Unreachable Roots for Global Homotopy Continuation Methods

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The development of a method for finding all real roots of general systems of nonlinear equations with probability one is important for the solution of many chemical engineering problems. Global homotopy continuation methods such as those proposed by Kuno and Seader (1988) and Seader et al. (1990) trace the homotopy path from a single starting point to find all real roots. Wayburn and Seader (1987) provided examples of homotopy paths for which all real roots were reachable through the complex space. Based on this experience, Kuno and Seader (1988) and Seader (1990) conjecture that all real roots are reachable from an arbitrary starting point if fixed point homotopy paths are traced in the complex space. However, examples are provided that demonstrate that some real roots are unreachable by following real or complex paths connected to the starting point. Examples of unreachable roots are given for both the Newton and fixed point homotopies, and the mapping techniques of Seader et al. (1990) are shown to fail to make all roots reachable in certain cases.

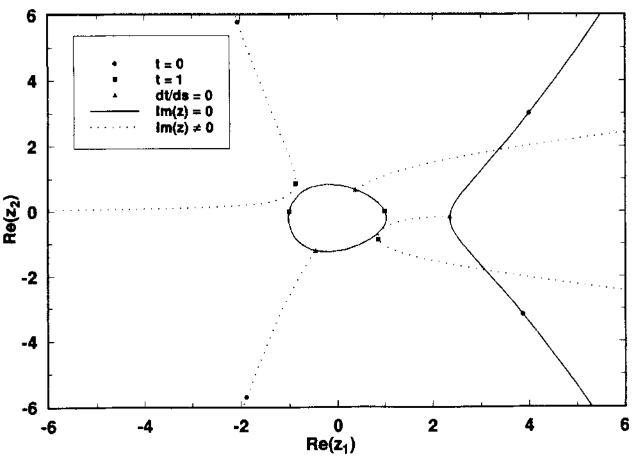

Figure 1. Homotopy paths for example 1 from the starting point (4, 3).

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Example 1. Newton Homotopy

A Newton homotopy such that $t=0$ at a starting point and $t=1$ at roots is constructed for the following system of equations:

$$z_1^2+z_2^2-1=0 \tag{1a}$$

$$z_1^3-z_1-z_2=0 \tag{1b}$$

These equations are easily reduced to a single equation, however, isolas cannot exist for a single equation. Nevertheless, were the conjecture true that all roots are reachable, then algebraic reduction to minimize dimensions should not be required.

Figure 1 shows the global homotopy paths for the starting point (4, 3). The solid lines represent the curves in the real space, and the dotted lines represent the projection onto the real space of the curves in the complex space. Each point on the projection of the complex curves corresponds to a conjugate pair of complex points. This problem has two real roots and four complex roots, but only one conjugate pair of complex roots are reachable from this starting point.

One possible method to make all roots reachable for this

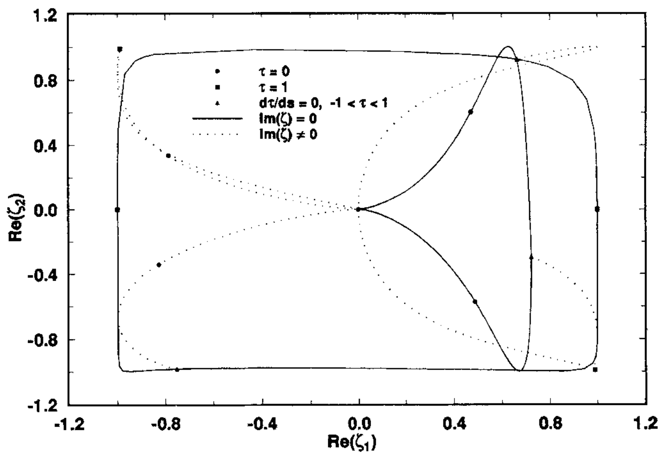

Figure 2. Boomerang-mapped homotopy paths for Figure 1.

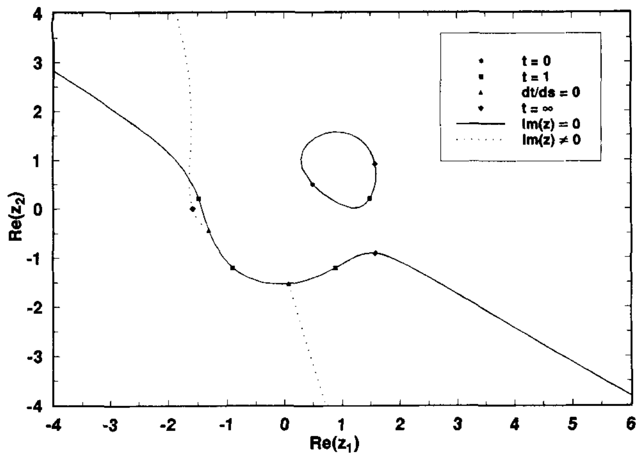

Figure 3. Homotopy paths for example 2 from the starting point (0.5, 0.5).

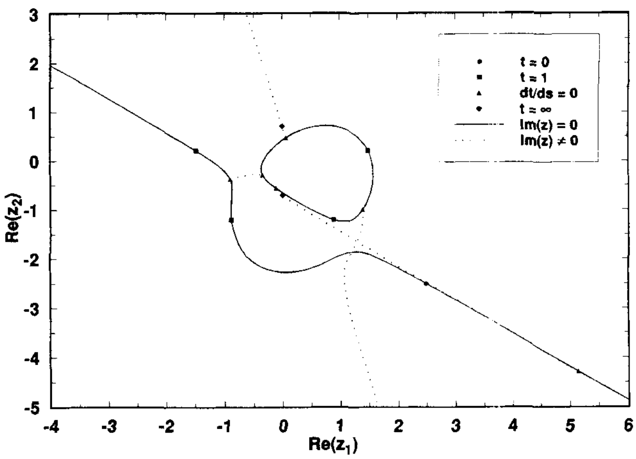

Figure 5. Homotopy paths for example 2 from the starting point (2.5, −2.5).

example problem is the boomerang mapping proposed by Seader et al. (1990) and reviewed by Seader (1990). Figure 2 shows the global homotopy paths obtained by mapping real parts of the variables, imaginary parts of the variables, and the homotopy parameter. Twelve branches meet at the origin, connecting all roots to the starting point. A general method for locating all branches was presented by Kearfott (1983). However, there are two inverse mappings for each variable when using the boomerang mapping. Therefore, a huge combinatorial problem arises when a large system of equations is to be solved.

Example 2. Fixed Point Homotopy

A fixed point homotopy is constructed for the following system equations:

$$z_1^2+z_2^2-1.5=0 \tag{2a}$$

$$-z_1^2-z_2-2=0 \tag{2b}$$

These equations are also easily reduced to a single equation. Figure 3 shows the global fixed point homotopy paths for the starting point (0.5, 0.5), one that does not fulfill the starting point criterion of Kuno and Seader (1988). This problem has four real roots. However, the homotopy path that contains the starting point passes only one real root and does not have any turning point with respect to the homotopy parameter from which to bifurcate into the complex space. Therefore, it is impossible to reach the other three roots. Additionally, the boomerang mapping, as shown in Figure 4, does not make all roots reachable from the starting point.

Figures 5, 6, and 7 show the global fixed point homotopy paths for starting points (2.5, −2.5), (2.6, −2.5) and (2.7, −2.5), respectively. Each of these three figures shows an isola which contains two real roots and the real main path containing the starting point and two real roots. Unfortunately, the isola in Figure 6 is not connected to the main path through the complex space. Without an appropriate mapping, the roots on that isola are unreachable from the starting point.

The basin boundaries for the characteristics of the homotopy paths with the starting points in the real space are shown in Figure 8. These boundaries were determined by exhaustive search. The shaded region on this graph, including its boundary represented by a dotted line, represents the locus of starting

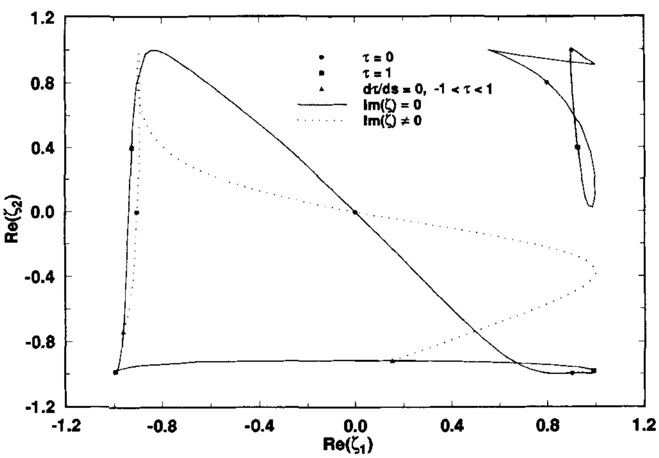

Figure 4. Boomerang-mapped homotopy paths for Figure 3.

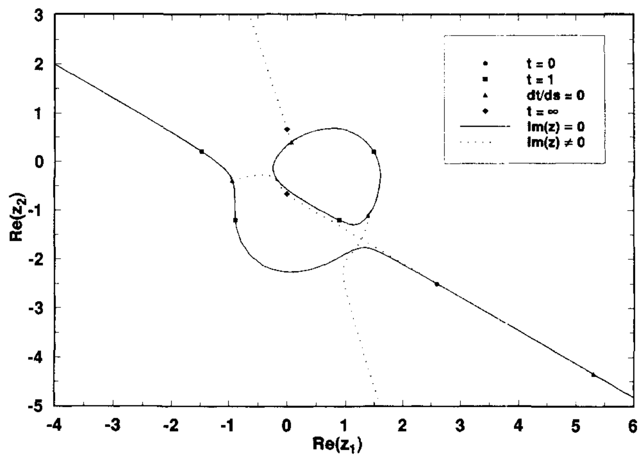

Figure 6. Homotopy paths for example 2 from the starting point (2.6, −2.5).

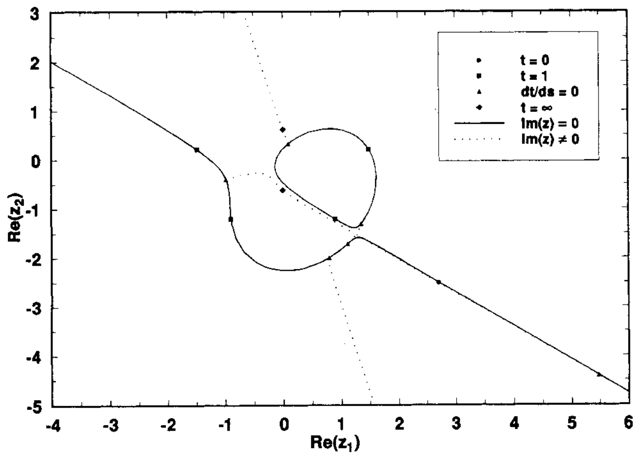

Figure 7. Homotopy paths for example 2 from the starting point (2.7, −2.5).

points that do not satisfy the starting point criterion of Kuno and Seader (1988). The solid lines on this graph represent the boundaries for starting points that produce homotopy paths that lead to the same roots in the real space and in the complex space, respectively. The nomenclature (0, 4) in a region in the figure indicates that no roots are reachable from the starting point by tracing paths in the real space. However, all four roots are reachable from the starting point by tracing paths in the complex space. For starting points in this region, all four roots lie on a real isola reachable through the complex space.

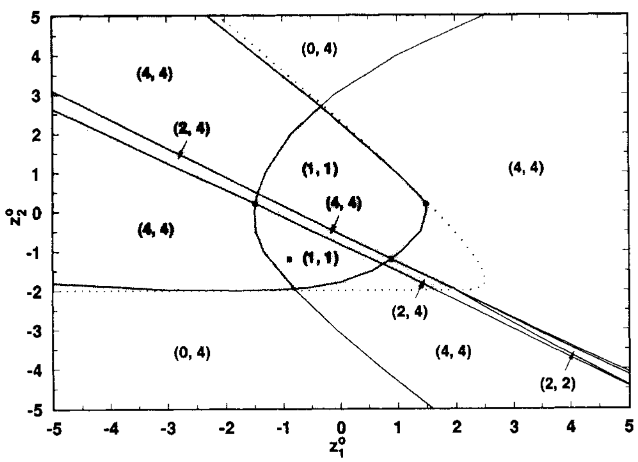

Figure 8. Basin boundaries for the starting points for example 2.

There are only three regions that do not have all four roots reachable through the complex space. Notably, two of these regions are near roots. Experience with global homotopy continuation methods indicates that, as a general rule, initial guesses near roots are less robust for reaching all roots. The starting points in both of these regions do not satisfy the starting point criterion. Experience also indicates that starting points that do not satisfy the starting point criterion tend to be less robust for reaching all roots.

There is one small region in which starting points satisfy the starting point criterion, however, all roots are not reachable from the starting point by tracing paths in the complex space. Although this region is small, its existence indicates that the global homotopy continuation methods cannot guarantee to find all roots from an arbitrary starting point.

Notation

s = arc length
t = homotopy parameter
z = variable

Greek letters

ζ = boomerang-mapped variable
τ = boomerang-mapped homotopy parameter

Superscript

o = starting point

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