Evaluating all Real Roots of Nonlinear Equations Using a Global Fixed-Point Homotopy Method

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The need for the evaluation of all the real roots in systems of nonlinear equations arises in many chemical engineering applications, ranging from the calculations of the steady states inside a CSTR reactor to the evaluation of multiphase equilibria. As all algorithms for the solution of nonlinear equations involve an iterative procedure, it is particularly important to have an algorithm that can guarantee that all real solutions have been found irrespective of the selection of the initial guess. Thus, there has been considerable enthusiasm toward the global fixed-point homotopy continuation method (Kuno and Seader, 1988), which is thought to have the potential to be such a method. Briefly, this technique involves the linear weighting of the function to be solved, $\underline{F}(\underline{x})$, $\underline{x}\in\mathbf{R}^n$ and a linear function, $\underline{x}-\underline{x}_0$, using a "homotopy" parameter t,

$$\underline{H}(\underline{x},\, t) = t\underline{F}(\underline{x}) + (1-t)(\underline{x}-\underline{x}_0), \tag{1}$$

with the roots of the new function, $\underline{H}(\underline{x},\, t)$, being evaluated using Newton's method with continuation with respect to t, starting from $(\underline{x},\, t) = (\underline{x}_0,\, 0)$.

The name "global" refers to the fact that the continuation path is, in general, followed in the extended $(\mathbf{R}U\{\infty\})^{n+1}$ space (i.e., allowing both the variables $\underline{x}$ and the parameter t to take infinite values) (Seader et al., 1990). Quite early in the development of the global homotopy technique it was realized that for a given initial guess some of the real roots might lie on a path that is not connected to the original path (isola). Based on a number of examples, it was found that these isolated paths could be connected through continuation lines in the (extended) complex $\mathbf{C}^n\times\mathbf{R}$ space by allowing the variables, $\underline{z}=\underline{x}$, to be complex (Wayburn and Seader, 1987). Therefore, it was conjectured that all the real roots can be found for an arbitrary function, $\underline{F}$, starting from any (single) arbitrary initial guess, $\underline{z}_0=\underline{x}_0$ (Kuno and Seader, 1988; Seader et al., 1990), despite the fact that there is no formal proof available. The work of Diener (1987) is the closest to supplying a formal proof, but it is applicable only if certain rather restrictive and in general difficult to test conditions are satisfied. Very recently, Choi and Book (1991) proved that Seader's conjecture is not in general true by examining a counterexample, example 2 in Choi and Book (1991). There they showed that for specific choices of the initial guess, $\underline{x}_0$, the continuation path cannot trace all the real roots, even if allowance for complex values for the variables, $\underline{x}$, is made. We show in this note that this failure can be rectified, in at least the counterexample of Choi and Book, if one of the variables, x_i, is used as a continuation parameter and the rest of the variables as well as the homotopy parameter are allowed to be complex and/or infinite. Whether a formal proof is possible that will guarantee this behavior for all possible cases or another counterexample can be found to disprove this extended conjecture remains an unanswered question.

Example 2 presented by Choi and Book (1991) corresponds to a simple system of two equations:

$$\underline{F}(z) = \begin{pmatrix} z_1^2 + z_2^2 - \left(2+\dfrac{5}{16}\right) \\ -z_1^2 + z_2 + 2 \end{pmatrix} = \underline{0}. \tag{2}$$

This system of equations admits four real roots, $(z_1, z_2)^T = \{(1.5, 0.25)^T, (-1.5, 0.25)^T, (\sqrt{3}/2, -1.25)^T, (-\sqrt{3}/2, -1.25)^T\}$. As Choi and Book (1991) have shown, the homotopy path, corresponding to the initial guess $\underline{z}_0 = (0.5, 0.5)^T$, is an isola that passes through only one of the four real roots. Furthermore, it is disconnected from all other real solution paths even if $\underline{z}$ is allowed to be complex. To understand the origin of this phenomenon it is instructive to show the projections of the homotopy path in the $Re(z_1)-t$ and $Re(z_2)-t$ planes, shown in Figure 1, instead of the projection on the $Re(z_1)-Re(z_2)$ plane, as shown in Figure 3 of Choi and Book (1991). As Figure 1 shows, the (primary) path emanating from $\underline{z}_0=(0.5, 0.5)^T$ exhibits no limit points with respect to t. Therefore, the homotopy path is isolated and cannot connect to any other real solution paths, even through the complex plane, as correctly concluded by Choi and Book, (1991). Since the system of equations is polynomial, the same number of solutions needs to exist for every parameter value, and thus limit points in the real space represent bifurcation points (where the solution changes from real to complex) in the complex space, and *vice*

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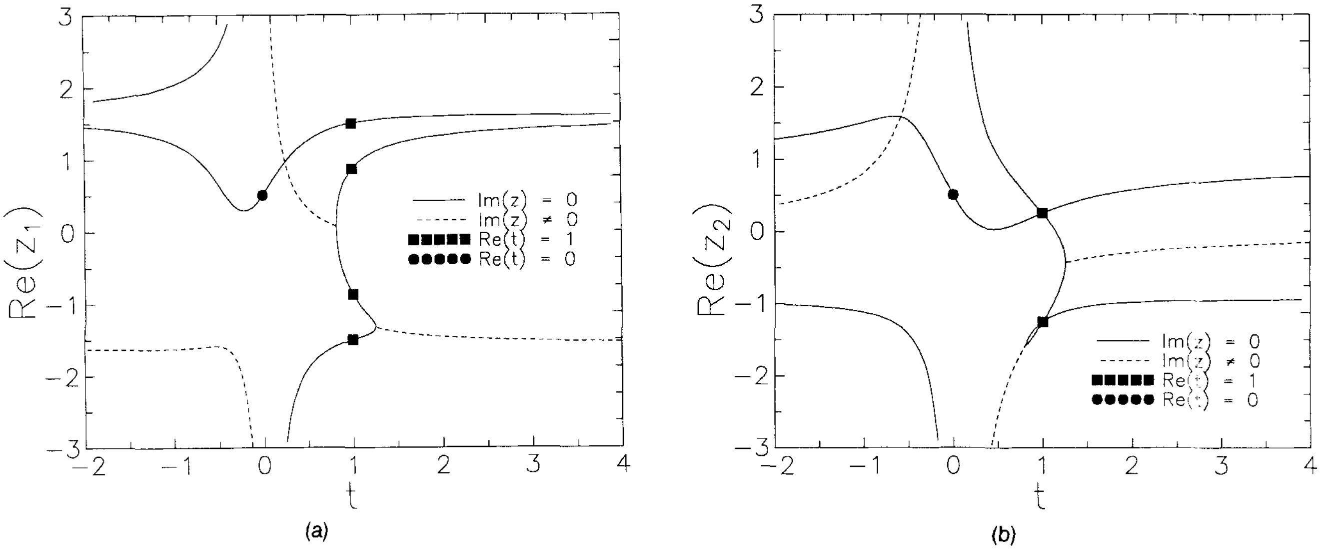

Figure 1. Projection of homotopy paths, starting from $\underline{z}_0 = (0.5, 0.5)^T$: (a) in the $Re(z_1) - t$ and (b) in the $Re(z_2) - t$ planes.

Dotted lines represent projection of complex data. Note that t is always real.

versa. Note that the limit points observed in the other (secondary) family of real solutions, also shown in Figure 1, do indeed connect to a family of complex solutions (actually two conjugate pairs) following the last argument. However, since these solutions cannot connect to the primary family of real solutions, they connect back to the secondary family after passing through infinity, as indicated by the projection represented by the dotted lines in Figure 1.

However, if Figure 1 is reexamined more carefully we cannot help but notice that there are limit points in the primary solution family, albeit not with respect to t, but with respect to either $x_1 \equiv Re(z_1)$ or $x_2 \equiv Re(z_2)$! Similarly, we can see from Figure 1 that the secondary solution family also exhibits additional limit points, although only with respect to x_2. Therefore, according to the discussion of the previous paragraph, the possibility exists that the primary and secondary solution families are connected through a family of complex solutions in the $z_1 \times t \epsilon \mathbf{C}^2$ with respect to x_2 as a parameter. Note that the original parameter t is allowed now to become complex. Numerically, all this represents is an exchange between x_2 and t with respect to their character as a parameter and a variable, respectively. To verify the above conjecture we have traced the solution paths within the parent "supermanifold" $\underline{z}xt \epsilon \mathbf{C}^3$, using different combinations of complex variables—real parameter. Thus, we have traced different one-dimensional solution families within the parent two-dimensional solution plane. This might raise the interesting question on how this plane can be exploited more efficiently, but this is beyond the point we would like to make in this note.

An efficient code has been developed using Newton's method, first-order continuation with provisions for arc-length continuation and an especially simple mapping ($1/x$) to trace the variables and/or the homotopy parameter through infinity (Gustafson, 1991). This code is used to apply the above-mentioned technique to the same example used by Choi and Book (1991), resulting in a connected solution manifold. In the current implementation, the homotopy equation, Eq. 1, is recasted into complex form,

$$\underline{H}(\underline{z}, t) = t\underline{F}(\underline{z}) + (1-t)(\underline{z} - \underline{z}_0), \tag{3}$$

where both $\underline{z}$ and t are complex, and then solved as a set of equations in real space by equating the real and the imaginary parts, respectively.

$$\begin{aligned} Re[\underline{H}(\underline{z}, t)] &= [1 - Re(t)][Re(\underline{z}) - \underline{x}_0] + Re(t)Re[\underline{F}(\underline{z})] \\ &\quad + Im(t)Im(\underline{z}) - Im(t)Im[\underline{F}(\underline{z})] = \underline{0} \\ Im[\underline{H}(\underline{z}, t)] &= [1 - Re(t)]Im(\underline{z}) + Re(t)Im[\underline{F}(\underline{z})] \\ &\quad - Im(t)[Re(\underline{z}) - \underline{x}_0] + Im(t)Re[\underline{F}(\underline{z})] = \underline{0}. \end{aligned} \tag{4}$$

Thus, a system of $2n$ equations in real space with $2n$ real variables and 2 real parameters must be solved. Note that in tracing the solution families through continuation, one of the parameters is always held constant [for example, $Im(t) = 0$ in classical homotopy] so that the solution families appear as one-dimensional parameterized curves.

The solution methodology is as follows. First, the primary solution family is traced in the real space from the initial point, $\underline{z}_0$. Subsequently, all limit points, with respect to $Re(t)$ or any of the $x_i = Re(z_i)$ variables taken as a parameter, are identified on the primary solution family. The one-dimensional solution families in the complex space, which originate from these limit points, are then traced by continuation in the real space of the variable with respect to which the limit point occurred, while allowing the other variables (including the homotopy parameter if applicable) to become complex. Each path in the complex space is traced until it bifurcates into the real space either on the primary solution family or on a secondary solution family.

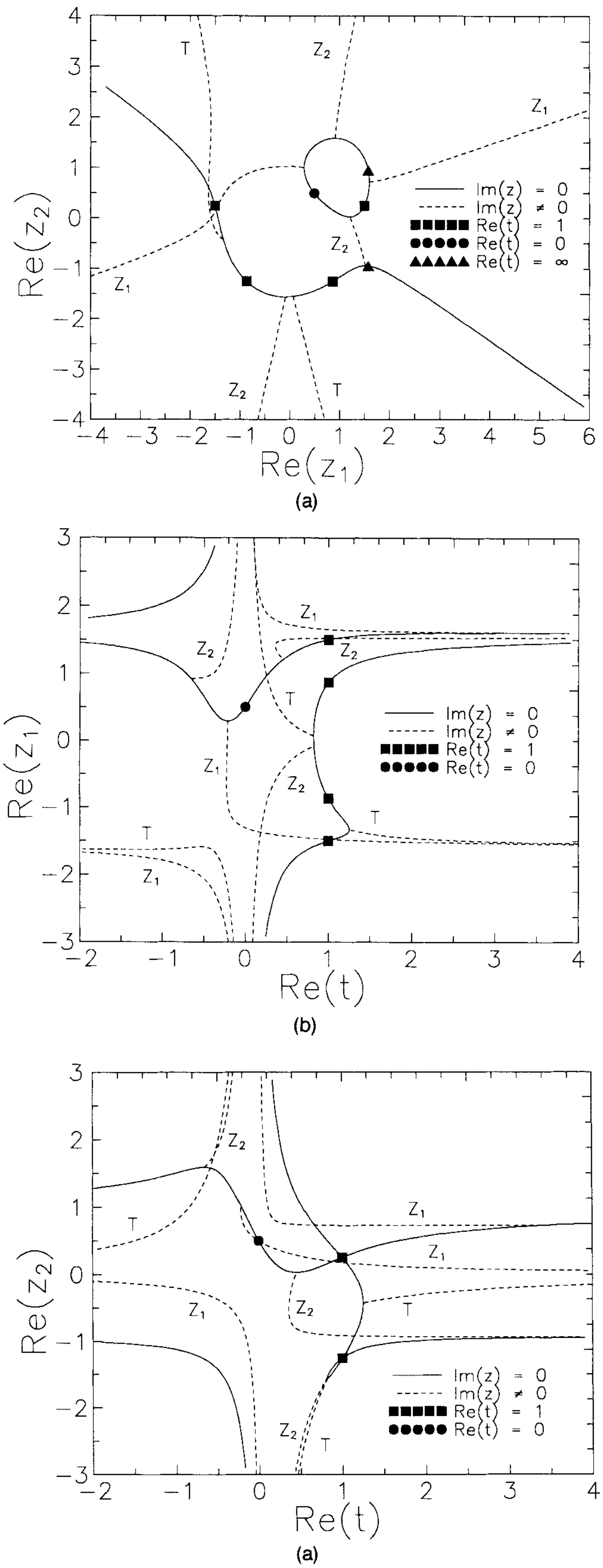

Figure 2. Projection of the interconnected one-dimensional solution manifold, starting from $\underline{z}_0 = (0.5, 0.5)^T$: (a) in the $Re(z_1) - Re(z_2)$, (b) in the $Re(z_1) - t$, and (c) in the $Re(z_2) - t$ planes.

The secondary solution families are then traced by continuation in the real space of the homotopy parameter. This procedure is repeated for all limit points on the primary and secondary solution families until all possible paths have been exhausted and thus all roots of the original equations are found from the same single initial guess. Note that each solution family in complex space connects two limit points and thus, an exhaustive search is not as large of a task as it might appear at first.

The projections onto the real planes, $Re(z_1) - Re(z_2)$, $Re(z_1) - t$, and $Re(z_2) - t$, of the interconnected manifold of the one-dimensional solution families for example 2 presented by Choi and Book (1991) are shown in Figures 2a, 2b, and 2c, respectively. In all cases, the primary and secondary solution families in the real space are shown as solid lines, while the families in complex space are shown by dashed lines. Note that only limit point bifurcations occur and thus any crossings of the homotopy paths, other than at the limit points, are only apparent and result from the projection of the solution families onto a dimensionally-reduced space. For clarity, the different solution families in the complex space are identified by the parameter, with respect to which the originating and terminating limit points are identified and which is used as the continuation parameter to generate the homotopy path. An important observation is that the solution families which are passing through infinity actually continue through it [that is, passing from $Re(z_i) = \infty$ to $Re(z_i) = -\infty$] as is more clearly seen in Figure 3. As stated by Choi and Book (1991), the only limit points with respect to $Re(t)$ occur in the secondary solution family and thus must and do connect back to each other after passing through infinity with respect to $Re(z_2)$. The same is true for the limit points in $Re(z_1)$ which occurs on the primary solution family, except that this family passes through

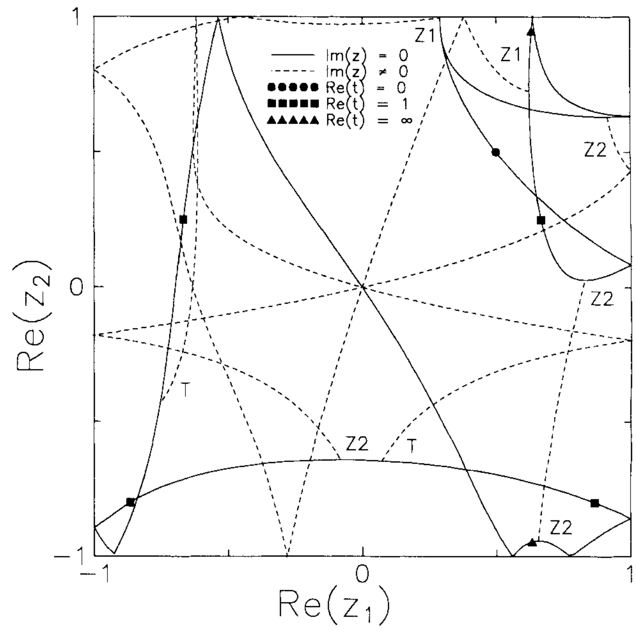

Figure 3. Projection of the innerconnected one-dimensional solution manifold, starting from $\underline{z}_0 = (0.5,\ 0.5)^T$, in the mapped $Re(z_1) - Re(z_2)$ plane.

infinity with respect to $Re(z_1)$. However, the primary and secondary solution families are connected by two paths through the complex space from limit points in the variable $Re(z_2)$. Thus, all roots were successfully found by tracing the complete manifold of solutions in the complex space from a single "arbitrary" initial guess.

The finite limits of the axes in Figure 2 prevent direct observation of the connection of the various solution families through infinity with respect to one or more of the variables. Numerically, in all cases, a simple inverse mapping ($1/x$) of the variables was used, when their absolute value exceeded unity, to allow the finite accuracy calculations performed in the computer to trace the solution families as they pass through infinity. Calculations were performed in the unmapped space for variables with absolute values less than unity. The major advantage of this mapping is that its reverse map is the same and has a one-to-one functional correspondence in the extended real space $\mathbf{R} \cup \{\infty\}$.

For illustrative purposes, the projection of the interconnected solution manifold in the extended real space $(\mathbf{R} \cup \{\infty\})^{2n+2}$ into the mapped $Re(z_1)$-$Re(z_2)$ space is shown in Figure 3. The connection of the various paths, both real and complex, through infinity, which is mapped into the origin as in the "boomerang" map proposed by Seader et al. (1990), is clearly shown. The "kinks" that appear in the paths at the boundaries of Figure 2 result from the minor imaging of the solution by the mapping as one of the absolute values of the variables passes through unity. This does not pose any difficulties numerically since all calculations are performed either in the mapped or in the unmapped space of each variable, respectively, depending on its true absolute value. Thus, any given solution family, each of which is identified by the variable that was used as the continuation parameter in real space to generate the family, can easily be followed from its originating limit point to its terminating limit point. (This designation is arbitrary since the paths can be traced in either direction.)

In this note, we have demonstrated a global fixed-point homotopy continuation strategy which successfully found all real roots of the system of equations corresponding to example 2 of Choi and Book (1991) starting from a single arbitrary initial guess. In this example, the solution families in the real space are connected by solution families in the complex space, provided that the continuation parameter t is also allowed to become complex. Thus, all real roots can be found by starting at a single, arbitrary initial guess and the validity of the conjecture made by Kuno and Seader (1988) and Seader et al. (1990) is preserved. However, it is recognized that much more work is needed to prove or disprove this conjecture in general. We hope that this note will stir enough interest in the applied mathematics community to pursue the proof or disproof of the conjecture. Even if this conjecture proves eventually to be false, we believe that the improvements brought upon the standard global fixed-point homotopy technique used here significantly increase its power to solve for all the real roots in most applications.

Notation

$\underline{F}$ = nonlinear system of equations
$\underline{H}$ = system of homotopy equations
$Im(f)$ = imaginary part of f, where f is a complex number
n = dimension of the system of equations
$Re(f)$ = real part of f, where f is a complex number
t = homotopy parameter, both real and complex
$\underline{x}$ = variable vector (real)
$\underline{z}$ = variable vector (complex)

Superscript

T = vector transpose

Subscript

0 = initial guess (starting point)

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