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HOMOTOPY CONTINUATION METHODS FOR COMPUTER-AIDED PROCESS DESIGN†

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Abstract—Homotopy continuation methods have been used by the authors and others to solve difficult chemical engineering flowsheeting and design problems involving the solution of simultaneous nonlinear equations. Such methods can fail when: (1) the homotopy path, which one follows from the solution of a simple problem to the solution of the original (difficult) problem, returns to a second solution of the simple problem; (2) the homotopy path strikes an interior boundary of the domain of definition of the original (vector-valued) function; and (3) the homotopy path goes off to infinity. For the first two modes of failure, the use of an affine homotopy is discussed here as a possible remedy. Failure due to an unbounded homotopy path is the subject of current research.

Scope—Many chemical process design problems require the solution of simultaneous nonlinear equations. Wayburn and Seader [1] used homotopy continuation to solve the equilibrium-stage model equations for complex systems of interlinked distillation columns. In many cases, homotopy continuation succeeded where Newton's method failed.

A *homotopy*, $h(x, t)$, is a continuous blending of two functions, $f(x)$ and $g(x)$, by means of a *homotopy parameter*, t. The homotopies used in this work belong to the class of *convex linear* homotopies, $h(x, t) = tf(x) + (1 - t)g(x)$. Different members in this class correspond to different choices of $g(x)$. Clearly, the convex linear homotopies are independent of the choice of $f(x)$; therefore, they are well-suited to general flowsheeting problems (heat and material balances for arbitrary processes). The *homotopy equation* $tf(x) + (1 - t)g(x) = 0$ reduces at $t = 0$ to $g(x) = 0$, an *easy problem* whose solution, x^0, is known or easily obtained. At $t = 1$, it reduces to $f(x) = 0$, a *difficult problem* whose solution, x^*, we seek. Since the homotopy equation consists of n equations in $n + 1$ unknowns, under reasonable assumptions, the solution set will contain a 1-D component, known as a *homotopy path*, connecting x^0 with x^*.

Differential arclength homotopy continuation is the method by which we follow the homotopy path from the solution of the easy problem to the solution of the difficult problem. It is analogous to providing a high-velocity gas flame [solving $f(x) = 0$] by, first, lighting the gas burner with a low flow rate of gas and, then, turning up the gas. Lighting the burner with a low flow rate of gas is like solving the easy problem $g(x) = 0$, whose solution is known or can be found easily. Turning up the gas is like varying the parameter t smoothly from 0 to 1. Solving the difficult problem without homotopy continuation is like lighting a gas burner whose valve is wide open. (Most of the time it works, but occasionally you get burned.) The path is followed by differentiating the homotopy equation as first discussed by Davidenko [2] and further developed by Keller [3] to obtain an initial-value problem, which is solved by a predictor–corrector algorithm.

The differential homotopy continuation method can be guaranteed to follow a homotopy path from an arbitrary starting point, x^0 [a solution of $g(x) = 0$], to a solution of $f(x) = 0$, provided that: (1) certain regularity conditions, discussed in the body of the paper, are satisfied; (2) x^0 is the *unique* solution of $g(x) = 0$; and (3) the homotopy path does not strike the boundary of D, the domain of definition of $f(x)$, i.e. the homotopy equation has no solutions on the boundary of D.

Unfortunately, many nonlinear equations used in chemical engineering are not defined for negative values of their variables. For example, if negative molar flows or mole fractions or temperatures are substituted into equilibrium-stage model equations, the computer subroutines that generate the enthalpies and K-values will generate error stops. Since some component molar flows or mole fractions can be very small at the solution, it is not surprising that, occasionally, the homotopy path *does* strike the boundary of D, in which case the method fails (or has to be patched).

In the approach presented here, the original vector-valued function is combined with the absolute-value function by replacing each independent variable (unknown) by its absolute value. The absolute-value sign is thought of as belonging to the function rather than belonging to the variable. In this manner, equations that are not defined for negative values of their independent variables are transformed into equations that are defined inside a large sphere centered at the origin.

Homotopies may be problem dependent or problem independent. Of the problem-independent homotopies discussed in the literature, the Newton homotopy has had the widest application. Unfortunately, the simple mapping in the Newton homotopy, $f(x) - f(x^0)$, can have multiple zeros, therefore the homotopy path generated by the Newton homotopy can double back to a second solution of the simple problem rather than lead to a solution of the original problem. An affine homotopy is presented here that

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blends the mapping $f(|x|)$, described above, with the simple mapping $f'(x^0)(x - x^0)$. The matrix $f'(x^0)$ is the ordinary Jacobian matrix of $f(x)$ evaluated at x^0, the so-called starting guess. This affine homotopy has most of the good properties of the Newton homotopy, particularly the scale invariance, but it avoids the most serious drawback of the Newton homotopy, namely, the possibility of multiple zeros of the simple mapping.

Conclusions and Significance—The homotopy continuation method is a powerful device for solving chemical engineering process design problems, including optimization problems, as well as nonlinear problems arising in other disciplines. It is a candidate for a "method of last resort" to be embedded in large user-friendly, or expert, systems. It can *almost* be guaranteed to converge from an arbitrary starting point to a solution of a system of nonlinear equations. Two of the most common causes of failure have been eliminated by implementing the problem-independent, convex linear, affine homotopy with the original equations combined with the absolute-value function. The method has been tested on a few small problems, but not on large process design problems as of this communication. Difficulties could be encountered as a result of introducing the absolute-value function whose derivative is undefined on the coordinate planes. In addition, intermediate solutions can become unbounded, i.e. the homotopy path can go off to infinity. This is perceived as a major drawback of the method and a topic of further research.

INTRODUCTION

Many chemical process design problems can be resolved by solving systems of nonlinear equations. We would like to have a reliable standard approach to solving such systems, but, instead, we have a bewildering array of methods. The comprehensive book by Ortega and Rheinboldt [4] is practically required reading for anyone seriously interested in this subject, as suggested by Sargent [5], who reviewed most of the methods current at the time his review was written. A newer and somewhat more elementary book by Dennis and Schnabel [6] covers most Newton-based methods other than the continuation methods. The recent article by Hiebert [7] reviews available software and documents the failure of existing software to solve all problems.

For many years to come, one expects that different methods will be required for different problems because of (1) vast differences in the size, form, complexity and difficulty of the problems and (2) differences in the budgets and computing power of the users of numerical methods. Nevertheless, the trend in computer-aided chemical process design and in many other important applications is to embed numerical methods in large, user-friendly programs or, possibly, expert systems. Failure of a nonlinear equation solver buried deeply within such a system would be catastrophic because of the waste of costly calculations completed before the failure occurred and because of the waste of even more costly manpower as the user waited for expert help to arrive. For such a system, we need a sequence of methods of monotonically increasing reliability (and operating cost) culminating in a single method (or family of methods) capable of solving all but the most pathological problems. Whenever more economical methods fail, the final method in the sequence could be employed as a method of last resort. We propose that homotopy continuation methods be considered for this "method of last resort".

In a large chemical process simulator or expert system, the specific nonlinear equations to be solved may not be known until execution time. They may be provided by the user as a subroutine. Therefore, we direct our attention to homotopies that do not depend on the specific choice of $f(x)$.

To develop a method of last resort, one must do more than devise a problem-solving technique, try it on a large set of problems and simply report the number of successes and failure. It is necessary to establish exact conditions under which a technique can be *guaranteed* to succeed or, failing that, conditions under which the probability of success is known. One then tries to develop methods that satisfy these conditions. That is the motivation for the research reported here.

Also, we would like to have an *a priori* estimate of the numerical effort that will be required; but results obtained so far, particularly from the field of complexity theory, are extremely pessimistic. For example, Boult and Sikorski [8] have shown that, in the class of infinitely differentiable functions from R^2 into R^2, there exist two functions that give rise to the same continuation steps, i.e. in the language of complexity theory, the same information, but whose roots are at opposite corners of their common domain or definition. Of course, for "practical" problems, one does not expect this "worst case" behavior, but no specific results are available. Further consideration of complexity is beyond the scope of this paper. Finally, there should be a system for selecting methods from a family of methods if it is necessary (or convenient) to provide more than one method to ensure global convergence or to reduce costs, but such a system will not be discussed here.

Methods for finding the zeros of a nonlinear function can be divided into local methods, which rely on information about the function at particular points in its domain of definition, and global methods, which depend on some property of the function that holds throughout the domain. The quasi-Newton methods, simplified Newton's method, and Newton's method itself are local methods, and a good approximation to the solution is required as a starting point. The Levenberg–Marquardt-type methods, including Powell's dogleg method and the trust-region methods are also local methods. They do expand the domain of attraction somewhat by combining Newton's method with the method of steepest

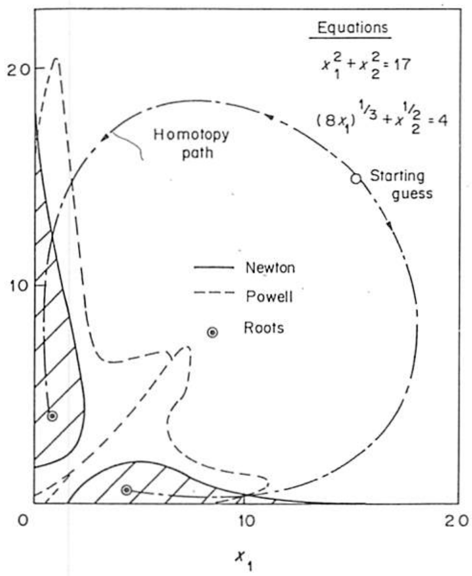


Fig. 1. Domains of attraction for the sample problem.

descent. The homotopy continuation methods are true global methods because they utilize a genuine global property of the mapping that is preserved under homotopy, namely, topological degree.

The difference between local and global methods is dramatically illustrated by the two-nonlinear-equation example of Fig. 1. The real positive roots, (1, 4) and (4.07, 0.65), are sought. With Newton's method, the initial guess for x_1 and x_2 must lie within either of the cross-hatched regions in order to achieve convergence to either of the roots. With Powell's dogleg method, which is available as a subroutine in a number of mathematical libraries, the region of convergence is expanded outward to the dashed lines. Both methods fail from a starting guess of (15, 15), which is marked by a circle. Differential homotopy continuation with $g(x) = f(x) - f(x^0)$ is convergent from the point (15, 15) as well as from any other point in the positive quadrant. Two branches of the homotopy path starting from the point (15, 15) and leading to the two solutions are shown as ––– curves. By continuing past either solution, a closed homotopy path containing both solutions is obtained.

Embedding, homotopy or continuation methods, referred to here as homotopy continuation methods, go back at least to the work of Lahaye [9], who developed numerical methods based on the theorems of Leray and Schauder [10, 11]. In 1950, Friedrichs [12] suggested a globalization of Newton's method. Early work in this area is summarized in the review paper of Ficken [13], who continued the work of Friedrichs and got an upper bound on the number of steps required for the classical homotopy continuation method.

Apparently Davidenko [2] was the first to differentiate the homotopy equation to get an initial-value problem (IVP). According to Allgower and Georg [14], the idea of stabilizing the integration of the IVP by applying Newton's method to the homotopy equation is due to Haselgrove [15]. According to Yamaguchi *et al.* [16], Riks [17] was the first to employ arclength parameterization, although Klopfenstein [18] seems to have had the idea earlier. His ideas were refined by Keller [3], who imposed an additional constraint upon the problem in such a way that: (i) solutions are parameterized by an approximation to a form of arclength; (ii) turning points "disappear"; (iii) bifurcations are easy to detect; and (iv) it is easy to switch branches.

The state of the art of homotopy continuation up to about 1970 is summarized in the book by Ortega and Rheinboldt [4]. The two reviews by Wacker [19] and by Allgower and Georg [14] cover developments up to their respective dates.

Kubicek [20] provided a computer code for continuing with respect to an actual parameter of the problem. Watson [21], who implemented the algorithm of Chow *et al.* [22], applied homotopy methods to a number of engineering problems [23]. den Heijer and Rheinboldt [24] suggested selecting a local continuation parameter corresponding to the component of the tangent whose absolute value was the greatest on the previous iterate. This is the technique used in our software. Also, den Heijer and Rheinboldt proved that no nonzero lower bound and no upper bound for the radius of convergence of the Newton correctors can be computed from previous iterates. Rheinboldt and Burkardt [25] provide an implementation of the methods of Rheinboldt and his coworkers that can be employed to solve small general problems.

Recently, Salgovic *et al.* [26], Byrne and Baird [27], Wayburn and Seader [1] and Bhargava and Hlavacek [28] have applied homotopy continuation to separation problems. The techniques employed by Byrne and Baird correspond to those developed by the Rheinboldt group. The methods of Wayburn and Seader are based on the work of Allgower and Georg [14], Georg [29, 30] and den Heijer and Rheinboldt [24]. The techniques of Bhargava and Hlavacek are related to those of Salgovic *et al.* [26].

In this study, we attempt to establish conditions under which the convergence of homotopy continuation methods is independent of the starting point. We employ existing results to establish a new and different viewpoint. In addition, we point out where results are lacking.

THEORY

Preliminary Discussion

In this section, we show that the differential homotopy continuation method can be guaranteed to follow a homotopy path from an arbitrary starting point, x^0 [a solution of $g(x) = 0$], to a solution of $f(x) = 0$, provided that: (1) certain regularity conditions, discussed below, are satisfied; (2) x^0 is the *unique* solution of $g(x) = 0$; and (3) the homotopy path does not strike the boundary of D, the domain of definition of $f(x)$ or, stated differently, there exists a bounded set E, a subset of D, such that the homotopy equation has no solutions on the boundary of E.

The vector-valued function f is a mapping from the closure of an open set D, a subset of R^n, into R^n. The problem we wish to solve can be stated mathematically as follows: find a zero of f, i.e. find a vector, x^*, belonging to D such that f maps x^* into the n-dimensional vector all of whose components are zero. (A brief review of the few mathematical terms used in this paper is provided in Appendix A.) Before we can discuss the homotopy continuation method and its probability of success for this general problem, we must introduce two important concepts, namely, topological degree and set of measure zero. Topological degree is the closest one can hope to come to an actual count *that depends continuously on the mapping* f of the number of zeros of f in D.

Topological degree

Let f be a continuous mapping from D, a subset of R^n, into R^n; let E be an open and bounded subset of D; and let y be an arbitrary vector in R^n. (In this application, y is usually taken to be the zero vector, represented in this paper by 0.) Then, the degree of f with respect to E and y, written deg(f, E, y), can be motivated by looking at a 1-D example. Consider the function f plotted in Fig. 2. We would like an integer measure *that depends continuously on* f of the number of solutions of $f(x) = y = 0$ in the open interval $E = (a, b)$. There are no solutions of $f(x) = 0$ on $\dot{E}$, the boundary of E, i.e. $f(a) \neq 0$ and $f(b) \neq 0$. Apparently a simple count of the zeros of f is unsatisfactory as that number can change discontinuously from 3 to 2 to 1 if f is perturbed slightly.

Returning to the n-dimensional case for a moment, suppose that: (i) f is continuously differentiable on the open and bounded set, E; (ii) the closure of E is within D, the domain of definition of f; (iii) $f(x) = 0$ has no solutions on $\dot{E}$, the boundary of E; and (iv) $f'(x)$, the $n \times n$ matrix representation of the Frechet derivative of f, is nonsingular on ψ, the set of all x belonging to E such that $f(x) = 0$. Then a valid formula for the degree of f with respect to E and 0 is

$$\deg(f, E, 0) = \sum_{x \in \psi} \operatorname{sgn} \det f'(x). \tag{1}$$

By the inverse function theorem, the zeros of f are isolated, and, since E is bounded, they are finite in number. (If there were an infinite number of zeros, there would be at least one accumulation point, thus contradicting the fact that the zeros are isolated.) So, the sum in equation (1) is well-defined and can be applied to the situation in Fig. 2. The sign or signum of a real number, x, is -1 if x is negative, $+1$ if x is positive, and 0 if x is zero. In the 1-D case, the

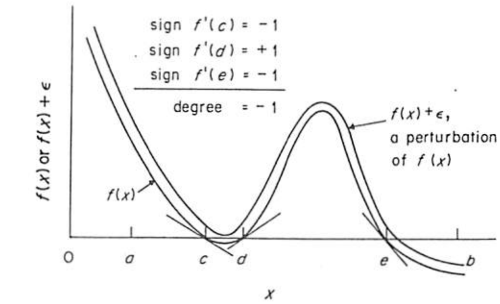


Fig. 2. Motivation for definition of degree.

matrix representing the Frechet derivative of f consists of one real number, the slope of the tangent to the curve. Therefore, the root at c contributes -1, the root at d contributes $+1$, and the root at e contributes -1. So, $\deg(f, E, 0) = -1 + (+1) + (-1) = -1$. Since the degree is nonzero, even if we know nothing else about the function, we know that there is at least one root in (a, b). If the degree had been zero, there may or may not have been a root in E.

For the sake of completeness, we provide, in Appendix B, a definition of degree that is independent of whether $f'(x)$ exists or is singular or not. This definition of degree can be shown to have a number of important properties not the least of which is invariance under homotopy. So, not only does degree theory play a role in homotopy but homotopy is crucial in developing the properties of degree. In the subsequent discussion, however, only the solution property of degree will be used.

It can be shown that, if $f(x) = 0$ has no solutions in the interior of the open set E, the degree of f with respect to E and 0, written deg(f, E, 0), is zero. This is logically equivalent to the following: if deg(f, E, 0) $\neq 0$, there exists an x belonging to E such that $f(x) = 0$. This is the solution property of degree. Notice that, if deg(f, E, 0) $= 0$, the solution property says nothing. On the other hand, if there is a unique solution, and the Frechet derivative of f is nonsingular at the solution, then the degree is certainly nonzero.

We shall see, in the following, that, if the easy problem has a unique solution with nonsingular derivative, then the homotopy path connects the starting point to a solution rather than doubling back to $t = 0$. If the converse were true, namely, that, if the solution is not unique, the homotopy path doubles back to $t = 0$ rather than connecting the starting point with a solution, we would not need the concept of topological degree. However, in many important cases, the easy problem does have multiple solutions, but the degree is nonzero and a connecting path can be found. More details on degree theory are given by Lloyd [31] and Garcia and Zangwill [32].

Sets of measure zero

A set of measure zero in R^n is a subset of R^n that can be contained in the union of a countable col-

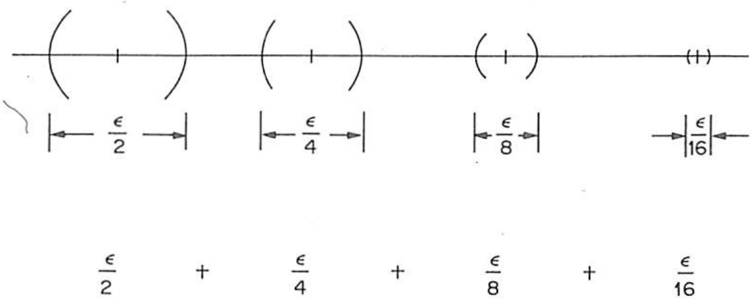


Fig. 3. A set of measure zero.

lection of little balls, themselves subsets of R^n, the sum of whose volumes is less than any positive number one can name. (The members of a countable collection bear a one-to-one correspondence with the ordinary counting numbers, 1, 2, 3, ...) Clearly a subset of a set of measure zero is itself a set of measure zero. An example of a set of measure zero is all the numbers in the computer. These are finite in number. Let them be represented on the real line by appropriate marks. Referring to Fig. 3, imagine that the lowest (most negative) number is contained in a small ball (an interval in R^1) of diameter $\epsilon/2$ centered at the number, where ϵ is an arbitrarily small positive number. The next highest (neighboring) number is contained in an interval of diameter $\epsilon/4$, and so on. Clearly, all the numbers in the computer are contained in a set of intervals the total volume of which is less than ϵ. (Note that in R^1 volume is length.)

If a real number is chosen *at random* from the *entire* set of real numbers, the probability of choosing a member of a set of measure zero is zero. If the success of an enterprise depended on a member of a set of measure zero *not* being chosen in some random choosing process, we could say that the enterprise would succeed *with probability 1*. However, it is not often in real life that a choosing process is truly random.

The Homotopy Path

The idea of the homotopy continuation method is to blend, by means of an artificial parameter, call it t, the function f whose root we seek with a function g whose root is known or can be found easily. The homotopy, $h(x, t)$, is defined on the closure of some open and bounded set Ω, a subset of the cartesian product of R^n with the closed interval $[a, b]$, written $R^n \times [a, b]$, as depicted by the shaded region in Fig. 4. A point in Ω is represented by a vector with $n + 1$ components. The first n components are those of an n-dimensional vector x belonging to R^n while the last component is a real number t belonging to the closed interval $[a, b]$. The set Ω does not have to be connected, but it usually is; so, we have drawn it as a connected set.

The homotopy equation $h(x, t) = 0$, represents n nonlinear equations in $n + 1$ unknowns, the n components of x and the artificial parameter t, which is a scalar. A typical slice through Ω at fixed t is labeled Ω_t. We shall be interested in the boundary of Ω_t because, in the following, we want to exclude solutions of the homotopy equation there. The homotopy, $h(x, t)$, with $t = a$ is $g(x)$, the simple mapping. The domain of $g(x)$ is Ω_a, the intersection of Ω with $R^n \times \{a\}$, the set of all $n + 1$-dimensional vectors whose $n + 1$st component is a. The set Ω_a is represented by the left-hand boundary of the shaded region in Fig. 4. The homotopy, $h(x, t)$, with $t = b$ is the original function, $f(x)$. The domain of $f(x)$ is Ω_b, the intersection of Ω with $R^n \times \{b\}$, represented by the right-hand boundary of the shaded region in Fig. 4.

The curved lines *within* the shaded region in Fig. 4 (not the upper and lower boundaries) represent a solution set of the homotopy equation, $h(x, t) = 0$. This solution set corresponds to a particular choice of $g(x)$, which, in our formulation, depends on the starting point, x^0. If Dh, the total Frechet derivative of h with respect to its variables, represented by the familiar $n \times n + 1$ Jacobian matrix, has full rank, i.e. at least one nonsingular $n \times n$ minor, then, according to the implicit function theorem, *all of the pieces*

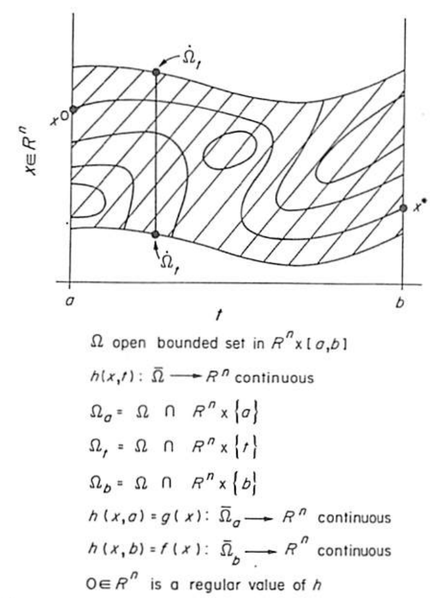


Fig. 4. Homotopy paths in an open bounded set.

of the solution set will be smooth curves without intersections.

A point where Dh has full rank is said to be a *regular point* of h. If, when Dh is evaluated at a point in Ω, *every* $n \times n$ minor of Dh is singular, that point is called a *critical point* of h. If the inverse image of a point y in R^n, i.e. the set of all points in Ω that are mapped by h into y, contains only regular points, then y is said to be a *regular value* of h. If the inverse image of y has at least one critical point of h, y is said to be a *critical value* of h.

The parameterized Sard's theorem states that, if h (twice continuously differentiable) is thought of as a function of x, t *and* x^0, and if 0 is a regular value of h when the dependence of h on x^0 is taken into account, then 0 is a regular value of $h(x, t)$ for all x^0 except for a set of x^0 of measure zero. Sard's theorem itself shows that, for the homotopies used in this work, the $n \times n$ matrix representing the derivative of h with respect to x^0 will be nonsingular for all x and t in Ω except for a set of $y^0 = f(x^0)$ of measure zero; therefore, 0 will be a regular value of $h(x, t, x^0)$ and, consequently, of $h(x, t)$ for fixed x^0. Mathematically rigorous statements of Sard's theorem and the parameterized Sard's theorem are given in Appendix C together with an elaboration of the above argument.

Even though we have encountered multiple solutions for $f(x) = 0$ in chemical engineering problems, we do not expect to encounter bifurcation points (points of intersection of two or more branches) on the homotopy path since we are continuing with respect to an artificial parameter. On the other hand, if t represents an actual parameter of the problem, such as the reflux ratio of a distillation column, the homotopy path might contain a point of bifurcation, i.e. a point where two or more branches of the homotopy path intersect in a critical point of h. When the continuation parameter, t, represents an actual parameter of the problem, the starting point, x^0, is not an arbitrary point. On the contrary, it is a solution of a physical problem.

Now that we know, with probability 1, that the solution set of $h(x, t) = 0$ is composed of smooth curves without intersection, we would like to establish conditions under which one of these smooth curves connects x^0 with x^*, a desired solution of $f(x) = 0$. Without loss of generality, we may specialize the interval $[a, b]$ to $[0, 1]$ as shown in Fig. 5, where, in addition, the domain of h is taken to be $D \times [0, 1]$, where D is the domain of definition of $f(x)$. (In order to prove theorems about degree and homotopy, it is necessary to define h on a domain as general as that of Fig. 4; but, for the purposes of the homotopy continuation algorithm, the simpler domain of Fig. 5 is adequate.)

For many problems it is possible to choose the boundary of Ω in such a way that $h(x, t) = 0$ cannot have solutions on the boundary of Ω_t as t varies between 0 and 1, i.e. such that there are no solutions on the top and bottom borders of the representation

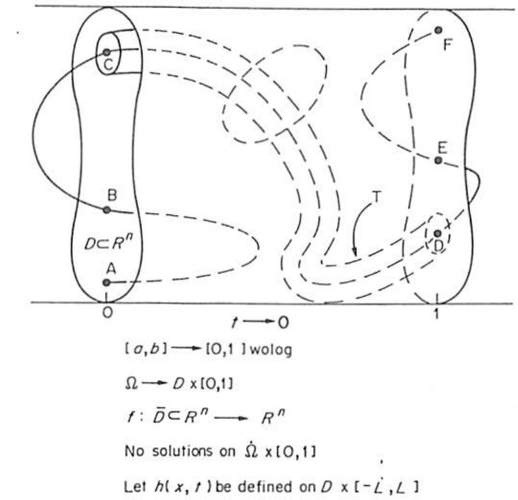


Fig. 5. Existence of a homotopy path.

of $\Omega = D \times [0, 1]$ in Fig. 5. Then, the Leray–Schauder [10] theorem, which is proved in Ref. [1], guarantees that, if there is at least one component of this solution set that starts out at $t = 0$ and does *not* return to $t = 0$, there will be a homotopy path connecting x^0 with x^*. The component that starts out at $t = 0$ does not return to $t = 0$; it cannot cross the sides of Ω; and, finally, the theorem shows that it cannot stop in the interior of Ω. Therefore, it must cross the hyperplane $t = 1$ at a solution of $f(x) = 0$.

A component of the solution set of $h(x, t) = 0$ that starts out at $t = 0$ and does not return to $t = 0$ will exist if the mapping $g(x) = 0$ has nonzero topological degree. If the contribution to degree from point A in Fig. 5 is $+1$, the contribution at point B must be -1; so, paths like AB do not contribute to degree. Clearly, if the solution to $g(x) = 0$ is unique, lies within D, and $g'(x)$ is nonsingular at x^0, then the degree of g with respect to D and 0 is nonzero (either 1 or -1). Suppose now that a path exists connecting x^0 and x^*. How can we be certain that it can be followed by differential arclength homotopy continuation?

Since the solution set of $h(x, t) = 0$ is closed and bounded, the Heine–Borel theorem can be used to prove that the homotopy path has finite length. In a later section, which discusses the implementation of differential homotopy continuation, it is shown that, to follow the homotopy path, it is necessary only to be able to solve linear systems whose matrices are nonsingular $n \times n$ minors of the $n \times n + 1$ Jacobian matrices that represent the total derivatives of $h(x, t)$ evaluated at various points inside a tubular neighborhood T of the homotopy path as illustrated in Fig. 5. The parameterized Sard's theorem and Sard's theorem itself lead us to expect regularity on the homotopy path. By simple continuity and compactness arguments, we can establish the existence of a tube T of radius ϵ surrounding the path such that the total derivative of h has full rank and the hypotheses of the Newton–Kantorovich theorem hold in the interior of T, as discussed in Appendix 3 of Wayburn [33]. This is all that is required to guarantee the success of our methods with probability 1, where, it must be remembered, "probability 1" has a technical meaning.

It should be pointed out that, sometimes, one can follow a homotopy path outside the region $D \times [0, 1]$ to find a desired solution. For example, if x^0 were taken to be point A or B in Fig. 5, a desired solution could be found at point D by going through point C. Solutions at E and F could be found by extending the path beyond $t = 1$. Some examples of this are given later.

OBJECTIONS

Unfortunately, there are a number of objections one might make to the above line of reasoning even if it were made completely rigorous. Some of these "objections" will help the reader understand what we mean by "success with probability 1". The more serious objections are addressed by the research described in the final section of this paper.

Objection 1

All of our proofs apply to continuous, infinite-precision arithmetic; but the computer has only a finite and discrete set of numbers. We would like to discretize our proofs; but, for the present, we will have to assume that the computer has "enough" numbers, and it usually does.

Objection 2

Sard's theorem and the parameterized Sard's theorem give us nonsingular matrices except for a set of x^0 of measure zero; but, all the numbers in the computer taken together represent a set of measure zero with respect to R^1, the real line. Therefore, they are capable of representing vectors in R^n that constitute only a set of measure zero with respect to R^n. The comment following Objection 1 applies to this objection as well and, probably, neither of these objections is important.

Objection 3

A more realistic objection is that, although the critical points of the homotopy, h, constitute a set of measure zero, every $n \times n$ minor of the total derivative (Jacobian matrix) of h could be so ill-conditioned on a set of positive measure that linear systems cannot be solved by row-reduction methods. We plan to implement a number of additional methods for solving linear systems such as the method of iterative refinement, QR-factorization, semi-direct methods, semi-iterative methods, conjugate gradients with a preconditioner and perturbation methods.

Objection 4

There is no hope of solving $f(x) = 0$ exactly. What we actually do is solve a problem $f(x) = y$, where the norm of y is small. It is easy to imagine a function for which the norm of y is as small as you please at a given point, but the correct location of the root is as far from the given point as you please. [Also, it is easy to imagine a function with a zero inside the interval (0, 1) on the real line but whose norm exceeds one for every number between 0 and 1 in the computer.] We do not expect this behavior in problems that come from models of physical systems. On the other hand, the observation that we are solving $f(x) = y$ rather than $f(x) = 0$ is encouraging from the point of view of avoiding the critical points of f; since, according to Sard's theorem, even if zero were a critical value of f, a point close to zero, but otherwise random, would not be.

Objection 5

Although the path length can be shown to be finite if the path is bounded, no bound has been found for the number of computations. In fact, Boult and Sikorski [8] proved that, for the class of infinitely-differentiable functions (C^∞), in a worst case scenario, the bound on the number of computations is infinity. The function, $f(x)$, whose root we seek in our practical engineering problem, probably belongs to a class much larger than C^∞, such as the class of piecewise differentiable functions, wherein functions even more pathological than Boult and Sikorskis' function could be found. Nevertheless, $f(x)$ could be restricted to a small enough subset of that class that a finite bound on the number of computations could be found. However, in the foreseeable future, estimates probably will be too pessimistic to be of any use. Although continuation methods tend to require relatively long computing times, the number of computations normally has the same order of magnitude as the number of computations required for Newton's method.

Objection 6

Some of the proofs used in the above arguments require $h(x, t)$ to be twice continuously differentiable (belong to C^2), but there may be isolated discontinuities in the second or even the first derivatives of our functions. For example, in the case of distillation equations, the thermodynamic properties routines often are treated as black boxes, but the mathematical functions used to compute thermodynamic properties are at least piecewise differentiable and, probably, piecewise C^∞. Perhaps some of the proofs can be extended to functions that are only piecewise C^2.

The next two objections are dealt with by introducing the scale-invariant affine homotopy combined with the absolute-value function. This increases the number of points at which our functions are nondifferentiable. We are interested in what the effect of this will be.

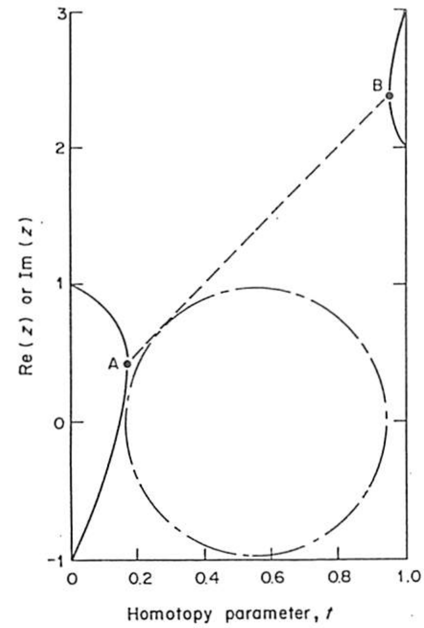


Fig. 6. Complex homotopy path for $f(x) = x^2 - 5x + 6 = 0$ with $g(x) = x^2 - 1$.

Objection 7

The solution of the simplified problem, $g(x) = 0$, could be nonunique or, worse, the degree of g with respect to D and 0 could be zero, in which case a hypothesis of the Leray–Schauder theorem is violated. Consider the single-equation example given by Garcia and Zangwill [32], where $f(x) = x^2 - 5x + 6$ and $g(x) = x^2 - 1$. The homotopy equation, then, is $h(x, t) = t(x^2 - 5x + 6) + (1 - t) \quad (x^2 - 1) = 0$ or $x^2 - 5xt + 7t - 1 = 0$. The degree of $h(x, 0) = g(x) = x^2 - 1$ with respect to the entire real line and zero is just the sum of sgn det $g'(x)$ evaluated at -1 plus sgn det $g'(x)$ evaluated at $+1$. [The roots of $g(x)$ are -1 and $+1$.] The derivative of $g(x)$ is $2x$, whose determinant is $2x$, itself. So, $\deg(g, R, 0) = \operatorname{sgn}(-2) + \operatorname{sgn}(+2) = -1 + (+1) = 0$. Thus, the hypothesis that degree is nonzero is violated.

Indeed, as shown in Fig. 6, the solutions, $+2$ and $+3$, of $h(x, 1) = f(x) = 0$ cannot be reached by a *real* homotopy path starting from $t = 0$ because the solution of $h(x, t) = 0$ is

$$x = \frac{5t \pm (25t^2 - 28t + 4)^{0.5}}{2},$$

which is complex in the region $0.1681 < t < 0.9519$. Thus, if only real numbers are used, the two —— line disconnected paths result. If complex numbers are used, these two real curves are connected as shown by the --- line for the real part and the ——— line for the complex part. Connected paths also can be obtained by selecting a different function for $g(x)$, e.g. $g(x) = x - x^0$, with x a real variable. Also, for this example the Newton homotopy, $g(x) = f(x) - f(x^0)$, with x real, provides a connected homotopy path.

A two-equation example given by Watson [23],

$$x_1^2 x_2 - 1 = 0$$
$$x_2^2 - 1 = 0,$$

fails to lead to either of the two pairs of roots, (1, 1) and $(-1, 1)$, for the selection of $g(x) = x - x^0$ with $x^0 < -1$ unless complex numbers are used. Use of the Newton homotopy with real numbers encounters similar difficulties. Thus, Watson, who has solved by homotopy continuation a large number of difficult engineering problems, states that "there is probably not a homotopy map for all seasons, but that some homotopy map, resulting in a globally convergent algorithm, may exist [for every problem]". That homotopy map may have to include the complex region.

Objection 8

Sometimes, it is impossible to find a bounded region $D \times [0, 1]$ where the homotopy, $h(x, t)$, is defined and such that there are no solutions of the homotopy equation, $h(x, t) = 0$, on the boundary of $D \times \{t\}$ as t varies from 0 to 1. For example, the equilibrium-stage model distillation equations are not defined for negative molar flows or temperatures. Indeed, one gets error stops in the thermodynamic properties subroutines if negative mole fractions or temperatures occur. But, the components of the solution of $f(x) = 0$ could be very close to zero; so, if the homotopy is viewed as a perturbation of the function, it is easy to see that the roots of f could be "mapped" to the boundary, thus violating a hypothesis of the theorem. This is a case of a solution of $h(x, t) = 0$ striking an *interior boundary*.

Objection 9

There will be a solution of $h(x, t) = 0$ striking an *exterior boundary* if the solution set of $h(x, t) = 0$ is unbounded. Stated differently, there may not exist a *bounded* subset E of D, the domain of definition of f, such that the solution set of $h(x, t) = 0$ does not strike the boundary of E. We perceive this as the single greatest difficulty with homotopy continuation methods. There are techniques that can be applied to polynomials to prevent this, but none of them are suitable for large numbers of equations. Moreover, most engineering equations are not polynomials. For many practical engineering problems, unbounded paths can be ruled out. Also, there are a number of theorems that give conditions under which a bounded path exists. We are interested in finding homotopies corresponding to the hypotheses of various theorems for a number of classes of functions. Also, there may be transformations of the functions and variables that result in bounded homotopy paths. This is the thrust of future work for one of the authors.

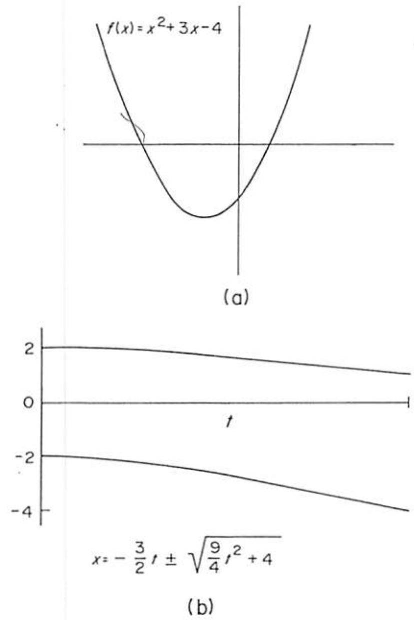


Fig. 7. For $f(x) = x^2 + 3x - 4 = 0$: (a) graph of function; (b) homotopy path with $g(x) = x^2 - 4$.

IMPLEMENTATION

In this section, various implementations of the homotopy continuation method are described in terms of examples.

Path Parameterization by the Homotopy Parameter

Assuming that the homotopy path exists, it is the object of the homotopy continuation method to follow the path from x^0, the arbitrary starting point and the zero of $g(x)$, to x^*, a desired solution of $f(x) = 0$, the original problem. We shall illustrate the procedure by applying it to the very simple function plotted in Fig. 7. Let us pretend that the problem $f(x) = x^2 + 3x - 4 = 0$ is difficult to solve, but the problem $g(x) = x^2 - 4 = 0$ is easy to solve. We could embed the two functions in a homotopy by taking a convex linear combination. Thus,

$$h(x, t) = t(x^2 + 3x - 4) + (1 - t)(x^2 - 4) = 0$$

or

$$h(x, t) = x^2 + 3xt - 4 = 0, \tag{2}$$

which could have been arrived at directly by contriving to cancel out the middle term for $t = 0$.

According to the implicit function theorem, if $\partial h/\partial x$, the $n \times n$ Jacobian matrix, is nonsingular on the homotopy path, Γ, then Γ can be parameterized by t, in which case the classical homotopy continuation method is guaranteed to succeed. This was proved in Appendix 3 of Wayburn [33] using the well-known Newton–Kantorovich theorem. In the *classical homotopy continuation method*, the interval [0, 1] is broken up into N parts with $t_{i+1} - t_i = 1/N$ for $i = 0, \ldots N$, $t_0 = 0$, and $t_N = 1$. Newton's method is applied to $h(x, t_{i+1}) = 0$, $i = 1, \ldots, N$, with the solution of $h(x, t_i) = 0$ as a starting point. The solution of $h(x, t_0) = h(x, 0) = 0$ is x^0, the known solution of $g(x) = 0$.

In our sample problem, the homotopy path connecting $+2$ to $+1$ and the homotopy path connecting -2 to -4 can be solved for directly as shown in Fig. 7. The number of equations, n, equals 1 and the 1×1 Jacobian matrix $\partial h/\partial x = 2x + 3t$ is nonzero on both homotopy paths; therefore the classical homotopy method is bound to succeed. (Normally, one would not know this unless the problem was already solved.) At $t = 0.5$, say, one could apply Newton's method to the equation $h(x, 0.5) = x^2 + 1.5x - 4 = 0$ with a starting guess of $+2$ and converge to the point (1.386, 0.5) on the upper homotopy path in Fig. 7. For that matter, Newton's method applied to $f(x)$ will converge to $+1$ from a starting guess of $+2$ and to -4 from a starting guess of -2; so t_1 could have been taken as 1. The classical homotopy method could be improved by choosing the t_is so as to minimize the computational expense.

Strangely enough, in the case of most realistic problems, the amount of computation can be reduced substantially by converting the nonlinear equations into an IVP for an ordinary differential equation as first shown by Davidenko [2]. Since the solution set of $h(x, t) = 0$ can be parameterized by t, the homotopy equation defines implicitly a function $x = x(t)$. Substituting this into equation (2) and taking the total derivative with respect to t, we get

$$\frac{\mathrm{d}}{\mathrm{d}t}[h(x(t), t)] = 2x\frac{\mathrm{d}x}{\mathrm{d}t} + 3x + 3t\frac{\mathrm{d}x}{\mathrm{d}t} = 0,$$

which leads to the IVPs:

$$\frac{\mathrm{d}x}{\mathrm{d}t} = -\frac{3x}{2x + 3t}, \quad x(0) = \pm 2. \tag{3}$$

These can be solved analytically to obtain

$$x = -\tfrac{3}{2}t \pm (\tfrac{9}{4}t^2 + 4)^{0.5},$$

the familiar formula for the roots of a quadratic equation, plotted in Fig. 7.

As long as we are pretending that $f(x) = x^2 + 3x - 4 = 0$ is difficult to solve, we might just as well pretend that the IVP of equation (3) is difficult to solve and employ Gear's method. This might be a good idea for some problems since sharp turns in the homotopy path could be interpreted as stiffness. Alternatively, we could employ Euler's method, but that would not take advantage of the fact that we have at our disposal the actual function that was differentiated to get the IVP. We can arrange matters so that the calculation does not depend on its history and eliminate all questions of stability by applying Newton's method to the homotopy equation with the point predicted by Euler's method as a starting "guess". We could use a higher-order predictor, but the experience of many workers [cf. 26], has indicated that the additional complexity is usually not justified.

Some experts disagree with this conclusion and higher-order predictors should be studied.

Returning to the general case, we differentiate the homotopy equation with respect to t while thinking of x as a function of t:

$$\frac{\mathrm{d}h(x(t), t)}{\mathrm{d}t} = \frac{\partial h}{\partial x}\frac{\mathrm{d}x}{\mathrm{d}t} + \frac{\partial h}{\partial t} = 0.$$

Normally, $\partial h/\partial x$ is an $n \times n$ matrix, $\mathrm{d}x/\mathrm{d}t$ is an $n \times 1$ column vector and $\partial h/\partial t$ is an $n \times 1$ column vector. To implement Euler's method, we need to solve the matrix equation

$$\frac{\partial h}{\partial x}\frac{\mathrm{d}x}{\mathrm{d}t} = -\frac{\partial h}{\partial t}$$

for $\mathrm{d}x/\mathrm{d}t$. For the case of $h(x, t) = x^2 + 3xt - 4$, $\partial h/\partial x$ is a nonsingular 1×1 matrix; therefore, to solve for $\mathrm{d}x/\mathrm{d}t$, it is necessary only to divide $-3x$, the single element in the column vector $-\partial h/\partial t$, by $2x + 3t$, the sole element in the 1×1 matrix $\partial h/\partial x$. This amounts to solving for $\mathrm{d}x/\mathrm{d}t$ by Gaussian elimination. At $t = 0$, with an initial guess of $x = 2$, we get $\mathrm{d}x/\mathrm{d}t = -1.5$, the same as we would have obtained from equation (3). [In the general case, of course, it would not be feasible to compute a formula like equation (3), which explicitly exhibits the dependence of $\mathrm{d}x/\mathrm{d}t$ on the data.] The predicted value of x is $x^0 + \Delta t(\mathrm{d}x/\mathrm{d}t)$. This value is used to start Newton's method. If Δt is taken to be 0.5, the predicted value of x is 1.25.

In general, the Newton correction vector, x, is obtained by solving the matrix equation

$$\frac{\partial h}{\partial x}\Delta x = -h(x, t).$$

The 1×1 Jacobian matrix of the example contains the single element $2x + 3t$ evaluated at $x = 1.25$ and $t = 0.5$, i.e. $\partial h(x, t)/\partial x = 4$. The homotopy, $h(x, t)$, evaluated at $x = 1.25$ and $t = 0.5$ equals -0.5625; therefore, the Newton correction is $\Delta x = 0.140625$ and the corrected value of x is 1.390625, which equals the correct value up to two decimal places. Of course, one could do another Newton iterate; but, since we need an accurate computation of the homotopy path only at $t = 1$, it is probably not worthwhile. To complete the procedure, one would compute the tangent vector at $x = 1.39$, $t = 0.5$, take another Euler step, correct with Newton's method etc.

Path Parameterization by Arclength

The case where the function $f(x) = x^3 - 30x^2 + 280x - 860$ is embedded in the convex linear homotopy $h(x, t) = f(x) - (1 - t)f(x^0)$, where $g(x)$ has been taken as $f(x) - f(x^0)$, is discussed in Ref. [1]. Newton's method fails for this function if x^0 is less than about 12.6. Also, for choices of x^0 less than about 12.6, the homotopy paths, which are plotted in Fig. 8 for a number of choices of x^0, cannot be parameterized by the homotopy parameter, t, over their entire length because they exhibit what are

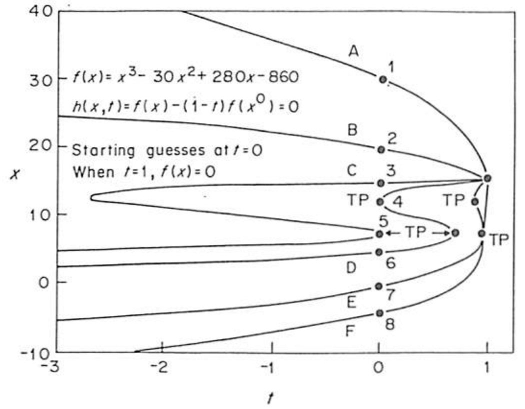


Fig. 8. Homotopy paths for $f(x) = x^3 - 30x^2 + 280x - 860 = 0$ with $g(x) = f(x) - f(x^0)$.

known as *turning points*. The turning points in Fig. 8 are identified by TP.

The methods of the previous section will fail if $x^0 = 0$, for example, in which case the homotopy equation is $h(x, t) = x^3 - 30x^2 + 280x - 860t = 0$. To accommodate this case and other cases that exhibit turning points, the modification by Klopfenstein [18] is employed, wherein x and t are taken to be functions of arclength, s, and the homotopy equation is differentiated with respect to arclength to obtain the following IVP:

$$\frac{\partial h}{\partial x}\dot{x} + \frac{\partial h}{\partial t}\dot{t} = 0, \tag{4}$$

$$\dot{x}^{\mathrm{T}}\dot{x} + \dot{t}^2 = 1, \tag{5}$$

$$x(0) = x^0,$$

$$t(0) = 0,$$

where $\mathrm{d}x/\mathrm{d}s$ is represented by $\dot{x}$ and $\dot{t} = \mathrm{d}t/\mathrm{d}s$.

This IVP can be solved conveniently by a simple Euler predictor with Newton corrections in the hyperplane orthogonal to the Euler predictor. Alternatively, the Newton corrections can be taken in the hyperplane orthogonal to the coordinate axis corresponding to a suitable local parameter, which can be either t, itself, or, in case $\dot{t}$ is close to zero, some x_i such that $\dot{x}_i$ is not close to zero. The process of switching parameters on a local basis is referred to as reparameterization. Even though $\partial h/\partial x$ is singular, one expects $\mathrm{D}h = [\partial h/\partial x \,|\, \partial h/\partial t]$ to be of full rank, n, because of Sard's theorem and the parameterized Sard's theorem. Identify t with x_{n+1}; let H'_{-i} be the $n \times 1 + n$ matrix, $\mathrm{D}h$, with the ith column removed; and let $\dot{x}_{-i}$ be the $n + 1$-dimensional column vector $\dot{x}$ with the ith component removed. Then, we can write

$$\left[\begin{array}{c|c} H'_{-i} & \dfrac{\partial h}{\partial x_i} \\ \hline \dot{x}^{\mathrm{T}}_{-i} & \dot{x}_i \end{array}\right]\left[\begin{array}{c|c} I & \dot{x}_{-i} \\ \hline 0^{\mathrm{T}} & \dot{x}_i \end{array}\right]$$

$$= \left[\begin{array}{c|c} H'_{-i} & H'_{-1}\dot{x}_{-1} + \dfrac{\partial h}{\partial x_i}\dot{x}_i \\ \hline \dot{x}^{\mathrm{T}}_{-i} & \dot{x}^{\mathrm{T}}_{-i}\dot{x}_{-1} + \dot{x}_i^2 \end{array}\right] = \left[\begin{array}{c|c} H'_{-i} & 0 \\ \hline \dot{x}^{\mathrm{T}}_{-1} & 1 \end{array}\right]. \tag{6}$$

The first matrix on the l.h.s., call it χ, is not singular because $(\dot{x}^{\mathrm{T}}_{-i}, \dot{x}_i)$ is orthogonal to every row of $[H'_{-1}|\partial h/\partial x_i]$, which itself has rank n; therefore,

$$\det \chi \cdot \det\left[\begin{array}{c|c} I & \dot{x}_{-i} \\ \hline 0^{\mathrm{T}} & \dot{x}_i \end{array}\right] = \det\left[\begin{array}{c|c} H'_{-i} & 0 \\ \hline \dot{x}^{\mathrm{T}}_{-i} & 1 \end{array}\right]$$

or

$$\dot{x}_i \det \chi = \det H'_{-i}. \tag{7}$$

This shows that H'_{-i} is singular iff $\dot{x}_i$ is zero. In other words, far from a turning point with respect to x_i, i.e. far from a point on the homotopy path were $\dot{x}_i = 0$, H'_{-i} should be far from singular, and x_i can be used as a local parameter for purposes of solving equations (4) and (5) for the unit tangent vector. Also, Newton corrections can be made safely in the hyperplane orthogonal to the x_i-axis, provided only that the predicted point lies within the tube T discussed in a previous section.

The above remarks can be illustrated by the example of this section. The homotopy equation, $h(x, t) = x^3 - 30x^2 + 280x - 860t = 0$, can be differentiated with respect to arclength, s, to obtain

$$\frac{\partial h}{\partial s} = \frac{\partial h}{\partial x}\dot{x} + \frac{\partial h}{\partial t}\dot{t} = \left[\begin{array}{c|c} \dfrac{\partial h}{\partial x} & \dfrac{\partial h}{\partial t} \end{array}\right]\begin{bmatrix} \dot{x} \\ \dot{t} \end{bmatrix}$$

$$= [3x^2 - 60x + 280| - 860]\begin{bmatrix} \dot{x} \\ \dot{t} \end{bmatrix}.$$

At $x = 0$, $\partial h/\partial x = 280 \neq 0$. To compute the unit tangent vector, u, we first solve

$$280v_1 - 860v_2 = 0,$$

corresponding to equation (4), where v_1 and v_2 are placeholders for $\dot{x}$ and $\dot{t}$. Since t does not vanish, we may set $v_2 = 1$. Then, $v_1 = 860/280 = 3.0714286$. Therefore,

$$u = \frac{(v_1\, v_2)^{\mathrm{T}}}{\|(v_1, v_2)\|} = \frac{(3.07, 1)^{\mathrm{T}}}{\|(3.07, 1)\|},$$

which satisfies both equations (4) and (5).

Given a steplength, the Euler predictor step can be taken followed by a Newton correction parallel to the x-axis with t fixed. This procedure can be repeated until $t \simeq 0.97$. At $t = 0.9702634$ and $x = 7.4180111$, the 1×1 matrix representing $\partial h/\partial t$ is singular, i.e. $3x^2 - 60x + 280 = 0$. This is a turning point with respect to t; and, at such a point, $\dot{t} = 0$. In this 1-D case, it is clear that the unit tangent vector is just $(1, 0)^{\mathrm{T}}$; nevertheless, we shall go through the formalities.

We must change the local continuation parameter from x_2 to x_1, where x_1 is to be identified with x and x_2 is to be identified with t. The 1×1 matrix H'_{-1}, consisting of the single element -860, is nonsingular and the scalar $\dot{x}_1$ is nonzero. Normally, we would set v_1 equal to 1 and compute the remaining components of v other than v_{n+1}, the placeholder for t. In this 1-D case, there are no additional components of v (other than v_{n+1}, which is zero). Therefore,

$$u = \frac{(v_1, v_2)^{\mathrm{T}}}{\|(v_1, v_2)\|} = \frac{(1, 0)^{\mathrm{T}}}{\|(1, 0)\|} = (1, 0)^{\mathrm{T}}.$$

In our software, we employ the algorithm of Georg [30] to compute the Euler step length, as described in Ref. [1]. Suppose that we wish to take a Euler step of length 0.5. The predicted value of x is $7.418 + 0.5 = 7.918$. To compute the first Newton corrector at $x = 7.918$ and $t = 0.9703$ in the direction orthogonal to the x-axis, i.e. with x fixed, we solve the "matrix" equation

$$\frac{\partial h}{\partial t}\Delta t = -h(x, t).$$

Since $h(x, t) = -1.8114974$, $\Delta t = +1.8114974/(-860)$ and the corrected value of t is $0.9702634 - 0.0021064 = 0.968157$, which is equal to the correct value on the homotopy path up to calculator accuracy. Calculations can proceed with a sequence of Euler steps and Newton corrections with either x or t as the distinguished local parameter, whichever is convenient.

THE SCALE-INVARIANT, AFFINE HOMOTOPY

For many engineering problems, it is possible to find a homotopy that takes advantage of special features of the problem. However, we are interested in problem-independent homotopies; therefore, we have studied the class of convex linear homotopies represented by the equation.

$$tf(x) + (1 - t)g(x) = 0, \tag{8}$$

where different members of the class correspond to different choices of $g(x)$ and $f(x)$ is any function. Both $g(x)$ and $f(x)$ are mappings from R^n to R^n.

If we let $g(x)$ equal $f(x) - f(x^0)$, we arrive at the Newton or global homotopy

$$h(x, t) = f(x) - (1 - t)f(x^0), \tag{9}$$

which is scale invariant with respect to variable changes of the form $y = \mathrm{A}x$ and $g = Bf$, as shown in Appendix C of Ref. [1]. Clearly, $g(x) = f(x) - f(x^0) = 0$ is satisfied by $x = x^0$.

Unfortunately, $g(x)$ could be satisfied by other values of x. If the contributions to degree of the roots of $g(x)$ cancel out in pairs, the degree of $g(x)$ with respect to D and 0 [$\deg(g, D, 0)$] could be zero and we are no longer guaranteed the existence of a homotopy path connecting at least one of the roots of $g(x)$ with a root of $f(x)$. The situation could be as in Fig. 9(a) with $\deg(g, D, 0) = 0$ and no connecting homotopy path. This difficulty was remedied in Objection 7, above, by taking x complex. We suspect that this can always be done; but, for large engineering problems, doubling the number of independent variables is highly undesirable. Also, the number of complex roots obtained before a real root is found might be excessive.

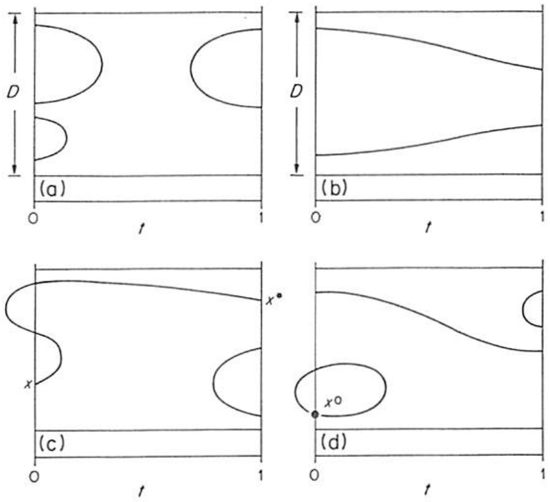


Fig. 9. Examples of degree.

An example of $\deg(g, D, 0) = 0$ with multiple connecting homotopy paths is given in Fig. 9(b). This presents no difficulties. On the other hand, the degree of g with respect to D and 0 could be nonzero; but, in order to trace out a connecting homotopy path between x^0 and x^*, it may be necessary to follow the path outside the region $D \times [0, 1]$ as in Fig. 9(c). Or, worse yet, the situation may be as in Fig. 9(d), where the degree is nonzero and a connecting path exists, but our choice of x^0 has been unfortuitous. In such a case, we must either complexify or choose another x^0.

Alternatively, we could let $g(x)$ equal $x - x^0$ to arrive at the so-called fixed-point homotopy

$$h(x, t) = tf(x) + (1 - t)(x - x^0), \qquad (10)$$

which has the virtue of a unique root at $t = 0$. Unfortunately, the fixed-point homotopy can have poor scaling properties arising from connecting the dependent variables with the independent variables. We could eliminate the scaling problem by introducing a scaling matrix A in the function $g(x)$. Thus, $g(x) = A(x - x^0)$, which leads to the homotopy

$$h(x, t) = tf(x) + (1 - t)A(x - x^0),$$

which retains the uniqueness at $t = 0$, provided A is nonsingular. If we choose A to be $f'(x)$ evaluated at x^0, i.e. $g(x) = f'(x^0)(x - x^0)$, we arrive at the affine homotopy

$$h(x, t) = tf(x) + (1 - t)f'(x^0)(x - x^0), \qquad (11)$$

which recaptures the scale invariance of the Newton or global homotopy and, since, according to Taylor's theorem, for x close to x^0, $f'(x)(x - x^0)$ is close to $f(x) - f(x^0)$, the affine homotopy recaptures some of the other nice properties of the Newton homotopy. Note that Sard's theorem gives us $f'(x^0)$ nonsingular except for a set of $y^0 = f(x^0)$ of measure zero.

This homotopy was referred to by Garcia and Gould [34] as the modified-Merrill homotopy and was attributed by them to Fisher *et al.* [35]. It was independently rediscovered by us and its properties were studied from a viewpoint different from that of Garcia and Gould. For example, Garcia and Gould showed that convergence was independent of the order of the equations and whether the equations were multiplied by -1 or not; we showed that the homotopy was invariant under arbitrary linear transformations of the dependent and independent variables. We have called it the affine homotopy since the simple function is the affine transformation $g(x) = f'(x^0)(x - x^0)$. (A translation composed with an arbitrary linear transformation is called an affine transformation since the point at infinity remains at infinity.) We continue to refer to it as the affine homotopy, mostly out of habit.

To overcome the situation in which the homotopy strikes the boundary of its domain of definition, which, for multicomponent, multistage separation problems, occurs whenever a molar flow or temperature is nonpositive, the absolute-value function is introduced into the function $f(x)$. The symbol $f(|x|)$ means that the absolute value of every component of x is taken. The absolute value is part of the function not part of x. For example, if $f(|x|) = |x|^{0.5} - 2$, and $x = -4$, $f(|x|) = 0$, but x still equals -4. If we are looking for the solution of $f(x) = x^{0.5} - 2 = 0$, $x = -4$ is *interpreted* as $+4$. The development of the scale-invariant, affine homotopy is illustrated by an example.

It is impossible to construct, for the Newton homotopy, given by equation (9), an example in one variable that exhibits negative solutions of the homotopy equation for $0 < t < 1$, when both $x^0 = g^{-1}(0)$ and $x^* = f^{-1}(0)$ are positive. However, for two or more variables, negative points on the homotopy path can occur. A simple example of this phenomenon in the case of two variables is provided by

$$f_1(x_1, x_2) = x_2 - 1 = 0$$

and

$$f_2(x_1, x_2) = 1.613 - 4(x_1 - 0.3125)^2 - 4(x_2 - 1.625)^2 = 0,$$

with a starting point of $x_1 = 0.2$, $x_2 = 2.0$. For the Newton homotopy, two homotopy paths, joined at x^0, are obtained with the projections in the x_1x_2 plane shown in Fig. 10(a), where the horizontal tick-marked axis corresponds to $x_2 = 1.5$. The left-hand path leads to the root $x_1 = 0.2$, $x_2 = 1$, but the path proceeds into and then out of the negative x_1 region. The right-hand path leads to the root $x_1 = 0.425$, $x_2 = 1$, without entering the negative x_1 region.

Let us focus our attention on the left-hand path. Suppose, for a moment, that for some reason f_1 and f_2 are undefined for negative values of x_1 and x_2. A hypothesis of the Leray–Schauder theorem is violated and the homotopy path runs "out the side" of the domain of definition of the homotopy rather than "out the end". A natural modification of the equations, which results in a domain of definition for the Newton homotopy equations that is symmetric with respect to the x_1t and x_2t coordinate planes, is the replacement of $f(x)$ by $F(x) = f(|x|)$, where the symbol $|x|$ means that the absolute value of each component of f is taken separately; thus,

$$F_1(x_1, x_2) = f_1(|x_1|, |x_2|) = |x_2| - 1$$

and

$$F_2(x_1, x_2) = f_2(|x_1|, |x_2|) = 1.613 - 4(|x_1| - 0.3125)^2 - 4(|x_2| - 1.625)^2.$$

This prevents the homotopy path from striking an "inner" boundary of the domain of definition of the homotopy since the inner boundaries have been eliminated. The homotopy path could still go off to infinity. To differentiate these equations, one takes

$$\frac{\mathrm{d}|x_i|}{\mathrm{d}x_i} = \begin{cases} +1, & x \geqslant 0 \\ -1, & x < 0 \end{cases}.$$

Unfortunately, if the Newton homotopy is applied to this problem with a starting point of (0.2, 2), one obtains the disconnected homotopy path whose projection is shown in Fig. 10(b).

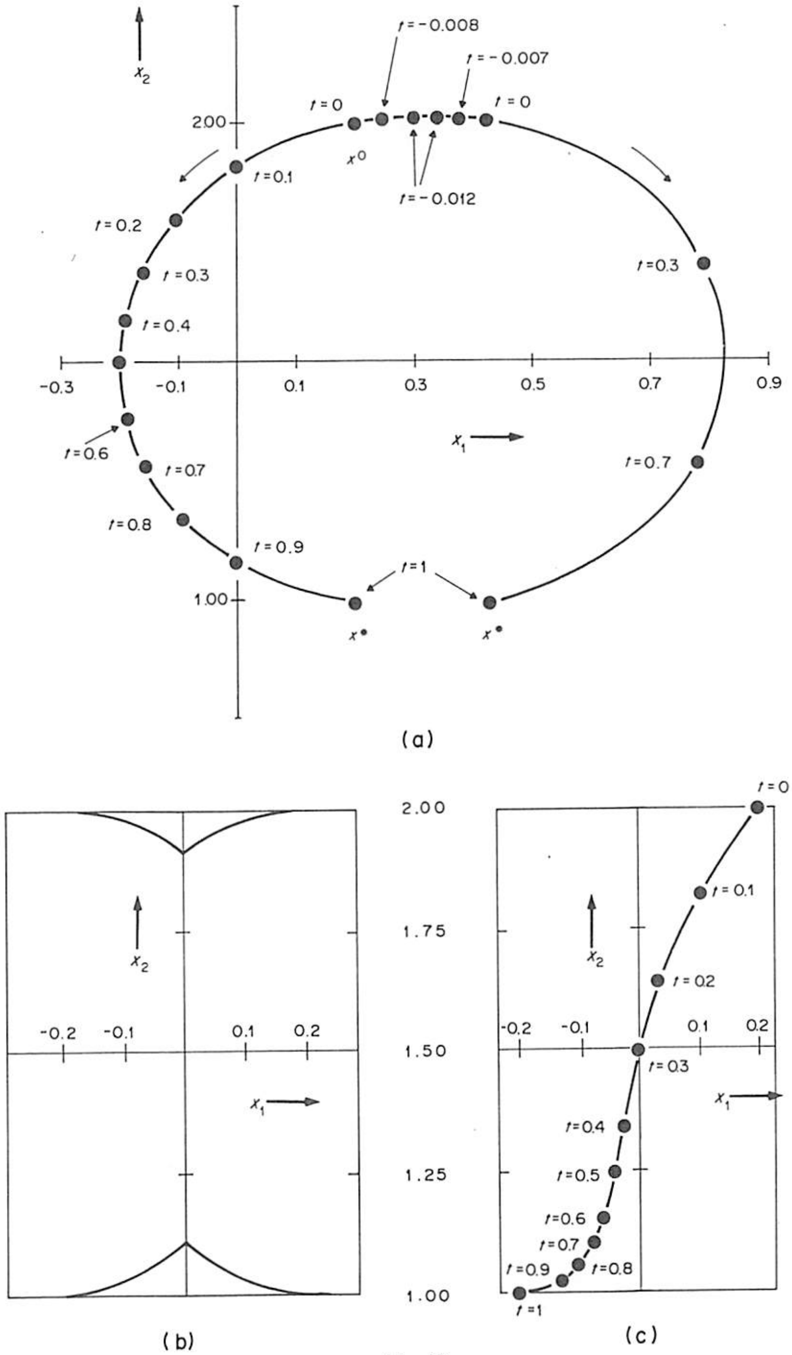
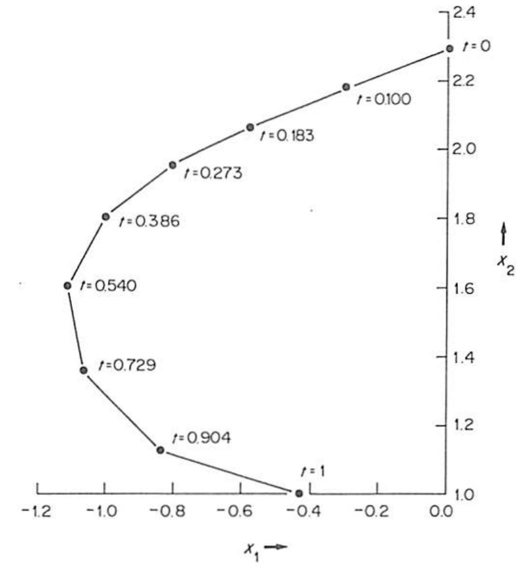


Fig. 10.



(d)

Fig. 10. Projection of the homotopy path for a two-function example: (a) Newton homotopy: (b) absolute value used in Newton homotopy; (c) absolute value used in fixed-point homotopy; (d) absolute value used in an affine homotopy.

Since the chief difficulty with this path, namely, its disconnectedness, could be eliminated if $g(x)$ had a unique root, one might consider trying the fixed-point homotopy, wherein $g(x) = x - x^0$. For the starting point $(-0.2, 2)$, this leads to the connected homotopy path whose projection is shown in Fig. 10(c); but, for a starting guess of $(0.01, 2.3)$, the path goes through a turning point near $t = 0.12$, $x_1 = -0.23$, $x_2 = 2.7$, after which it heads off to infinity in the x_2 direction coming closer and closer to the $t = 0$ plane, which, of course, it can never reach.

The affine function, $g(x) = f'(x^0)\,(x - x^0)$, however, also has a unique root, if $f'(x^0)$ is nonsingular, which, according to Sard's theorem, will be the case, except for a set of $y^0 = f(x^0)$ of measure zero. Also, as discussed above, one expects the affine homotopy, $tf(x) + (1-t)f'(x^0)\,(x - x^0)$, to have good scaling properties. When this homotopy was applied, the homotopy path whose projection (in the x_1x_2 plane) is shown in Fig. 10(d) resulted. This path leads from $(0.01, 2.3)$ at $t = 0$ to $(-0.425, 1.0)$ at $t = 1.0$ which, of course, is interpreted as $(+0.425, 1.0)$, the second root of the original problem. Differential homotopy continuation applied to this homotopy converged to a root of $f(x)$ from every starting point that was tried. [The starting point farthest from the root was (100,100).] This affine homotopy is currently being incorporated in a code to solve multicomponent, multistage separation problems.

For many problems, including this last example, it is easy to show that the homotopy path is bounded for the Newton homotopy. This is because in the Newton homotopy $f(x)$ equals something that does not depend on x. Therefore, we are interested in investigating the properties of the following restart version of the affine homotopy:

$$\frac{t - t_k}{1 - t_k} f(x) + \frac{1 - t}{1 - t_k} f'(x^k)\,(x - x^k).$$

If x is close to x^k, $f'(x^k)(x - x^k)$ is close to $f(x) - f(x^k)$, the simple function in the restart version of the Newton homotopy whose behavior is indistinguishable from that of the Newton homotopy itself.

Another important advantage of the affine homotopy over the Newton homotopy arises from the uniqueness of the starting point for the former homotopy. This sometimes permits us to obtain all solutions, if more than one exists, from a single starting point if we allow the homotopy parameter, t, to take on values >1. For example, suppose we wish to determine all roots of $f(x) = x^2 - 3x + 2 = 0$. The roots obviously are $x = 1$ and 2. If we use the fixed-point homotopy with $g(x) = x - 3$, i.e. $x^0 = 3$, the path shown in Fig. 11 is obtained which traces through both roots if t is allowed to continue past a value of 1.2. Note that a closed path can not be obtained because h is satisfied for only one value of

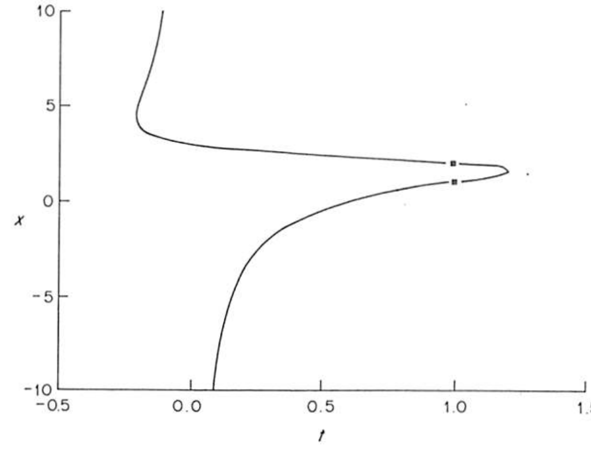


Fig. 11. Homotopy path for $f(x) = x^2 - 3x + 2 = 0$ with $g(x) = x - 3$.

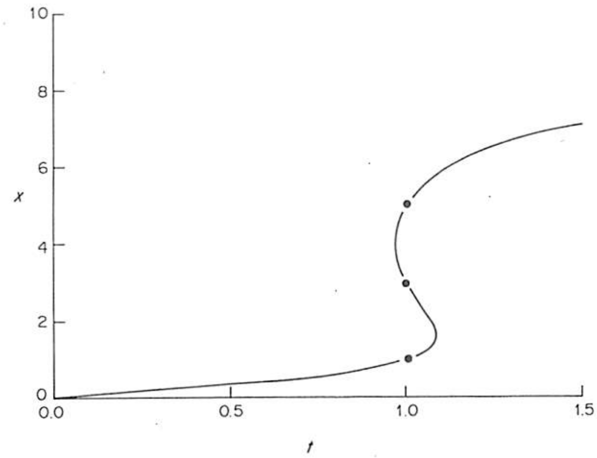


Fig. 12. Homotopy path for $f(x)=x^3-9x^2+23x=0$ with $g(x)=f(x)-f(x^0)$ and $x^0=0$.

x at $t=0$. Instead, as shown, the two legs of the path run off to $+\infty$ and $-\infty$ at $t=0$.

In a similar manner, all three roots of the function $f(x)=(x-1)\ (x-3)\ (x-5)=x^3-9x^2+23x-15=0$ can be obtained from one starting point using the affine homotopy. The path for a starting point of $x^0=0$ is shown in Fig. 12. Again a closed path is not obtained, but we trace through all three roots.

As a final example, consider an optimization application. We desire to optimize the function, $P=\frac{2}{3}x_1^3-8x_1^2+33x_1-x_2x_1+5$, with respect to x_1 and subject to the equality constraint, $f_1=(x_1-4)^2+(x_2-5)^2-4=0$. If we apply the Gauss–Newton method, we set $\partial P/\partial x_1=f_2$ to zero to give $f_2=2x_1^2-16x_1+33-x_2=0$. If we solve f_1 and f_2 simultaneously using the affine homotopy from a starting point of $(x_1^0, x_2^0)=(0, 0)$, all four roots of f_1 and f_2 are obtained from a single path by allowing t to be >1, with the following interpretation:

x_1^*	x_2^*	P
2.944	3.311	40.078 (global maximum)
5.056	3.311	36.77 (local minimum)
2.389	6.187	32.49 (local maximum)
5.611	6.187	21.35 (global minimum)

Application of this technique to Himmelblau's optimization function, as described by Reklaitis *et al.* [36], leads to four local minima and five saddle points. To handle additional equality constraints or inequality constraints, it is necessary only to introduce Lagrange multipliers and/or slack variables to convert inequality constraints to equality constraints. The ability to obtain all local maxima, local minima and saddle points, from a single initial guess, for an optimization problem would appear to have a distinct advantage over other conventional methods.

NOMENCLATURE

A, B = Constants sets
$B^n_{\epsilon,r}$ = The rth member of a sequence of n-dimensional balls, the sum of whose volumes is less than ϵ
C^0 = The class of continuous functions
C^1 = The class of continuous functions whose first derivatives exist and are continuous
C^k = The class of continuous functions all of whose derivatives up to and including the kth derivative exist and are continuous
C^∞ = The class of continuous functions for which all orders of derivatives exist and are continuous
C^n = The vector space of n-tuples of complex numbers
D = The domain of definition of, for example, f
$\mathrm{D}h$ = The total Frechet derivative of h with respect to x *and* t
$\dot{D}$ = The boundary of D
E = An arbitrary open and bounded set
$\dot{E}$ = The boundary of E
$E_t=E\times\{t\}$
f = The mapping or function in the original problem to be solved; an arbitrary function
f^{-1} = The inverse of f
$f'(x)$ = The Frechet derivative of the vector mapping f, with respect to its variable, the vector, x, represented by the Jacobian matrix; the ordinary derivative of a real-valued function of one real variable
g = A simple function, one of whose roots is known or can be found easily
$G(\cdot,\cdot)$ = An arbitrary function of an independent variable and a parameter
$G_Q(\cdot)=G(Q,\cdot)$
h = A homotopy
$h^{-1}(0)$ = The image of zero under the inverse of the homotopy, h
$H(x,t,x^0)$ = The homotopy, $f(x)-(1-t)f(x^0)$, with x^0 thought of as variable
$H_{x^0}(x,t)=H(x,t,x^0)$ with x^0 fixed
H'_{-i} = $\mathrm{D}h$ with its ith column removed
I = The identity matrix
n = Dimension of the space
N = An integer
R^n = The vector space of n-tuples of real numbers
S = A sphere in R^n
t = The homotopy parameter
$\dot{t}$ = The derivative of t with respect to arclength
T = The unit triangle in R^2, i.e. the triangle whose vertices are $(0, 0)$, $(0, 1)$ and $(1, 0)$; as a superscript, T stands for the transpose of a matrix or column vector, e.g. 0^{T} is the transpose of the n-dimensional column vector all of whose components are zero

u = Unit tangent vector
U = An arbitrary open set
v_1, v_2 = Placeholders
x = The vector of independent variables; an independent variable
x^0 = The (guessed) values of x at the beginning of a homotopy calculation
x^* = A value of x such that $f(x) = 0$
x_{-i} = The vector, x, with its ith component removed
$\dot{x}$ = The derivative of x with respect to arclength
$|x|$ = The vector whose components are the absolute values of the components of x
y = A point in the range of f

Greek letters

α = The index of a weight function; a small real and positive number
β = A small real and positive number
Γ = A homotopy path
δ = Lower bound for support of ω; bound on independent variable in definition of continuity
ϵ = A small parameter
Φ = A special function used in the definition of degree
ψ = The solution set of $f(x) = 0$
ω = The weight function used in the definition of degree
Ω = An arbitrary open and bounded subset of $R^n \times [0, 1]$

Abbreviations

Cl(D) = The closure of D
deg(f, E, y) = The degree of f with respect to E and y
det = Determinant
lim = Limit
min = Minimum
max = Maximum
sgn = Signum or sign
sup = Supremum
TP = Turning point

Special symbols

$\rightarrow$ = Approaches
$\|\cdot\|$ = Euclidean norm; an arbitrary norm
(a, b) = The open interval on the real line between a and b, i.e. not including a or b; a point in the plane whose first coordinate is a and whose second coordinate is b
$[0, 1]$ = The closed interval between 0 and 1 on the real line, i.e. including 0 and 1
$\{\cdot\}$ = Sequence; set
$\{t\}$ = The set consisting of t alone
$\emptyset$ = The null or empty set

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APPENDIX A

Review of Fundamental Notions from Higher-dimensional Nonlinear Analysis and General Topology

It is understood that the terms n-dimensional vector, point in R^n, and n-tuple of real numbers are synonymous; moreover, if it is agreed to let $\|\cdot\|$ stand for the *Euclidean* norm, R^n is, effectively, the Euclidean space of n dimensions.

A set is any collection of objects whatever. The sets in this paper are point sets; for example, collections of vectors (or points) in R^n. A set, A, is a subset of a set, D, written $A \subset D$, if x belongs to A implies x belongs to D. The null set, $\emptyset$ is the set that contains no objects at all, i.e. is empty.

An ϵ-neighborhood, U_ϵ, of a point, x, can be taken to be the set of all points y such that $|y - x| < \epsilon \ll 1$. By an open set, O, is meant a set such that for every point, x, in the set, O, there can be found a U_ϵ that contains x and is entirely contained in O. By an accumulation point, p, of a set, D, is meant a point such that every ϵ-neighborhood of the point, p, contains at least one point, x, that is a member of D. The closure of a set, D, is the set $\bar{D}$ consisting of all the points in D plus all the accumulation points of D. A closed set is a set that contains all of its accumulation points. The boundary of a set, D, is the set of all points, x, such that every U_ϵ of x contains points of D and points that are not in D. The boundary of D is written $\dot{D}$ or ∂D. For the purposes of this paper, it is sufficient to note that every closed and bounded set in R^n is *compact*.

The union of two sets A and B, written $A \cup B$, is the set of all points, x, such that x belongs to A *or* x belongs to B. The intersection of two sets A and B, written $A \cap B$, is the set of all points, x, such that x belongs to A *and* x belongs to B. By the cartesian product of two sets, A and B, written $A \times B$, is meant the collection of all ordered pairs (a, b), where a belongs to A and b belongs to B.

By a map from a subset, D, of R^n to R^m (written $f: D \subset R^n \to R^m$) is meant an m-dimensional vector-valued function of n real variables, i.e. for each n-tuple of real numbers, $x = (x_1, x_2, \ldots, x_n)^T$, belonging to D, the mapping (or function) f prescribes a unique vector (or point) in R^m. The subset, D, of R^n in the above definition of f is called the *domain* of f.

It is necessary for the development in this paper to make clear what is meant by the derivative of a vector-valued function of a vector. If

$$\lim_{t\to 0} \frac{1}{t} \|f(x + th) - f(x) - tA_x h\| = 0$$

for all h belonging to R^n, we say f is Gateaux differentiable and A_x is the G-derivative of f at x. If

$$\lim_{\|h\|\to 0} \frac{1}{\|h\|} \|f(x + h) - f(x) - A_x h\| = 0$$

for all h belonging to R^n, f is Frechet differentiable at x and its F-derivative at x is A_x, written simply $f'(x)$. The derivative, $f'(x)$, which in this paper is always the F-derivative, is a linear transformation from R^n into R^m, which can be represented by the well-known Jacobian matrix, whose components are the ordinary partial derivatives of the component functions of f with respect to the components of x, i.e. if

$$f = \begin{bmatrix} f_1(x_1, x_2, \ldots, x_n) \\ f_2(x_1, x_2, \ldots, x_n) \\ \vdots \\ f_n(x_1, x_2, \ldots, x_n) \end{bmatrix},$$

then

$$f'(x) = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \cdots & \frac{\partial f_2}{\partial x_n} \\ \vdots & & & \\ \frac{\partial f_m}{\partial x_1} & \frac{\partial f_m}{\partial x_2} & \cdots & \frac{\partial f_m}{\partial x_n} \end{bmatrix}$$

an $m \times n$ matrix.

Suppose now that our function, f, is specialized to the case where $m = n$. An example of such a function is the relations that describe a multicomponent, multistage separation column modeled in the simulation mode, i.e. the situation where the number of unknowns (the scalar elements of x) exactly matches the number of equations (the individual real-valued component functions of f). The problem of finding the temperatures and the component liquid and vapor flows on each stage of the column can then be stated as follows: given f: $D \subset R^n \to R^n$, find an x such that $f(x) = 0$. (The symbol 0 represents the n-dimensional vector, all of whose components are zero.) The domain D would be a bounded subset of the positive orthant since the equations are not defined for negative flow rates and temperatures. (The word "orthant" is a generalization of the word "quadrant".)

APPENDIX B

A Rigorous Definition of Topological Degree

Motivated by the discussion in the text, we introduce a definition for degree, for the class of functions continuous on Cl(E) with no zeros on $\dot{E}$, that is independent of whether $f'(x)$ exists or is singular or not. Following Ortega and Rheinboldt [4], we first remove the requirement that $f'(x)$ be nonsingular on the solution set, ψ, then we show how to extend our new definition to functions that are merely continuous.

A real-valued function, ω, defined on $[0, \infty]$ is a *weight function of index* α if, for $\alpha > 0$, there is a δ such that, for t outside the interval $[\delta, \alpha]$, $\omega(t) = 0$. Assume the following conditions are satisfied: (i) f is continuously differentiable on the open and bounded set, E; (ii) the closure of E is within D, the domain of definition of f; (iii) $f(x) = 0$ has no solutions on $\dot{E}$, the boundary of E. Then

$$\deg_\omega(f, E, 0) = \int_{R^n} \Phi(x)\,\mathrm{d}x,$$

where

$$\Phi\colon R^n \to R^n,\ \Phi = \begin{cases} \omega(\|f(x)\|)\det f'(x), & x \in E \\ 0, & \text{otherwise} \end{cases}$$

and ω is a weight function of index α. As shown by Ortega and Rheinboldt [4], this definition is independent of ω and α provided

$$\int_{R^n} \omega(\|x\|)\,\mathrm{d}x = 1$$

and $0 < \alpha < \min\{\|f(x)\| \mid x \in \dot{E}\}$ where all integrations are taken in the sense of Riemann. Finally, a mapping, f, that is merely continuous on E and satisfies conditions (ii) and (iii) can be approximated by a sequence of mappings, $\{f_k(x)\}$, continuously differentiable in E, that satisfy conditions (i), (ii) and (iii). We assert without proof that the definition of topological degree,

$$\deg(f, E, 0) = \lim_{k\to\infty} \deg_\omega(f_k, E, 0)$$

is independent of the sequence $\{f_k(x)\}$ provided

$$\lim_{k\to\infty} \|f_k - f\| = 0.$$

Admittedly, this definition does not appeal much to geometric intuition, but it is not hard to show that, for the case of $f'(x)$ nonsingular on the solution set, it breaks down to equation (1) in the main text of this paper. We can prove that the topological degree defined above satisfies the following four properties, or we can take the four properties as axioms:

(*1*) Normality: $\deg(id, E, 0) = \begin{cases} 1 \text{ if } 0 \text{ belongs to } E \\ 0 \text{ otherwise;} \end{cases}$

(*2*) *Additivity*: if E_1 and E_2 are open subsets of E, and, if there are no solutions of $f(x) = 0$ in the part of Cl(E) outside the union of E_1 *and* E_2, then $\deg(f, E, 0) = \deg(f, E_1, 0) + \deg(f, E_2, 0)$.

(*3*) *Continuous dependence on f*: if

$$\min_{x\in\dot{E}} \|f(x)\| > \beta > 0$$

then $\deg(f, E, 0) = \deg(g, E, 0)$ for any continuous mapping, g, from Cl(E) into R^n such that

$$\sup_{x\in \mathrm{Cl}(E)} \|f(x) - g(x)\| < \tfrac{1}{7}\beta.$$

By taking E_1 to be E and E_2 to be the empty set, $\emptyset$, in axiom (2), we see that $\deg(f, E, 0) = \deg(f, E, 0) + \deg(f, \emptyset, 0)$; so, $\deg(f, \emptyset, 0) = 0$. If U is an open subset of E, let E_1 in axiom (2) be U and E_2 be $\emptyset$ to prove:

(*5*) *Excision property*: if U is an open subset of E and $f(x) = 0$ has no solution in the part of E that is not in U, then $\deg(f, E, 0) = \deg(f, U, 0)$.

Using the excision property with $U = \emptyset$ and $\deg(f, \emptyset, 0) = 0$ as shown above, one sees that, if $f(x) = 0$ has no solutions in Cl(E), $\deg(f, E, 0) = \deg(f, \emptyset, 0) = 0$. This is logically equivalent to the following important result:

(*4*) *Solution property*: if $\deg(f, E, 0) \neq 0$, then there exists an x belonging to E such that $f(x) = 0$.

Alternative definitions of degree are given in Refs [37–39].

APPENDIX C

Sard's Theorem and the Parameterized Sard's Theorem

Following Sternberg [40], a few definitions and the statement of Sard's theorem are given. Then, following Chow *et al.* [22], the statement of the parameterized Sard's theorem is given.

Definitions of criticality and regularity

Let G be a continuously differentiable (C^1) map of R^m into R^n. The points of R^m where the rank of the Jacobian matrix of G is less than n, i.e. where the Jacobian matrix of G does not have at least one nonsingular $n \times n$ minor, are the *critical points* of G. All other points are *regular points*. A point, P, of R^n such that $G^{-1}(P)$, the inverse image of P under G, contains at least one critical point is a *critical value*. All other points of R^n are *regular values*.

Sard's theorem

Let G be a map from R^m to R^n having continuous kth derivatives, i.e. belonging to C^k. If $k - 1 \geqslant \max(m - n, 0)$, the critical values of G form a set of measure zero in R^n.

There are numerous statements of Sard's theorem in the literature having greater or less generality. This statement, which is proved in greater generality in Ref. [40], i.e. for the case where R^m and R^n are m- and n-dimensional C^k manifolds, is adequate for our purposes.

Parameterized Sard's theorem

Let V be an open subset of R^q, let U be an open subset of R^m, and let G be a mapping from $V \times U$ into R^n with continuous kth derivatives (G belongs to C^k) $k - 1 \geqslant \max(m - n, 0)$. If 0, a point of R^n, is a regular value of G, then, except for a set of measure zero, for every point Q belonging to V, 0 is a regular value of $G_Q(\cdot) = G(Q, \cdot)$. A sketch of the proof of this theorem can be found in Ref. [22].

We now apply the parameterized Sard's theorem to the Newton homotopy by embedding it in a larger space where the components of x^0, the starting point, are thought of as additional parameters:

$$H\colon R^n \times [0, 1] \times R^n$$

$$\to R^n \text{ (twice continuously differentiable)}$$

$$H(x, t, x^0) = f(x) - (1 - t)f(x^0).$$

According to Sard's theorem, itself, $y^0 = f(x^0)$ is a regular value of f, continuously differentiable, for all y^0 in R^n, except for a set of measure zero. So, we expect that, for an arbitrary $y^0 = f(x^0)$, $f'(x^0)$ will be nonsingular, in which case 0 is a regular value of $H(x, t, x^0)$ for $0 \leqslant t < 1$, since $\partial H/\partial x^0 = (t - 1)f'(x^0)$. Then, by the parameterized Sard's theorem, 0 is a regular value of $H_{x^0}(x, t) = h(x, t)$, except for a set of starting points, x^0, of measure zero. Again, since x^0 is arbitrary, we expect regularity. In order to have regularity along the entire homotopy path including the end point at $t = 1$, which is necessary for the path to have finite length, we must assume that 0 is a regular value of $f(x)$. If zero is an arbitrary point in R^n, it will be a regular value of $f(x)$ with "probability 1", according to Sard's theorem.

We would like to apply the parameterized Sard's theorem to the scale-invariant, affine homotopy, $H(x, t, x^0) = tf(x) + (1 - t)f'(x^0)\ (x - x^0)$ in the above straightforward way. Unfortunately, this is impossible since both $\partial H/\partial x^0 = (1 - t)\ [f''(x^0)\ (x - x^0) - f'(x^0)]$ and

$\partial H/\partial x = tf'(x) + (1-t)f'(x^0)$ depend on x and singular points cannot be ruled out. To avoid this difficulty, we could perturb the homotopy somewhat. Instead of using $f'(x^0)$ as the scaling matrix, we could take $f'(x)$ evaluated at a point x^1 close to x^0. Then $H(x, t, x^0, x^1) = tf(x) + (1-t)f'(x^1)(x - x^0)$ is close to the original affine homotopy and is still scale invariant. Now, $\partial H/\partial x^0 = (t-1)f'(x^1)$ and the previous argument holds.