

A New Imbedding Method for Computing all Real Solutions of Nonlinear Algebraic Equations

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ABSTRACT

The applications of nonlinear equations arise in science and engineering. A new continuation method that seeks all real solutions to single nonlinear algebraic equations is developed and analyzed. The new continuation method comprises of new homotopy function that is a combination of the fixed-point and Newton homotopies, is developed for seeking all real solutions to a single nonlinear equation $f(x) = 0$ without having to specify a bounded interval. Path tracking is carried out with MATLAB, using the continuation toolbox of MATCONT. The new method has been applied, without failure, to numerous nonlinear equations including those with transcendental functions.

Keywords: *Imbedding method, Fixed-Point and Newton Homotopies, Nonlinear Equation*

1. INTRODUCTION

The applications of nonlinear equations arise in many areas in science and engineering. Many mathematical models consist of systems of algebraic and or transcendental equations. When all equations in the system are linear and independent of each other, only a single solution exists, which is readily obtained by many robust numerical schemes. However, more commonly, the system of equations contains some nonlinear equations. In that case, multiple solutions may exist, where the unknowns may be real (positive or negative) or complex conjugate pairs. Solutions sets consisting of real positive values are of interest when the unknowns are absolute temperature, absolute pressure, flow rate or composition variables and so on.

Occurrence of multiple solutions of interest in science and engineering problem have been known for decades, a robust methods have been devised to compute the multiple solutions. Some of these numerical methods that seek to find multiple solutions includes, Newton's method with deflation, e.g. Press. et al (1992), Parallel-path homotopy continuation methods for systems of polynomial, which use Bezout's theorem for determining the maximum number of multiple solutions and finds all solutions, real and positive, e. g., Morgan (1987) and Global homotopy continuation methods, which attempts to find all sets of real solutions, e. g. Keller (1977, 1978), Garcia and Zangwill (1981), Allgower and Georg (2003), Watson et al (1997), Gritton et al (2001), Verschelde (1999) and Sommese and Wampler (2005).

The first method is unreliable. The second method, though restricted to polynomial systems, is very reliable and easy to implement. In this paper, we concentrate on the third method and we consider only a single nonlinear algebraic equation. A new homotopy is introduced and applied to the determination of all real roots in this regard. Unlike the method of Gritton et al

(2001), the homotopy path of our method consists of branches that are only connected at opposite infinities, or by branches in the complex domain. Instead our new homotopy only consists of one path, which is quickly tracked in the forward and backward directions, called *Branches 1 and 2*, from the starting point or tracking initiation point. See Fig. 1 below.

2. THE NEW HOMOTOPY

$H(x, t)$ is widely used homotopy function. It consists of a linear combination of two real functions: a base function, $g(x)$, for which a zero x^0 is known or readily selected or obtained; and $f(x)$, whose zeroes x_i^* are sought. Both functions must be smooth with twice-differentiable derivatives. Thus,

$$H(x, t) = tf(x) + (1 - t)g(x) = 0 \quad (1)$$

where t , the homotopy parameter, allows tracking of a solution path that connects the starting point, x^0 , at $t = 0$, to all x_i^* , which are all solutions of $f(x) = 0$. With numerical continuation, the parameter t is gradually varied, starting at $t = 0$ and without being confined, leading to a series of solutions to Eqn. (1). The solution of $f(x) = 0$ is found whenever the homotopy path crosses $t = 1$.

One important thing that comes up when attempting to determine all roots $f(x) = 0$ is the choice of the base function or the start function $g(x)$. The three most widely used start functions are the fixed-point function

$$g(x) = (x - x^0), \quad (2)$$

the affine function, which only adds a factor, A , to the fixed point function to improve scaling in the homotopy function

$$g(x) = A(x - x^0), \quad (3)$$

where A is often taken as the derivative of $f(x)$ evaluated at x^0 , and the Newton function

$$g(x) = f(x) - f(x^0) \quad (4)$$

When Eqn. (2) or Eqn. (3) are applied to Eqn. (1), the homotopy is satisfied by only root at $t = 0$, the usual starting point.

When Eqn. (4) is applied, $f(x) = f(x^0)$ at $t = 0$ and multiple starting points and multiple branches may exist. Here, we introduce a new formulation of the homotopy function of Eqn. (1), which incorporates a new $g(x)$ function. At first, the new homotopy appears to be considerably more complicated than Eqn. (1) with Eqn. (2), (3) or (4). However, after simplification, the new homotopy is less complex, avoids the disadvantages of fixed-point, affine and Newton functions, and possesses superior characteristics for tracking the homotopy path to determine all solutions to $f(x) = 0$. Since our new homotopy uses elements of the fixed-point and Newton's functions, we refer to the new homotopy as **fixed-point-Newton homotopy**. Most important, the fixed-point-Newton homotopy does not have multiple starting points and the path is not connected at opposite infinities.

The fixed-point-Newton homotopy is formulated in two stages. In the first stage, multiply the target function, $f(x)$, by the fixed-point function to give a new function,

$$F(x) = f(x)(x - x^0) \quad (5)$$

Now, Eqn. (1) becomes

$$H(x, t) = tF(x) + (1 - t)g(x) \quad (6)$$

In the next step, the function $g(x)$ is formed by a combination of the fixed-point and Newton functions to give

$$g(x) = \{(x - x^0) + [F(x) - F(x^0)]\} = 0 \quad (7)$$

substitution of Eqn. (7) into Eqn. (6), we have

$$H(x, t) = tF(x) + (1 - t)\{(x - x^0) + [F(x) - F(x^0)]\} = 0 \quad (8)$$

Our new homotopy given in Eqn. (8) seems to be more complicated than homotopies formed from Eqn. (1) with Eqns. (2), (3), or (4). It is simplified by first noting that Eqn. (5) causes $F(x^0)$ to be zero. Thus, putting Eqn. (5) into Eqn. (8), after simplification, gives

$$H(x, t) = (x - x^0)[1 + f(x) - t] = 0 \quad (9)$$

which is quite simple. Eqn. (9) is the new homotopy for the continuation method presented here.

3. STEPS FOR FINDING ALL ROOTS WITH THE FIXED-POINT-NEWTON HOMOTOPY

The steps for finding all real roots with the fixed-point-Newton homotopy, as used in this research, are as follows, with reference to Fig. 1, which shows an example of homotopy paths.

Step 1 Write the equation to be solved in the form $f(x) = 0$, if it is not in this form. While doing this, examine the function and determine if it can be reduced to a simpler form. Remove variables from any denominator terms where possible. Consider changing variables or scaling.

Step 2 Multiply $f(x)$ by $(x - x^0)$ to give a new function $F(x) = f(x)(x - x^0)$

Step 3 Form the fixed-point-Newton homotopy $H(x, t) = tF(x) + (1 - t)\{(x - x^0) + [F(x) - F(x^0)]\} = 0$

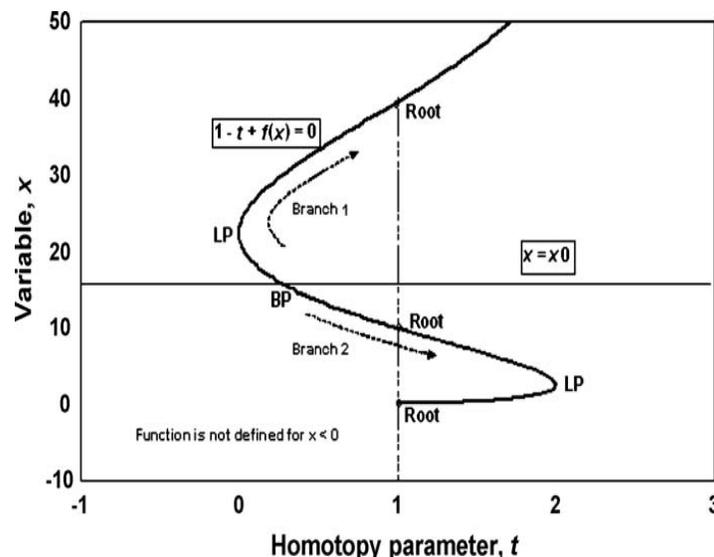


Fig. 1

Example of homotopy branches.

Step 4 Simplifying the fixed-point-Newton homotopy to its working form

$$H(x, t) = (x - x^0)[1 + f(x) - t] = 0$$

Step 5 Select the starting point, x^0 , as zero, unless $f(x^0)$ is not defined; in which case, select a value of x^0 (e. g. one) such that $f(x^0)$ is defined. This starting point is the bifurcation (branch) point, (BP). Note that although x^0 is a root of $F(x) = 0$. In Fig. 1, the function is not defined for $x < 0$ and x^0 is arbitrarily chosen as 16. When $f(x)$ is not defined within certain

bounds, starting points on either side of the bounds can be used to find all roots.

Step 6 Note that the value of the homotopy parameter, t , for the starting point is readily calculated from $t = 1 + f(x^0)$, and is usually not zero as in the application of other homotopy methods. Note in Fig. 1, that at the starting point, BP, $t = 0.21$.

Step 7 Ignoring the branch, $x - x^0$, track the paths of Branches 1 and 2 of $1 + f(x) - 1 = 0$ that stem from the starting point in the $x-t$ plane, proceeding carefully around any existing limit (turning) points, LP. Branch 1 is computed by initially continuing backward in t , while Branch 2 is computed by initially computing forward in t .

Step 8 Verify any turning point by applying the condition $t = 1 + f(x)$ when $\frac{df(x)}{dx} = 0$. If possible, check for additional turning points, which if found may require that extensions of the branches be calculated.

Step 9 The value of x each time the path of a branch crosses $t = 1$ is a root of $f(x) = 0$. In Fig. 1, three roots are shown, one on branch 1, and two on Branch 2. If Branch 2 were continued, more roots might be found on that branch. If neither branch crosses $t = 1$, it may be assumed that no real roots exist (see Problem 2).

Step 10 Verify that each root satisfies $f(x) = 0$.

4. APPLICATION OF FIXED-POINT-NEWTON

Using the global fixed- point homotopy method, Gritton et al (2001) successfully solved many single nonlinear equations for all roots, real and complex. These equations were also solved successfully for all real roots with the fixed-point-Newton homotopy method described above. However, we limit our discussion here to three of these equations and point out the significant difference between the two methods.

Problem 1 This problem consists of the following second degree polynomial equation, which has complex roots, and was formulated to see how the fixed-point-Newton homotopy method behaves when no real roots exist. The function is

$$f(x) = x^2 - 4x + 13 = 0 \tag{10}$$

Equation (10) has a complex conjugate roots, $x = 2 + 3i$ and $2 - 3i$. A starting value of 0 was selected for x^0 , corresponding to a value of 14 for the homotopy parameter, t . The homotopy curve, as computed with MATCONT is shown in Fig. 5, where it can be seen that the path does not intersect the vertical line for $t = 1$. Thus, there are no real roots.

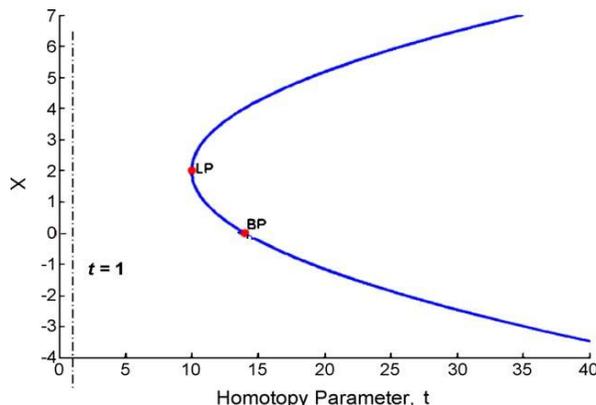


Fig. 5

FPN homotopy path for Problem 2 using $x^0 = 0$

Problem 2 This problem was designed to test the ability of fixed-point-Newton homotopy to track the path of a trigonometrical function, complicated by the addition of an exponential term in the form of a hyperbolic function, as follows;

$$f(x) = \sin(x) - \frac{\cosh(x)}{1000} + 0.5 = 0 \tag{11}$$

A starting point of $x^0 = 0$ was selected, which gave a bifurcation point at $t = 1.5$. The homotopy path is shown in Fig. 6. Tracking of the forward branch found three real roots at $x = 3.643, 5.975,$ and 8.000 . Tracking of the backward branch found three real roots at $x = -0.522, -2.626,$ and -6.464 . After finding the roots, the ends of both branches tends to trail off to $t = -\infty$.

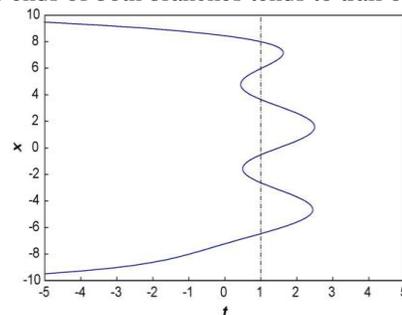


Fig. 6

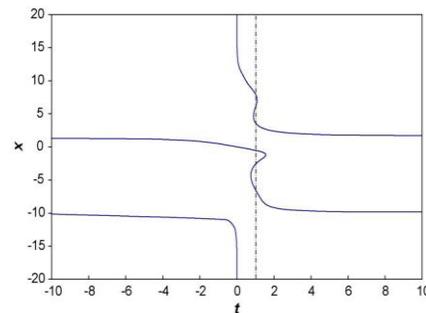


Fig. 7

FPN homotopy path for Problem 2 using $x^0 = 0$
 GFPH homotopy path for Problem 2 using $x^0 = 0$

Problem 2 was also solved using GFPH method, with $x^0 = 0$. The homotopy path is shown in Fig. 7, which exhibits some of the characteristics of the complicated GFPH paths in Fig. 4. Although the GFPH method finds all six roots, the paths go in and out of $x = \pm \infty$ at $t = 0$.

5. DISCUSSION OF RESULTS

We presented the homotopy continuation methods where we observed that the method operates in two stages: Firstly, homotopy methods exploits the structure of the system $f(x) = 0$ to find a root count and to construct a start system $g(x) = 0$ that has exactly as many regular solutions as the root count. This start system is embedded in the homotopy $H(x, t) = \eta(1 - t)g(x) + tf(x) = 0$, $t \in [0, 1]$ with $\eta \in \leq$ a random number. Secondly, as t moves from 0 to 1, numerical continuation methods trace the path that originates at the solution of the start systems towards the solution of the target system.

PHCpack (a general-purpose solver for polynomial) is a software package that contains many homotopy methods to solve polynomial systems. The first public release of the source code (Version 1.0) of PHCpack is achieved in [Verschelde, 1999]. In [Verschelde, 2005], 22 algorithms are explicitly listed as part of PHCpack. We used the software in constructing a large database of interesting polynomial systems that can serve the same polynomial.

Another result obtained, which is less superior to the method described above is the development of a new continuation method that seeks all real solutions to a single nonlinear algebraic equations. The new continuation method comprises of new homotopy function that is a combination of the fixed-point and Newton homotopies, is developed for seeking all real solutions to a single nonlinear equation $f(x) = 0$ without having to specify a bounded interval. Path tracking is carried out with MATLAB, using the continuation toolbox of MATCONT. The new method has been applied, without failure, to numerous nonlinear equations including those with transcendental functions. The new homotopy is used in chemical equilibrium problem and compare the result with the one obtained by Gritton *et al* (2006) using global fixed-point homotopy.

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