

Least Squares and Chaotic Behavior in Initial Value Problems

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Abstract

We describe an unconventional method for treating initial value problems. The system of differential equations is discretized on a fixed interval, the initial value is left unspecified, and the underdetermined system is solved by a least squares minimization procedure. When applied to the celebrated Lorenz equations, it produces a simple smooth curve that terminates at a stationary point rather than producing the ‘butterfly’ attractor. As far as we know this is the first method that produces a non-chaotic orbit.

1 Introduction

This paper is addressed to the relationship between numerical experimentation and differential equations. Of particular interest are instances in which numerical results indicate some kind of chaotic behavior. We use the term chaotic in a broad general sense here. Since it is often impossible to obtain good error bounds for numerical approximations, it can be difficult to distinguish between chaotic dynamics and chaotic behavior that is purely an artifact of numerical roundoff and discretization error.

As an example, consider continuous Newton’s method for finding zeros of a nonconstant complex polynomial p . A trajectory for p is a continuous function $z : R \rightarrow C$ such that

$$p(z)' = -p(z), \tag{1}$$

or, in a more familiar form,

$$p'(z(t))z'(t) = -p(z(t)), \quad t \in R.$$

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For a discretization, pick $T > 0$ such that $p'(z(t)) \neq 0$ for $t \in [0, T]$, choose a positive integer n and denote $\frac{T}{n}$ by δ . Then Euler's method yields

$$z_k = z_{k-1} - \delta \frac{p(z_{k-1})}{p'(z_{k-1})}, \quad k = 1, \dots, n.$$

This is damped Newton's method (ordinary Newton's method if $\delta = 1$). Now consider the polynomial $p(z) = z^3 - 1$ for $z \in \mathbb{C}$. Figure 1 depicts the domains of attraction of the three zeros of p for Newton's method ($\delta = 1$); i.e., the color associated with a point in the complex plane is defined by the zero to which the Newton iteration converges when started from that point as initial value. (The background color is assigned to the few points for which the iteration fails to converge to a zero, but these are not noticeable.)

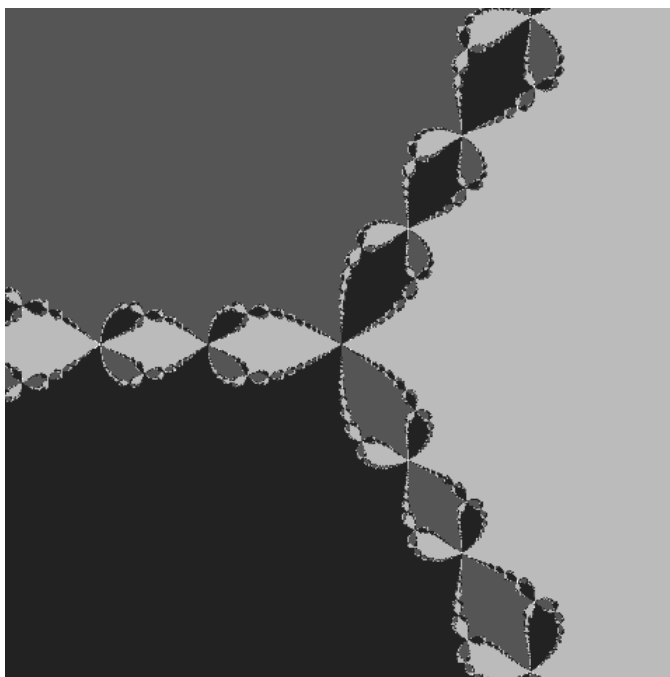


Figure 1: Newton's method for cube roots of 1.

It is well known that the domains of attraction depicted in the figure have fractal boundaries implying chaotic dynamics. In [3], however, it is proved that no such chaos occurs in the continuous case defined by (1). Starting from a point z_0 that does not lie on one of the rays $\theta = \pi/3$, $\theta = -\pi/3$, or $\theta = \pi$, $\lim_{t \rightarrow \infty} z(t)$ is the nearest zero to z_0 . The only 'chaos' in the differential equation (1) is that introduced by discretization.

The above example raises the question of how to separate chaos that is intrinsic to the solution of a differential equation from chaos that arises from numerical

approximation. Our primary purpose here is to illustrate a non-conventional numerical technique that may be helpful in addressing this question. We apply the method to a system of ordinary differential equations, but the method applies equally well to the more important case of partial differential equations. For example, an important unresolved question is the existence of classical solutions to the incompressible Navier-Stokes equation in three dimensions [1]. The crux of the matter seems to be whether or not there is turbulence and, if so, whether a classical solution ceases to exist at the onset of turbulence. Numerical results are inconclusive. An alternative approach such as suggested here, might help to resolve this issue.

2 Least Squares Method

Suppose m is a positive integer, $T > 0$, and $F : R^m \rightarrow R^m$ is continuous. We consider the system of differential equations

$$y'(t) = F(y(t)), \quad t \in [0, T] \quad (2)$$

with or without a specified initial value $y(0)$. A discretization of (2) is, with $\delta = \frac{T}{n}$ and $Y = (Y_0, Y_1, \dots, Y_n) \in (R^m)^{n+1}$,

$$Y_k = Y_{k-1} + \delta \frac{F(Y_k) + F(Y_{k-1})}{2}, \quad k = 1, \dots, n.$$

When applied in a step-by-step manner, this method is referred to in the literature as the trapezoidal method. It is a second-order implicit method with no restriction on the step-size δ required for stability. Rather than single-stepping from an initial value, however, we define $\phi : (R^m)^{n+1} \rightarrow R$ by

$$\phi(Y) = \frac{1}{2} \sum_{k=1}^n \left\| Y_k - Y_{k-1} - \delta \frac{F(Y_k) + F(Y_{k-1})}{2} \right\|^2, \quad (3)$$

and we find a zero of ϕ by means of a least squares minimization procedure.

A standard method for treating an underdetermined system, such as a damped Newton iteration with a pseudo-inverse Jacobian, works extremely well for this particular problem, requiring very few iterations. However, we present an alternative method that has been shown to work well even when Newton's method fails. This is the method of steepest descent with a Sobolev gradient. Our general reference for Sobolev gradients is [2], but we give a sketch here for this special case. Clearly ϕ has a gradient in the ordinary sense, but it is widely understood that such gradients have extremely poor numerical properties in problems arising from differential equations. With an appropriate gradient, however, steepest descent becomes an effective method. A Sobolev gradient for ϕ is one with respect to a metric that emulates the norm associated with the Sobolev space $H^{1,2}([0, T])$, i.e.

$$\|Y\|_S^2 = \sum_{k=1}^n \left(\left\| \frac{Y_k + Y_{k-1}}{2} \right\|_{R^m}^2 + \left\| \frac{Y_k - Y_{k-1}}{\delta} \right\|_{R^m}^2 \right),$$

$$Y = (Y_0, Y_1, \dots, Y_n) \in (\mathbb{R}^m)^{n+1}. \quad (4)$$

The Sobolev gradient of ϕ , $\nabla_S \phi$, is defined by

$$(\phi'(Y))h = \langle h, (\nabla_S \phi)(Y) \rangle_S, \quad Y, h \in (\mathbb{R}^m)^{n+1},$$

where the inner product is the one associated with $\|\cdot\|_S$ in 4). Computationally, $\nabla_S \phi(Y)$ is the solution of a linear system in which the right hand side is the ordinary gradient $\nabla \phi(Y)$, and the matrix (inverse smoothing operator) is $I + D_1^t D_1$ for the first difference operator D_1 . This matrix is tridiagonal and diagonally dominant.

Using this gradient, we employ a steepest descent iteration:

$$Y \rightarrow Y - \alpha(\nabla_S \phi)(Y), \quad (5)$$

with α chosen to minimize

$$\phi(Y - \alpha(\nabla_S \phi)(Y)).$$

A line search is used to approximate α . If a specified value for Y_0 is to be retained, we project the gradient $\nabla_S \phi(Y)$ onto the subspace of vectors that have zero first components before updating Y at each step.

3 Numerical Results

Our test results were computed using IEEE standard double precision. We applied the least squares method to the Lorenz equations with standard parameters:

$$\begin{aligned} x' &= 10(y - x), \\ y' &= 28x - y - xz, \\ z' &= xy - \frac{8}{3}z. \end{aligned} \quad (6)$$

As far as we know all previous numerical approximations to (6) over even moderately long time intervals result in the famous ‘butterfly’ pattern as depicted in Figure 2 ([4]). The least squares method, however, with initial estimate for Y taken to have all $n + 1$ components equal to $(10, 12, 14)$ and no enforcement of an end condition, produces a trajectory that follows a smooth curve from a point p_1 to a point p_2 near the critical point $c = (\sqrt{72}, \sqrt{72}, 27)$, spirals in toward the critical point, and then spirals out in approximately the same plane. The curve between p_1 and p_2 is nearly normal to the plane of the spiral with p_2 in the plane and, in some cases, agreeing with c in almost all significant digits (in which cases there is no spiraling in, only spiraling out). This is the case for time interval $T = 800$ with the number of grid points $n = 160000$ corresponding to mesh width $\delta = .005$. The first endpoint (initial value) is $p_1 = Y_0 =$

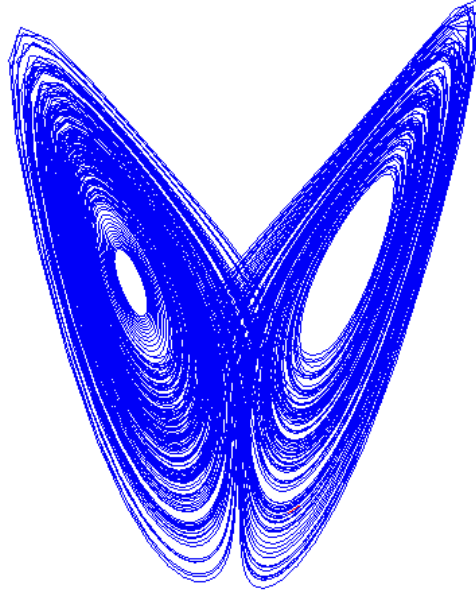


Figure 2: Lorenz attractor

(10.0094834215091, 7.87724239501250, 26.3369924246729), the distance from p_2 to c is about 10^{-15} , and the last point on the curve is (8.8968, 8.9385, 27.453). The radius of the spiral increases very slowly with T .

Using the same (constant) step-size δ and the initial value Y_0 computed by the least squares procedure, we ran the trapezoidal method in step-by-step mode to $T = 800$. The computed trajectory reproduced the curve from p_1 to p_2 but not the spiral. More precisely, the iterates stopped changing after about 500 steps, the final value agreeing with c in all but the last decimal place. We then perturbed the third component of the initial value by 10^{-15} and reran the experiment. This tiny perturbation resulted in the ‘butterfly’ attractor.

When the nonchaotic orbit (p_1 to p_2) produced by the trapezoidal method was used as initial estimate for the least squares code, with or without prescribed initial value, that orbit was nearly reproduced in a single iteration with a smaller residual than that of the original spiraling solution ($\phi = 8.2 \times 10^{-27}$ versus $\phi = 4.2 \times 10^{-25}$). This strongly indicates that the spiraling is a numerical artifact.

As a final test, we ran the least squares code with a prescribed initial value obtained by perturbing Y_0 . With the remaining values taken to be initially constant, the method failed to converge, stopping with an uphill search direction. With the computed solution from the trapezoidal method (with perturbed initial

value) as initial estimate, the method converged to the butterfly attractor with $\phi = 5.6 \times 10^{-25}$. We conclude that, as in the case of single-stepping methods, the least squares method with prescribed endpoint value leads to the butterfly attractor when Y_0 is perturbed. This conclusion must be qualified, however, by the fact that the method fails without a reasonably good initial estimate.

Additional test results indicate the existence of at least one non-chaotic orbit for each of the three stationary points. Further testing with different initial estimates for the least squares procedure may reveal additional non-chaotic orbits. Given the extreme sensitivity of these orbits to perturbations in initial values, it is hardly surprising that standard methods fail to produce them. What makes the least squares method work is that at each step, it computes a minimum-norm update to the current approximation, thus producing a solution that is, in some sense, close to the initial estimate, which we took to be a simple constant.

We make no claim for the accuracy of our approximate solutions. In unstable systems such as (6) global error cannot be bounded by controlling local discretization error. A computed solution cannot be assured of having any relationship to the actual solution regardless of the computational method. We merely observe the possibility that our method may be capable of picking out solutions that are not accessible to any step-by-step method.

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