different tangent vectors that might result in the same stemming branch. However, to make sure that all the existing branches are tracked, all three tangent vectors, including the one obtained in Step 7 and the other two vectors obtained in this step, are used. The code avoids duplicate tracking of the similar branches. The additional tangent vectors for the four roots were found to be

$$\text{v2R1}: v_1 = -0.65467 \quad v_2 = -0.61008 \quad v_3 = 0.44634 \quad v_t = 1.9237\text{e-}017$$

$$\text{v2R2}: v_1 = -0.72584 \quad v_2 = -0.57962 \quad v_3 = 0.3704 \quad v_t = 1.4827\text{e-}018$$

$$\text{v2R3}: v_1 = 0.66503 \quad v_2 = 0.60692 \quad v_3 = 0.43519 \quad v_t = -2.5516\text{e-}017$$

$$\text{v2R4}: v_1 = 0.7014 \quad v_2 = 0.56337 \quad v_3 = 0.43663 \quad v_t = -2.6661\text{e-}017$$

$$v\text{3R1}: v_1 = -0.35836 \quad v_2 = -0.75347 \quad v_3 = 0.55125 \quad v_t = 2.3758\text{e-}017$$

$$\text{v3R2}: v_1 = -0.3147 \quad v_2 = -0.79982 \quad v_3 = 0.51112 \quad v_t = 2.046\text{e-}018$$

$$\text{v3R3}: v_1 = 0.34469 \quad v_2 = 0.76287 \quad v_3 = 0.54701 \quad v_t = -3.2072\text{e-}017$$

$$\text{v3R4}: v_1 = 0.31153 \quad v_2 = 0.75107 \quad v_3 = 0.58211 \quad v_t = -3.5544\text{e-}017$$

Step 9

The stemming branches from the four roots using the tangent vectors obtained in Steps 7 and 8 are tracked. The branch stemmed from R1 using v2R1 found the following additional two roots and four limit points:

$$\text{R5}: x_1 = 0.64171 \quad x_2 = 0.80107 \quad x_3 = 0.39919$$

$$\text{R6}: x_1 = 0.67919 \quad x_2 = 0.82413 \quad x_3 = 0.38071$$

$$\text{LP4}: x_1 = 0.70402 \quad x_2 = 0.81479 \quad x_3 = 0.38725$$

$$\text{LP5}: x_1 = 0.64351 \quad x_2 = 0.76317 \quad x_3 = 0.421695$$

$$\text{LP6}: x_1 = 0.65597 \quad x_2 = 0.81574 \quad x_3 = 0.38858$$

$$\text{LP7}: x_1 = 0.70258 \quad x_2 = 0.77696 \quad x_3 = 0.41646$$

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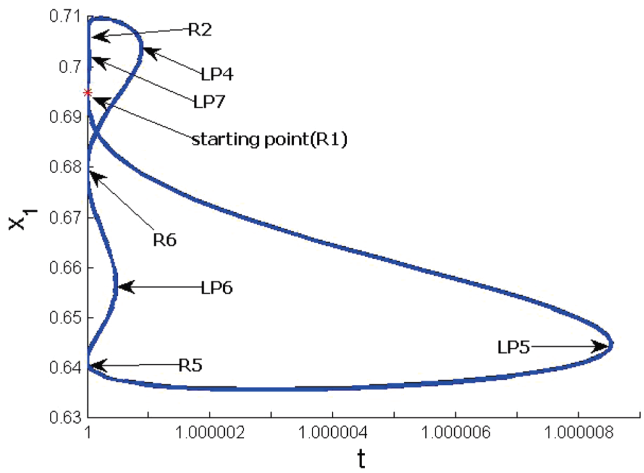

Figure 4. Stemming Path from R1, using v2R1 in Step 9 of the Example for x_1.

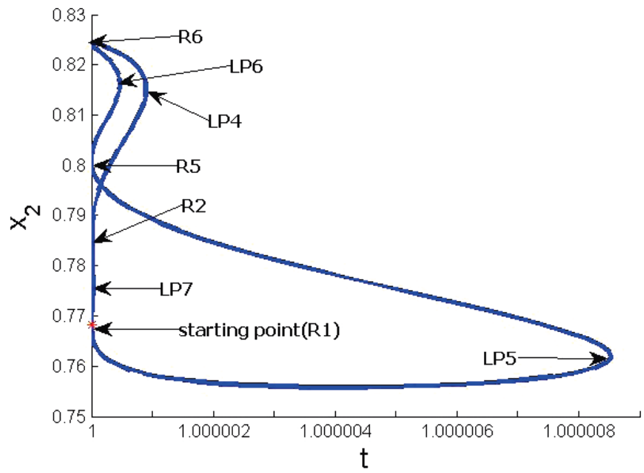

Figure 5. Stemming Path from R1, using v2R1 in Step 9 of the Example for x_2.

Figures 4, 5, and 6 show the homotopy paths for x_1, x_2, and x_3, respectively. Unlike the paths in Figures 1, 2, and 3, the stemming paths in this example are isolas.

Tracking the stemming branches from R1 using v1R1 generates another isola, but with no additional roots, while using v3R1 results in the same branch that was already traced in Step 6. All stemming branches from R2 were tracked previously.

The last two roots are found by tracking the branches that stem from R3 by using v2R3 as shown in Figure 7 for x_3. The homotopy paths for x_1 and x_2 are exactly the same as in Figures 4 and 5, respectively. It is observed in Figure 7 that again the homotopy path is an isola, containing the following two additional roots and four limit points:

$$\mathrm{R7}: x_1 = 0.64171 \quad x_2 = 0.80107 \quad x_3 = -0.39919$$

$$\mathrm{R8}: x_1 = 0.67919 \quad x_2 = 0.82413 \quad x_3 = -0.38071$$

$$\mathrm{LP8}: x_1 = 0.64516 \quad x_2 = 0.76176 \quad x_3 = -0.42942$$

$$\mathrm{LP9}: x_1 = 0.65665 \quad x_2 = 0.81619 \quad x_3 = -0.38644$$

$$\mathrm{LP10}: x_1 = 0.70382 \quad x_2 = 0.81503 \quad x_3 = -0.38949$$

$$\mathrm{LP11}: x_1 = 0.7012 \quad x_2 = 0.77614 \quad x_3 = 0.41666$$

The homotopy path stemming from R3 using v1R3 is another isola, but with no additional roots. The other stemming branches, including those from R4, were already traced.

Step 10

Steps 7, 8, and 9 are repeated for the new roots until no additional roots are found. The only new homotopy paths were those stemming from R5 using v3R5 (an isola) and from R6 using v1R6. These paths did not contain any additional roots, and as a result the algorithm terminated and printed the eight roots that were found.

4. TEST RESULTS AND DISCUSSION

The efficient f^2 method was applied to the 20 test problems listed in Table 1. The problems included nonlinear functions with algebraic, square-root, trigonometric, exponential, and logarithmic terms. The number of equations varied from 2 to 13,

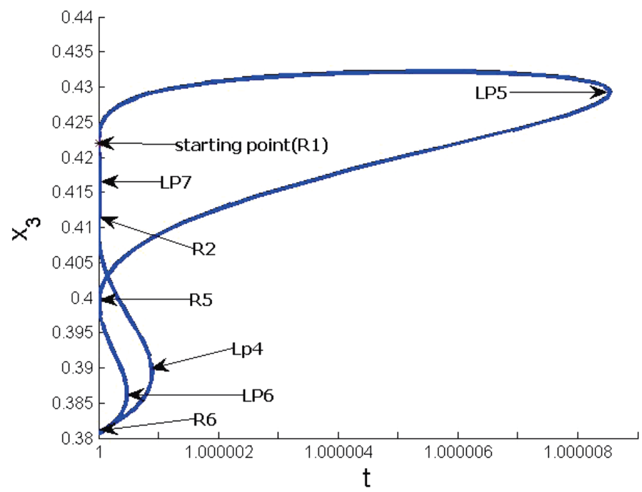

Figure 6. Stemming Path from R1, using v2R1 in Step 9 of the Example for x_3.

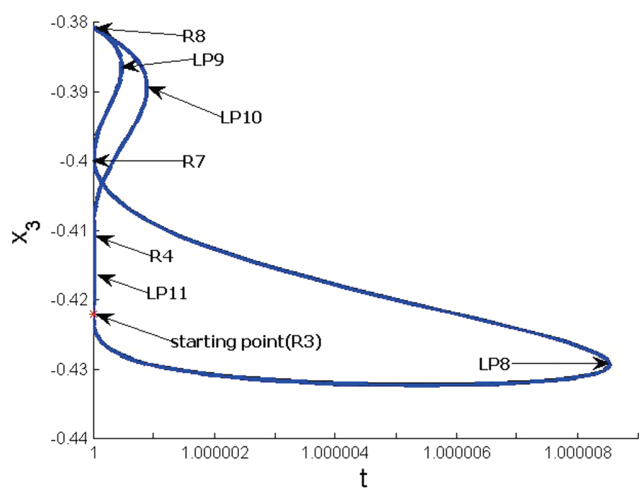

Figure 7. Stemming Path from R3, using v2R3 in Step 9 of the Example for x_3.

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Table 1. Test Results for the Efficient f^2 Method

no.	problem name	reference	no. of eqs	transcendental terms	no. of real roots	computing time (s)	isola paths?	no. of stemming roots
1	Kuno	19	3	trigonometric	8	13.37	yes	4
2	Branin1	21	2		1	3.4	no	0
3	Branin2	21	2	trigonometric	123	975.43	yes	121
4	Branin4	21	3	trigonometric	9	20.83	yes	7
5	Choi1	13	2		2	4.42	no	0
6	Choi2	13	2		4	6.54	yes	0
7	Georg1	22	2	trigonometric	27	117.85	yes	12
8	Georg2	22	3		18	206.57	yes	15
9	Georg3	22	4	trigonometric	13	280.52	yes	8
10	Heidemann	23	4	exponential	6	49.87	no	4
11	Himmelblau	24	2		9	8.39	no	5
12	Kubicek1	25	2	exponential	3	5.87	no	0
13	Kubicek2	25	4	exponential	5	18.04	yes	2
14	Seydel	26	6	exponential/trigonometric	3	22.62	no	0
15	Shacham62	27	7		11	1445.87	no	8
16	Shacham63	27	7		8	27.49	yes	0
17	Shacham70	27	10	square root	1	13.65	no	0
18	Shacham73	27	13	logarithmic	1	53.46	no	0
19	Skogestad	28	6		7	56.67	no	6
20	Stability_SRK_6	29	6	logarithmic	3	137.65	no	0

and the number of real roots, all of which were found, varied from 1 to 123. The table includes information on isolas and stemming. Computation times varied from 3 to 1446 s, with an average time per root found of 13 s. References for the test problems are included in the table and specifically addressed in the reference citations. For each test problem, the equations, starting guesses, roots, and sum of squared functions are tabulated in Appendix B in the Supporting Information, with the exception of the equations for Test Problem 20, which can be obtained from ref 29 and the 123 roots for Test Problem 3, which can be obtained from the first author of this paper. For all test problems, the fsolve function of MATLAB was used to find the precise values of the roots. However, in Appendix B in the Supporting Information, the roots are only reported to five significant digits.

For Problem 6, the form of the trigonometric functions in the Georg3 equations led to an infinite number of roots. Therefore, the search for roots was arbitrarily bounded to values of x_1 and x_2 from $-\pi$ to $+\pi$. One of the most difficult problems to solve was Problem 10, Heidemann. In addition to the two equations for liquid−liquid equilibrium, four equations had to be added to satisfy material balance constraints for the two-component system. As a result, an initial guess with the inconsistency of all values of $x = 0$, 1 or some intermediate value failed. A more reasonable starting guess of [0, 1, 1, 0, 0.5, 0.5] readily converged. Again, the search for roots was bounded, this time between the only feasible values of 0 and 1.

Problem 15 was the most difficult problem to solve. To obtain all 11 real roots, it was required to use three different values [1e-17,1e-15,1e-12] for the parameter "a" defined in Step 7. It was observed that there were multiple stemming paths from some roots, and as a result it was necessary to calculate different tangent vectors.

5. CONCLUSIONS

A new homotopy continuation method, which combines fixed-point and Newton homotopies, is developed for finding all real roots to a system of nonlinear equations, including those with transcendental terms. To do this, a new system of equations is formulated by squaring each function followed by multiplication of each squared function by $(x_i - x_i^0)$, where the 0 superscript indicates a starting value. The new system of equations generates bifurcation points that can reach all real roots, including those that might lie on isolas, which are all reachable from the bifurcations points. The method, called the *efficient f^2 method*, was applied successfully to 20 test problems.

APPENDIX

The bifurcation point test function of eq 6 is given by the Kuznetsov ([14]) criterion

$$\phi(\underline{x}, t) = \det \begin{pmatrix} \frac{\partial H_1}{\partial x_1} & \frac{\partial H_1}{\partial x_2} & \cdots & \frac{\partial H_1}{\partial x_n} & \frac{\partial H_1}{\partial t} \\ \frac{\partial H_2}{\partial x_1} & \frac{\partial H_2}{\partial x_2} & \cdots & \frac{\partial H_2}{\partial x_n} & \frac{\partial H_2}{\partial t} \\ \vdots & & & & \\ \frac{\partial H_n}{\partial x_1} & \frac{\partial H_n}{\partial x_2} & \cdots & \frac{\partial H_n}{\partial x_n} & \frac{\partial H_n}{\partial t} \\ \nu_1 & \nu_2 & \cdots & \nu_n & \nu_{n+1} \end{pmatrix}$$

The partial derivatives are calculated as follows:

$$\begin{cases} \frac{\partial H_1}{\partial x_1} = 1 + f_1^2 - t + 2f_1\left(\frac{\partial f_1}{\partial x_1}\right)(x_1 - x_1^0) \\ \frac{\partial H_1}{\partial x_2} = 2f_1\left(\frac{\partial f_1}{\partial x_2}\right)(x_1 - x_1^0) \\ \vdots \\ \frac{\partial H_1}{\partial x_n} = 2f_1\left(\frac{\partial f_1}{\partial x_n}\right)(x_1 - x_1^0) \\ \frac{\partial H_1}{\partial t} = x_1^0 - x_1 \end{cases}$$

$$\begin{cases} \dfrac{\partial H_2}{\partial x_1} = 2f_2\left(\dfrac{\partial f_2}{\partial x_1}\right)(x_2 - x_2^0) \\ \dfrac{\partial H_2}{\partial x_2} = 1 + f_2^2 - t + 2f_2\left(\dfrac{\partial f_2}{\partial x_2}\right)(x_2 - x_2^0) \\ \cdots \\ \dfrac{\partial H_2}{\partial x_n} = 2f_2\left(\dfrac{\partial f_2}{\partial x_n}\right)(x_2 - x_2^0) \\ \dfrac{\partial H_2}{\partial t} = x_2^0 - x_2 \end{cases}$$

$$\begin{cases} \dfrac{\partial H_n}{\partial x_1} = 2f_n\left(\dfrac{\partial f_n}{\partial x_1}\right)(x_n - x_n^0) \\ \dfrac{\partial H_n}{\partial x_2} = 2f_n\left(\dfrac{\partial f_n}{\partial x_2}\right)(x_n - x_n^0) \\ \cdots \\ \dfrac{\partial H_n}{\partial x_n} = 1 + f_n^2 - t + 2f_n\left(\dfrac{\partial f_n}{\partial x_n}\right)(x_n - x_n^0) \\ \dfrac{\partial H_2}{\partial t} = x_n^0 - x_n \end{cases}$$

Since at all roots, f_i and the homotopy parameter, t, are 0 and 1, respectively, the test function becomes as follows:

$$\phi(\underline{x}, t) = \det\begin{pmatrix} 00 \cdots 0x_1^0 - x_1 \\ 00 \cdots 0x_2^0 - x_2 \\ \cdots \\ 00 \cdots 0x_n^0 - x_n \\ \nu_1\ \nu_2 \cdots \nu_n\ \nu_{n+1} \end{pmatrix} = 0$$

Thus, all roots are bifurcation points.

ASSOCIATED CONTENT

Supporting Information. Appendix B. This material is available free of charge via the Internet at http://pubs.acs.org.

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NOMENCLATURE

F = New function
f = Original function
G = Combination of the fixed point and Newton functions
H = Homotopy function
t = Homotopy parameter
x = Unknown variable
BP = Bifurcation point
LP = Limit point
R = Root
ν = Tangent vector

REFERENCES

(1) Churchill, S. W. *The Interpretation and Use of Rate Data: The Rate Concept*. McGraw-Hill Book Co.: New York, 1974.
(2) Carnahan, B.; Luther, H. A.; Wilkes, J. O. *Applied Numerical Methods*. John Wiley & Sons, Inc.: New York, 1969.
(3) Lucia, A.; Feng, Y. Global Terrain Methods. *Comput. Chem. Eng.* **2002**, *26*, 529.
(4) Lahaye, E. C.R. Une methode de resolution d'une categorie dequations transcendantes. *Acad. Sci.* **1934**, *198*, 1840–1842.
(5) Wayburn, T. L.; Seader, J. D. *Solution of Systems of Interlinked Distillation Columns by Differential Homotopy-Continuation Methods. Proceedings of the Second International Conference on Foundations of Computer-Aided Process Design*. CACHE. 1984, 765−862.
(6) Conte, S. D.; de Boor, C. *Elementary Numerical Analysis*, 3rd ed.; McGraw-Hill Book Co.: New York, 1980.
(7) Davidenko, D. On a New Method of Numerically Integrating a System of Nonlinear Equations. *Dokl. Akad. Nauk SSSR.* **1953**, *88*, 601–602.
(8) Kloppenstein, R. W. Zeros of nonlinear functions. *J. ACM.* **1961**, *8*, 366–373.
(9) Kubicek, M. Algorithm 502 Dependence of Solution of Nonlinear Systems on a Parameter. *ACM Trans. Math. Software* **1976**, *2* (1), 98–107.
(10) Keller, H. B. Numerical solution of bifurcation and nonlinear eigenvalue problems. In *Applications of Bifurcation Theory*; Rabinowitz, P.H., Ed.; Academic Press, 1977, 359−384.
(11) Khaleghi Rahimian, S.; Farhang, J.; Seader, J. D.; White, R. E. A New Homotopy for Seeking All Real Roots of a Nonlinear Equation. *Comput. Chem. Eng.* **2011**, *35*, 403−411.
(12) Seader, J. D.; Kuno, M.; Lin, W.-J.; Johnson, S. A.; Unsworth, K.; Wiskin, J. W. Mapped Continuation Methods for Computing All Solutions to General Systems of Nonlinear Equations. *Comput. Chem. Eng.* **1990**, *14*, 71–85.
(13) Choi, S. H.; Book, N. L. Unreachable Roots for Global Homotopy Continuation Methods. *AIChE J.* **1991**, *37*, 1093–1095[Choi1 is Eqs. (1a, 1b); Choi2 is Eqs. (2a, 2b)].
(14) Kuznetsov, Yu. A. *Elements of Applied Bifurcation Theory*, Springer-Verlag: New York, 1988.
(15) Edgar, T. F.; Himmelblau, D. M.; Lasdon, L. S. *Optimization of Chemical Processes*, 2nd ed.; McGraw Hill: Boston, 2001.
(16) Dhooge, A.; Govaerts, W.; Kuznetsov, Yu. A. MatCont: A Matlab package for numerical bifurcation analysis of ODEs. *ACM Transactions on Mathematical Software* **2003**, *29* (2), 141–164.
(17) Dhooge, A.; Govaerts, W.; Kuznetsov, Yu.A.; Mestrom, W.; Riet, A. M.; Sautois, B. MATCONT and CL MATCONT: Continuation toolboxes in MATLAB. (http://www.matcont.ugent.be/manual.pdf). 2006.
(18) Penrose, R. A Generalized Inverse for Matrices, *Proceedings of the Cambridge Philosophical Society*. 1955, *51*, 406.
(19) Kuno, M.; Seader, J. D. Computing All Real Solutions to Systems of Nonlinear Equations with a Global Fixed-Point Homotopy. *Ind. Eng. Chem. Res.* **1988**, *27*, 1320–1329.
(20) Brown, K. M.; Gearhart, W. B. Deflation Techniques for the Calculation of Further Solutions of a Nonlinear System. *Numer. Math.* **1971**, *16*, 334–342.
(21) Branin, F. H., Jr.; Widely Convergent Method for Finding Multiple Solutions of Simultaneous Nonlinear Equations. *IBM J. Res. Develop.* **1972**, September, 504−522. [Branin1 is Eqs. (15a, 15b) with $a = 4$, $b = 2$, and $c = 1$; Branin2 is Eqs. (41a, 41b) with $a = 1$, $b = 2$, $c = 2$, $d = 4\pi$, $e = 1.9$, and $f = 2\pi$; Branin4 is Eqs. (47a, 47b, 47c) with $a = 2$, $b = 0.4\pi$, $c = 2.5$, $d = 1$, $e = 0.75$, $f = 2\pi$, $g = 1$, $h = 0.8$, and $k = 2\pi$].
(22) Georg, K. A new exclusion test. *J. Comput. and Applied Math.* **2003**, *152*, 147–160[Georg1 is *6.1. Example*; Georg2 is *6.2. Example*; Georg3 is *6.3. Example*].
(23) Heidemann, R. A.; Mandhane, J. M. Some properties of the NRTL equation in correlating liquid-liquid equilibrium data. *Chem. Eng. Sci.* **1973**, *28*, 1213–1221[Heidemann is NRTL equations with parameters of Eq. (18)].
(24) Reklaitis, G. V.; Ravindran, A.; Ragsdell, K. M.; *Engineering Optimization*; John Wiley and Sons: New York, 1983. [Himmelblau is obtained by taking partial derivatives of the Himmelblau Function of Figure 3.1 on page 69].
(25) Kubicek, M.; Marek, M.; *Computational Methods in Bifurcation Theory and Dissipative Structures*; Springer-Verlag: New York, 1983.

[Kubicek1 is the steady-state form of Eqs. (E1.1, E1.2) on page 28 with $\Lambda = 0.9$, Da = 0.07, $\gamma = 20$, $B = 20$, $\beta = 1.975$, and $\theta_c = 0$; Kubicek2 is the steady-state form of Eqs. (E3.1 to E3.4) on page 29 with $\Lambda = 1.0$, $Da_1 = Da_2 = 0.02$, $\gamma = 1000$, $B = 22$, $\beta = 3.0$, and $\theta_{c1} = \theta_{c2} = 0$]

(26) Seydel, R.; *From Equilibrium to Chaos*; Elsevier: New York, 1988. [Seydel is Eq. (5.22) on page 151]

(27) Shacham, M.; Brauner, N.; Cutlip, M. B.; A web-based library for testing performance of numerical software for solving nonlinear algebraic equations. *Comput. Chem. Eng.* **2002**, *26*, 547−554 [Shacham62, Shacham63, Shacham70, and Shacham73 are cited in Table 7 and given in detail in the NLE library at the website, http://www.polymath-software.com/library]

(28) Christiansen, A. C.; Morud, J.; Skogestad, S.; A Comparative Analysis of Numerical Methods for Solving Systems of Nonlinear Algebraic Equations. *Proc. 38th Scandinavian Simulation Soc. Conf,* June 11−13, 1996, pages 1−14. [Skogestad is Example 2, Eq. (21)]

(29) Jalali-Farahani, F.; Seader, J. D. Use of homotopy-continuation method in stability analysis of multiphase, reacting systems. *Comput. Chem. Eng.* **2000**, *24*, 1997–2008[Stability_SRK_6 is *8.1. Problem 1*].

(30) Jalali, F. Process Simulation Using Continuation Method in Complex Domain. *Comput. Chem. Eng.* **1998**, *22* (Supplement 1), S943–S946.