Computing All Real Solutions to Systems of Nonlinear Equations with a Global Fixed-Point Homotopy

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A global fixed-point homotopy has not found wide application in chemical engineering for solving systems of nonlinear equations by continuation. Rather, the Newton and problem-dependent homotopies have been favored. However, it is conjectured here that the fixed-point homotopy would be expected to always place all real roots of the system on a global homotopy path because the path is forced to begin from a single starting point. If so, all roots could be computed by following the single path with a suitable continuation method. This would be particularly desirable when the number of real roots to a system cannot be predetermined and one wishes to compute all solutions. In this study, it was found that such a path does exist provided that a criterion is used for selecting a starting point which minimizes the number of real roots of the global fixed-point homotopy function at an infinite value of the homotopy parameter. Several examples, including an adiabatic reactor with multiple solutions are presented to illustrate the application of the criterion. While methods have been devised recently to find all roots of polynomial equations, this is the first method for systematically locating all roots to general systems of nonlinear equations.

The necessity of solving systems of nonlinear equations often arises in simulating and designing a chemical plant or optimizing a process. Newton's method or Powell's method are commonly applied to solve such systems. However, as described by Seader (1985), both methods have well-known disadvantages such as the requirement that the starting point (initial guess of the solution) must be in the neighborhood of a root. That is, these methods are only locally convergent. In addition, both methods are designed to locate, at best, just one root even though multiple solutions may exist.

Continuation methods are rapidly being applied to numerous problems in engineering analysis as summarized in a recent review by Seydel and Hlavacek (1987). A solution method for nonlinear equations that is globally convergent from any starting point is the homotopy continuation method. This method, as described, e.g., by Garcia and Zangwill (1981), does not solve the nonlinear equations directly, but gradually reaches a root by beginning from a starting point which satisfies a second, simpler system of equations. Both systems of equations are embedded into a so-called homotopy function. Thus, if \( f(x) \) is the system of nonlinear equations to be solved and \( g(x) \) is a second simpler system of the same number of equations, the homotopy function might be constructed as

\[
H(x, t) = tf(x) + (1-t)g(x) = 0
\]

where \( t \) is a scalar homotopy parameter which is gradually varied from 0 to 1 as the path is tracked from the starting point to a solution.

The homotopy function can be constructed in accordance with the characteristics of each system of nonlinear equations, but this effort can be time consuming. Alternatively, canonical homotopy functions can be used, two of which, as described by Garcia and Zangwill (1981) and Wayburn and Seader (1987), are the Newton homotopy and the fixed-point homotopy, where \( g(x) = f(x) - f(x^0) \) and \( x - x^0 \), respectively.

Until now, most studies have focused on the use of homotopy continuation to obtain only one root even though other roots may exist. Studies to obtain all roots are recent and have been restricted largely to systems of polynomial equations, as discussed by Morgan (1987), where multiple starting points are used to obtain multiple solutions. Allgower and Georg (1980, 1983) discuss methods for approximating additional, but not necessarily all, roots of general systems of nonlinear equations.

The aim of this paper is to present a method for determining a starting point from which one can find all the roots along one branch of the path when using a global fixed-point homotopy. The homotopy parameter is permitted to take on values greater than one, but the homotopy path remains bounded for all values of the homotopy parameter within the region where the real path connects all the zeros of \( f(x) \). The real path may form an isola, which is a closed loop that does not contain the starting point.

In general, the global Newton homotopy and global fixed-point homotopy encounter difficulties when an at-