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A linear condition determining local or global existence for nonlinear problems

Research Article

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Abstract: Given a nonlinear autonomous system of ordinary or partial differential equations that has at least local existence and uniqueness, we offer a *linear* condition which is necessary and sufficient for existence to be global. This paper is largely concerned with numerically testing this condition. For larger systems, principals of computations are clear but actual implementation poses considerable challenges. We give examples for smaller systems and discuss challenges related to larger systems. This work is the second part of a program, the first part being [Neuberger J.W., How to distinguish local semigroups from global semigroups, Discrete Contin. Dyn. Syst. (in press), available at http://arxiv.org/abs/1109.2184]. Future work points to a distant goal for problems as in [Fefferman C.L., Existence and Smoothness of the Navier–Stokes Equation, In: The Millennium Prize Problems, Clay Mathematics Institute, Cambridge/American Mathematical Society, Providence, 2006, 57–67].

MSC: 35A01, 35L61

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1. Introduction

Is there a function u so that

$$u' = 1 + u^2$$

on a given connected subset S of $\mathbb{R}$? A moments thought gives an answer 'yes' if S has length less than π and 'no' if S has length exceeding π.

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It is an enduring problem for autonomous nonlinear ODE and PDE to try to determine maximal intervals of existence for solutions to such problems. In [4] there is given a necessary and sufficient condition for a wide class of autonomous ODE and PDE in order that existence, unlike the above example, be global. The condition is a *linear* one, but on a usually large space of functions.

Before going further with our development, we give some background. The problem of forging a close connection between dynamical and semidynamical systems with differential equations (we will speak here about semidynamical systems, i.e., semigroups, almost exclusively) was pursued for about thirty years before it, arguably, was solved in [1]. The main new ingredient in [1], in a sense, is a shift from the conventional notion of generator to generators in the sense of Sophus Lie [3]. Lie's ideas, in turn, can be traced to fundamental ideas of Riemann, and his teacher Gauss, concerning differentiation of functions with domain a manifold. In [4], the work of [1] was partially extended to *local* semigroups. In the process, the condition indicated in the second paragraph was discovered.

In [6] a start is made toward implementing a numerical means of investigating this condition. Applications are made there to simple ODEs, so simple that the condition can be recognized in closed form. It is noted that agreement between numerical results with closed form results is very good. In the present paper, this numerical work is extended to more substantial examples. An ultimate goal is to investigate unsettled problems such as the Navier–Stokes problem in the Clay Millennium collection [2]. A second, but main objective of the present work is to outline a path toward implementing the basic idea of [4, 6] in very substantial problems as in [2].

The program mentioned in the abstract can be elaborated as follows: to

- replace a finite difference setting with a more efficient bases such as given by finite element, Fourier, or wavelets methods;
- search for graphical representations for high dimensional data (much of this can come from existing literature);
- improve theoretical calculations;
- implement parallel computation.

One might ask why a new method, as in the present program, is timely to consider. As indicated in [2], numerical results which point to global (versus only local) existence for many important problems, have been 'inconclusive', this despite some sixty years of intense effort. It has so far been essentially impossible, for many problems, to infer whether a theoretical solution is ceasing to exist at a given time or whether there is a point of seeming turbulence which numerically might be traversed. The present method replaces considerations based on time-forward step-by-step methods with a very large linear eigenvalue problem, clearly a different approach. The huge size of our eigenvalue problems, as hinted by the difference between our 1D and 2D examples, is an obstacle, but it is not hard to see that advances in the speed, size, and particularly communication facility between processors, all will have a positive impact on the size of problem that can be handled by our methods.

Section 2 contains some needed definitions and gives the main result upon which this present note is based.

2. Definitions and basic result

Definition 2.1.
If X is a set, then a *semigroup* on X is a function from $[0, \infty)$ into the collection of all transformations from X to X so that if $x \in X$ and $t, s \geq 0$ then

$$T(t)(T(s)x) = T(t+s)x.$$

The composition of $T(t)$ and $T(s)$ is written $T(t)T(s)$.

Theorem 2.2.

Suppose X is a subset of a Banach space Y and $B\colon X \to Y$ is such that if $x \in X$, then there is a unique function $u\colon [0,\infty) \to X$ such that

$$u(0) = x, \qquad u'(t) = B(u(t)), \qquad t \geq 0. \tag{1}$$

Then there is a unique semigroup T on X so that if $s \geq 0$, $x \in X$, then

$$T(s)x = u(s)$$

where u satisfies (1).

In the above case, B is said to be the conventional generator of T.

From here on in this note, X is to be a complete, separable metric space, i.e., a Polish space. A semigroup T on X is said to be jointly continuous provided that if $g\colon [0,\infty)\times X \to X$ and

$$g(t,x) = T(t)x, \qquad t \geq 0, \quad x \in X,$$

then g is continuous. Denote by $\mathrm{CB}(X)$ the Banach space, under sup norm, of all bounded and continuous functions from X to $\mathbb{R}$.

Definition 2.3.

Suppose that X is a complete separable metric space. The statement that T is a *local semigroup* on X means that:

- There is ω so that $0 < \omega \leq \infty$ and so that if $0 \leq t < \omega$, then $T(t)$ is a function from a subset of X into X.
- $T(0)x = x$, $x \in X$.
- There is a continuous function $m\colon X \to (0,\infty]$ such that $x \in D(T(t))$ iff $t \in [0, m(x))$.
- $m(x) < \infty$ for some $x \in X$.
- If $t, s \geq 0$ and $x \in X$, then $T(t)T(s)x = T(t+s)x$ iff $t+s < m(x)$.
- T is jointly continuous.
- T is maximal, i.e., if $\lim_{t\to s-} T(t)x$ exists, then $s < m(x)$.

Observe that if, in the definition, the forth item is omitted and the function m is identically ∞, then the resulting function T is a jointly continuous semigroup on X. A semigroup on X is said to be *global*.

Definition 2.4.

Suppose that T is either a jointly continuous semigroup on X or a jointly continuous local semigroup on X. Then the *Lie generator* of T is

$$A = \left\{ (f,g) \in \mathrm{CB}(X)^2 \,:\, g(x) = \lim_{t\to 0+} \frac{f(T(t)x) - f(x)}{t},\ x \in X \right\}. \tag{2}$$

The key result on which this note is based is from [4] and is the following.

Theorem 2.5.

Suppose T is either a local or a global jointly continuous semigroup on X and A is the Lie generator of T. Then A has a positive eigenvalue if and only if T is local.

Suppose that X is a Banach space and T is a semigroup generated by a function B as in Theorem 2.2. What is, at least roughly, a relationship between the conventional generator B of T and the corresponding Lie generator A from Definition 2.4? For f, g in the set A, (2) gives

$$g(x) = \lim_{t\to 0+} \frac{f(T(t)x) - f(x)}{t}, \qquad x \in X.$$

Granted that

$$B(x) = \lim_{t\to 0+} \frac{T(t)x - x}{t},$$

as it must be for $T(\cdot)x$ to be a solution of (1), it follows that if f is itself differentiable, then at least formally

$$(Af)(x) = (f'(x))(B(x)). \tag{3}$$

(We will write $(f'(x))(B(x))$ more simply as $f'(x)B(x)$, leaving it to a reader to mentally put in the parentheses.)

It is from appropriate discretizations of A in (3) that we make our eigenvalue tests of Theorem 2.5.

A point of the present note is to further develop the numerical testing of Theorem 2.5. Section 3 elaborates on the four items of Introduction.

3. An eigenfunction theorem

Theorem 3.1.
Suppose that T is a local semigroup on X and $m\colon X \to (0, \infty]$ is the stopping time function for T, i.e., the function m in the third item of Definition 2.3. Let A be the Lie generator of T. Define $f \in \mathrm{CB}(X)$ so that

$$f(x) = \exp(-m(x)), \qquad x \in X. \tag{4}$$

Then f is an eigenfunction of A with eigenvalue one. Moreover, suppose $g \in \mathrm{CB}(X)$, $Ag = g$ and $x \in X$. Then there is $c \in \mathbb{R}$ so that

$$g(T(t)x) = cf(T(t)x), \qquad t \in [0, m(x)).$$

Proof. Define f as in (4). Then

$$\frac{f(T(t)x) - f(x)}{t} = \frac{\exp(-m(T(t)x)) - \exp m(x)}{t} = \frac{\exp t - 1}{t}\exp(-m(x)) \to \exp(-m(x)) = f(x)$$

as $t \to 0+$, since

$$m(T(t)x) = m(x) - t \qquad \text{if} \quad 0 < t < m(x), \tag{5}$$

equation (5) being a key point in this development.

Suppose now that $x \in X$ such that $m(x) \neq \infty$ and that $g \in \mathrm{CB}(X)$ so that $Ag = g$. Note that $f(T(s)x) \neq 0$ for $0 < s < m(x)$. For such an s, $y = T(s)x$ and $0 < t < m(x) - s$,

$$\frac{g}{f}(T(t)y) - \frac{g}{f}(y) = \frac{(g(T(t)y) - g(y))f(y) - (f(T(t)y) - f(y))g(y)}{f(y)f(T(t)y)}$$

so

$$\frac{1}{t}\left(\frac{g}{f}(T(t)y) - \frac{g}{f}(y)\right) \to \frac{(Ag)f - (Af)g}{f^2(y)} = 0$$

as $t \to 0+$. Therefore,

$$\left(\frac{g}{f}(T(\cdot)x)\right)' = 0 \qquad \text{on} \quad [0, m(x))$$

and hence

$$\frac{g}{f}(T(\cdot)x) \qquad \text{is constant on} \quad [0, m(x)).$$

□

The theorem gives that all eigenfunctions of A with eigenvalue one can be constructed in a simple way from f of the theorem. This will be useful in interpreting graphs of numerical eigenfunctions in Section 5, which is dedicated to systems of two autonomous ODEs.

For any $\lambda > 0$, the function f_λ,

$$f_\lambda(x) = \exp(-\lambda m(x)), \qquad x \geq 0,$$

can be used to characterize, as in Theorem 3.1, all eigenfunctions for A corresponding to the eigenvalue λ. Knowledge of the precise nature of the positive spectrum of the Lie generator A might lead to improved computations as well as a better understanding of an underlying semigroup T.

4. Some one dimensional examples and their numerics

The examples in this section are largely taken from [6].

Example 1

Consider the local semigroup on $[0, \infty)$ generated by solutions u to

$$u(0) = x \in [0, \infty), \qquad u' = u^2. \tag{6}$$

In the notation of Theorem 2.2 this is written as $X = [0, \infty)$ and $B(x) = x^2$, $x \in X$.

For $x \geq 0$, the solution u to

$$u(0) = x, \qquad u'(t) = B(u(t)), \qquad t \in \left[0, \frac{1}{x}\right),$$

is given by

$$u(t) = \frac{x}{1 - tx}, \qquad x \geq 0, \quad t \in [0, m(x)),$$

where $m(x) = 1/x$, $x \in [0, \infty)$.

One can see this by solving (6) and noticing that $[0, m(x))$ is the maximal connected subset of $[0, \infty)$ containing zero over which there is a solution. Note that the local semigroup T so that

$$T(t)x = \frac{x}{1 - tx}, \qquad x \in [0, \infty), \quad t \in [0, m(x)),$$

is associated with (6) in the sense that if u satisfies (6), then

$$T(t)x = u(t), \qquad x \in [0, \infty), \quad t \in [0, m(x)).$$

Solving (3) for this case, one has from

$$Af = f \tag{7}$$

that

$$f(x) = \exp\left(-\frac{1}{x}\right) = \exp(-m(x)), \qquad x \geq 0, \qquad f(0) = 0, \tag{8}$$

is a solution, i.e., an eigenvector of A with eigenvalue one. We note that satisfying (7) is essentially equivalent in this example to finding a suitable solution of

$$f'(x)B(x) = f(x), \qquad x \in [0, \infty).$$

While f must be defined and continuous on the entire interval, one cannot insist on differentiability at singular points (as seen in the next example).

Hence, it is consistent with Theorem 2.5 that T is a local semigroup, which may readily be seen anyway. Note that (7) is actually a singular equation and that any positive multiple of (8) is also a solution and hence an eigenfunction of A with eigenvalue one, consistent with the tradition that for linear eigenvalue problems, any non-zero multiple of an eigenfunction is also an eigenfunction. Quite generally, zeros of a conventional generator B seem to correspond to singularities of the associated differential equation (for f) in (7). This in a sense corresponds to the important role of rest points of semidynamical systems, only here the point x which is a rest point of T appears as a coefficient which renders (7) singular. This point, in our opinion, deserves more thought.

Figure 1 shows an eigenfunction of the Lie generator A for this problem. It was computed independently using two different algorithms, whose corresponding *Matlab* programs are described in Section 6. The first method uses iterations of Sobolev gradient steepest descent. The second, direct (non-iterative) method used the supplementary condition $f(20) = 1$. When the approximate eigenfunctions obtained by the two methods are normalized to account for the arbitrary multiplicative constant by dividing by their maximums over the interval, they are in close agreement.

The Lie generator for this problem is given by A based on

$$(Af)(x) = f'(x)x^2, \qquad x \in \mathbb{R}, \quad f\colon [0,\infty) \to \mathbb{R}.$$

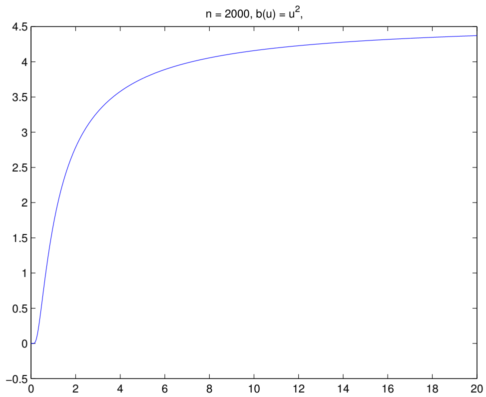

Figure 1. Lie generator eigenfunction for $u' = u^2$

Example 2

Figure 2 shows an eigenfunction for eigenvalue one for the local semigroup, generated by solutions to the differential equation

$$u(0) = x \geq 0, \qquad u' = u(u-1). \tag{9}$$

The Lie generator for this problem is given by A based on

$$(Af)(x) = f'(x)x(x-1), \qquad x \in \mathbb{R}, \quad f\colon [0,\infty) \to \mathbb{R}.$$

Perhaps of particular interest in Figure 2 is the flat spot over $[0, 1]$. That this flat spot is correct can be seen in several ways:

- By plotting a vector field for the equation in (9) and noting that integral curves from 0 to 1 must be flat, in light of the existence and uniqueness facts for this equation.

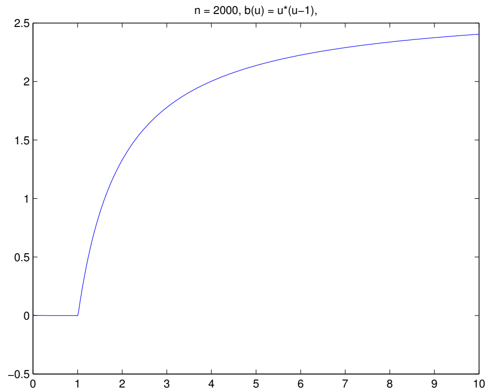

Figure 2. Lie generator eigenfunction for $u' = u(u-1)$

- By solving (9) in closed form and observing m in this case, using Definition 2.3.
- By solving the singular equation $f'(x)x(x-1) = f(x)$ on $[0,\infty)$, taking special care with the singularities at 0 and 1.
- Numerically using several different eigenvector methods.

This solution was also computed independently using the two different algorithms described in Section 6. We note here that the second method required enforcing $f(0) = 0$, and also used the supplementary condition $f(10) = 1$. Of course that eigenfunction differed from the one obtained by steepest descent, visualized in Figure 2, by a multiplicative constant.

Example 3

Figure 3 is generated by the problem

$$u(0) = x \geq 0, \qquad u' = -u^2.$$

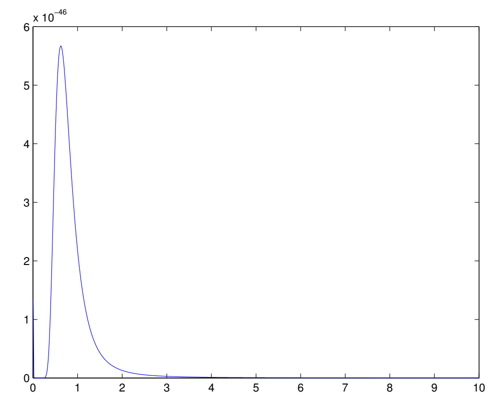

Figure 3. Lie generator eigenfunction for $u' = -u^2$

The Lie generator for this problem is given by A based on

$$(Af)(x) = f'(x)(-x^2), \qquad x \in \mathbb{R}, \quad f : [0,\infty) \to \mathbb{R}.$$

Some reflection yields that this problem has global existence for all $x \geq 0$. The test of Theorem 3.1 indicates that there should be no eigenfunction with positive eigenvalue. The steepest descent *Matlab* code gives an eigenvector reply to the chosen finite dimensional problem, nevertheless. However, examination of Figure 3 shows that the amplitudes of points on the graph are very small. One can infer that this is a numerical analyst's zero function and conclude that this figure represents only the zero function, that it does not represent an eigenfunction. An alternative indication of a non-eigenvalue might be a function that is rising steadily such that a doubling of the computational interval continues this trend. In such a case one might infer that one is looking at an unbounded solution f to $f'(x)(-x^2) = f(x)$, $x \geq 0$, not an eigenfunction due to this unboundedness.

As more use is made of the setting of this note, it is expected that the consequent experience will continue to add to the lore of interpreting computational results.

5. Examples for pairs of equations

In this section we provide several examples of systems, whereby the equation we need to solve is a partial differential equation.

Example 4

A first example of two equations is the decoupled system:

$$u(0) = x \geq 0, \qquad u' = u^2, \qquad\qquad v(0) = y \geq 0, \qquad v' = v^2.$$

The Lie generator for next two figures is given by A based on

$$(Af)(x, y) = f_1(x, y)x^2 + f_2(x, y)y^2, \qquad x \geq 0, \quad y \geq 0, \quad f\colon [0, \infty)^2 \to \mathbb{R}.$$

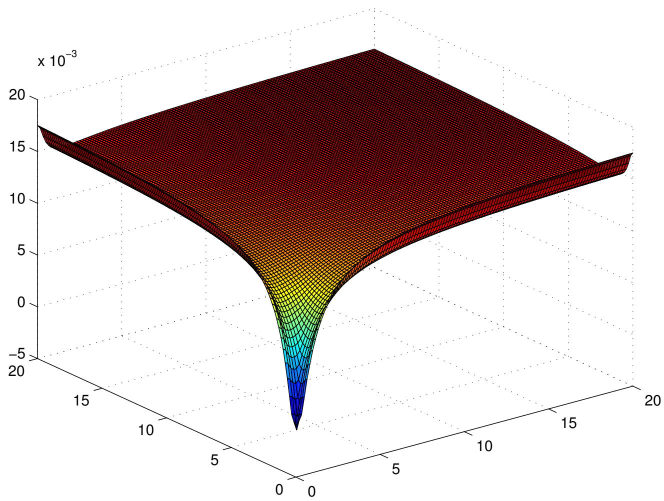

Figure 4. Lie generator eigenfunction for $u' = u^2$, $v' = v^2$

For this case, solving separately the two above equations, one may see that

$$m(x, y) = \min\left(\frac{1}{x}, \frac{1}{y}\right), \qquad x, y \geq 0.$$

The solution depicted in Figure 4 is in good agreement with this choice of m, but the figure itself is not precisely f, where

$$f(x,y) = \exp(-m(x,y)), \qquad x,y \geq 0.$$

A different initial estimate results in the different eigenfunction depicted in Firgure 5. In light of Theorem 3.1, any acceptable eigenfunction is obtained from f by multiplying f by appropriate constants *along trajectories of the underlying semigroup* T, subject only to the requirements that the resulting function is bounded, non-zero and continuous.

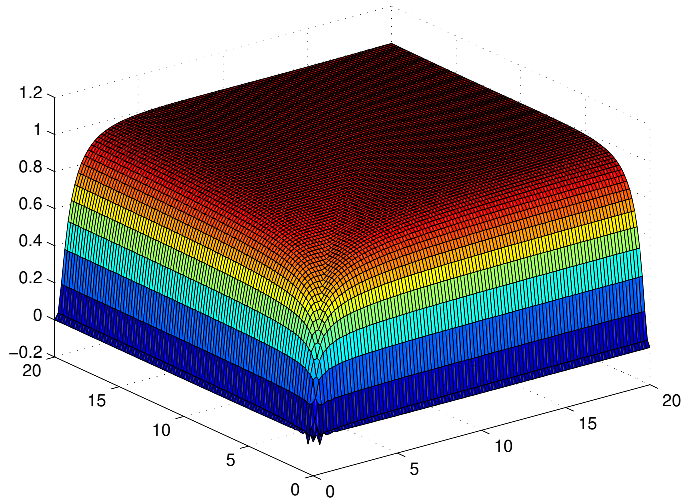

Figure 5. Lie generator eigenfunction for $u' = u^2$, $v' = v^2$, using a different initial estimate than in Figure 4.

Solutions equal or very close to those depicted in Figures 4 and 5 were again computed independently using the two different algorithms described in Section 6. In the first case, the second (direct) method enforced $f(x,y) = 1$ along the outer edges corresponding to $x = 20$ and $y = 20$. Again, that eigenfunction differs by a multiplicative constant from the steepest descent solution visualized in Figure 4. In the second case, the process of obtaining a solution via the second method was a bit strange. We enforced $f(x,y) = 1$ along the inner edges corresponding to $x = 0$ and $y = 0$. The resulting solution had a huge amplitude, and when normalized, gave a solution visually indistinguishable (up to a multiplicative constant) from the steepest descent solution found in Figure 5, where it appears that the eigenfunction is identically zero along the inner two edges.

Example 5

A second two equation example, with a solution represented by Figure 6, comes from another decoupled system:

$$u(0) = x \geq 0, \qquad u' = u^2, \qquad\qquad v(0) = y \geq 0, \qquad v' = -v^2.$$

The Lie generator for this problem is given by A based on

$$(Af)(x,y) = f_1(x,y)x^2 + f_2(x,y)(-y^2), \qquad x \geq 0, \quad y \geq 0, \quad f\colon [0,\infty)^2 \to \mathbb{R}.$$

For this case, solving separately the two above equations, one may see that

$$m(x,y) = \frac{1}{x}, \qquad x,y \geq 0.$$

Figure 6 is in good agreement with this choice of m:

$$f(x,y) = \exp(-m(x,y)), \qquad x,y \geq 0.$$

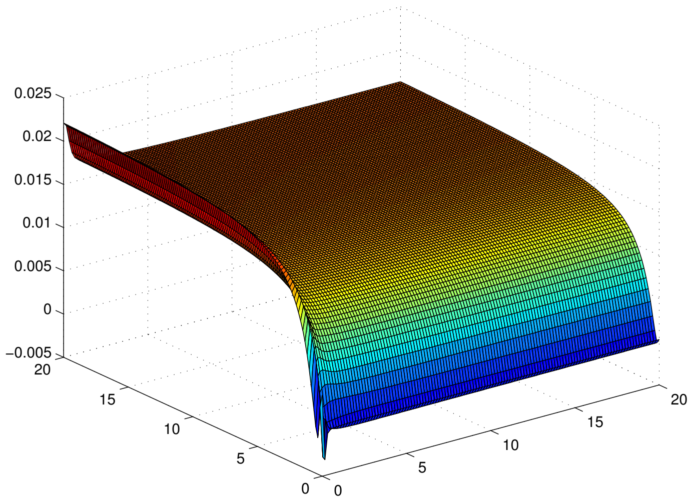

Figure 6. Lie generator eigenfunction for $u' = u^2$, $v' = -v^2$

Example 6

A third two equation example (Figure 7) is given by the coupled system

$$u(0) = x \geq 0, \qquad u' = v^2, \qquad\qquad v(0) = y \geq 0, \qquad v' = u^2.$$

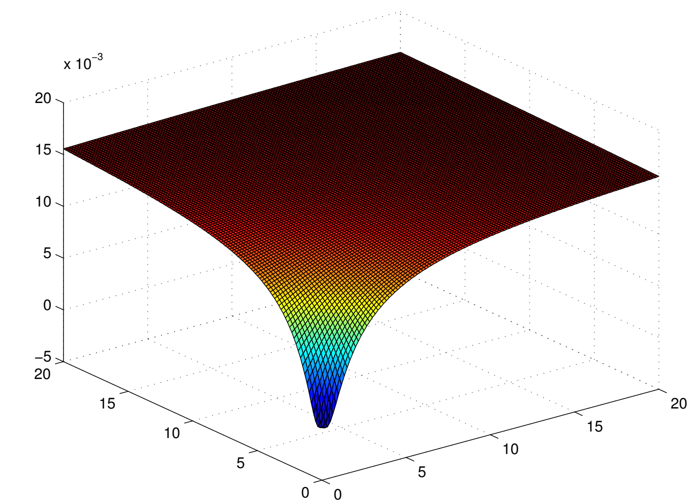

Figure 7. Lie generator eigenfunction for $u' = v^2$, $v' = u^2$

The Lie generator for this problem is given by A based on

$$(Af)(x,y) = f_1(x,y)y^2 + f_2(x,y)x^2, \qquad x \geq 0, \quad y \geq 0, \quad f\colon [0,\infty)^2 \to \mathbb{R}.$$

We can not offer an explicit expression for the associated function m, but note that some elementary calculations show that for $x, y > 0$, the trajectory of the underlying semigroup T starting at (x, y) ends in finite time. Hence this semigroup is indeed local. By Theorem 2.5, there is such a function m, however. Actually this case is more typical of intended applications.

5.1. Comparisons of numerical and theoretical eigenfunctions

We can make a check that the numerical solutions in our examples are in reasonable agreement with the theory. In the example depicted in Figure 4, we observe that the system has a trajectory following the diagonal. Along this trajectory, we can compute that it takes time $t = 1/2$ to proceed from $(u, v) = (1, 1)$ to $(u, v) = (2, 2)$, and then verify that equation $f(1, 1)e^{1/2} - f(2, 2) = 0$ is closely satisfied and converging as the number of gridpoints increases. In the related case depicted in Figure 5 (same differential equation, different initial guess/boundary condition), we chose a different trajectory for our test. We can see that it again takes time $t = 1/2$ to proceed from $(u, v) = (1, 1/2)$ to $(u, v) = (2, 1)$, and that $f(1, 1/2)e^{1/2} - f(2, 1) = 0$ is again nearly satisfied. For example, using $n = 60$ divisions leading to 3721 grid points, we obtained nearly four decimal places of accuracy in this last equation.

It is nice if for a given semigroup T, a stopping time function m is known explicitly so that all the facts about local versus global existence are already known, but this cannot generally be expected.

A main problem connected with the present work is the interpretation of graphical results to make accurate deduction of the global or local existence of an underlying semigroup when the function m is not known.

6. Description of some codes

We generated the example results from the previous two sections using two methods, namely Sobolev steepest descent and a direct, non-iterative linear solver. In this section we give a description of each algorithm.

Sobolev gradient steepest descent

In this subsection we provide some details about applying a descent method for finding approximate solutions to (7) assuming the underlying space is a Hilbert space. The interested reader should consult [5] for more details concerning the general technique. For a given semigroup T with Lie generator $\overline{A}$, we seek to determine whether or not $\overline{A}$ has eigenvalue one (we could just as well picked any other positive number to test). We take an appropriate discretization A of $\overline{A}$ on some grid. Pick a vector space H of appropriate dimension and a nonzero vector $y \in H$. Seek to determine the closest vector z to y so that z satisfies

$$(I - A)z = 0.$$

Choose

$$\phi(u) = \frac{1}{2}\,\|(I - A)u\|^2, \qquad u \in H. \tag{10}$$

The customary gradient $\nabla\phi$ is given by

$$(\nabla\phi)(u) = (I - A)^T (I - A)u. \tag{11}$$

That this gradient may not be a good choice for steepest descent is suggested by the fact that $\overline{A}$ is an unbounded differential operator and hence everywhere discontinuous and only densely defined. Especially for a fine enough grid to permit reasonable fidelity to the function space problem, the operator inherits poor numerical properties from $\overline{A}$ (see [5] for a discussion, especially Chapter 2 of that work). To remedy this, we take a gradient with respect to a metric on H which yields a preconditioned version of the customary gradient. The second gradient is effectively the weighted graph metric for A, specifically

$$\|u\|_S^2 = \|u\|_H^2 + \|wA\|^2, \tag{12}$$

where the second norm is a Euclidian one and w is an appropriate diagonal weight matrix depending on B, assuming that B is the conventional generator of the underlying semigroup T. The gradient used in our calculations is $\nabla_S\phi$ so that

$$(\phi'(u))h = \langle h, (\nabla_S\phi)(u)\rangle_S, \qquad u, h \in H.$$

This gradient is a good approximation to the associated gradient in the function space $\mathrm{CB}(X)$. It is a continuous, everywhere defined gradient, in distinction to what one gets in attempting construction of an ordinary gradient in this setting. Our gradient picks out, in an orderly way a nearest zero of $I - A$ to a selected initial approximation.

Thus, we seek knowledge of the global versus local existence of solutions to systems of the form

$$U' = B(U), \qquad U\colon [0,\infty) \to \mathbb{R}^d, \quad B\colon \mathbb{R}^d \to \mathbb{R}^d,$$

by approximating solutions $f\colon [0,X]^d \to \mathbb{R}$ to the associated eigenvalue problem

$$\left(\sum_{i=1}^{d} B_i D_i\right) f = f,$$

where B_i is the i^{th} component function of B, D_i is the first derivative differential operator with respect to the i^{th} variable, and X is a suitably large positive real number. The steepest descent method for obtaining these approximations is presented in Algorithm 6.1.

Algorithm 6.1 (steepest descent).

Let $n \in \mathbb{N}$ be the number of divisions of $[0,X]$, set $N = (n+1)^d$, and take $x = \{x_1, \ldots, x_N\}$ be regularly spaced gridpoints in $[0,X]^d$.

I. Initialize:

Compute first difference matrices $\mathbf{D}_i \in M_{n^d \times N}$, with respect to the i^{th} coordinate, $i \in \{1, \ldots, d\}$.

Compute matrix $\mathbf{I}_n^* \in M_{n^d \times N}$ (non-square averaging "identity" at cell centers).

Compute $\mathbf{B}^{(i)} = \operatorname{diag}(B_i(x_j)) \in M_{N \times N}$.

Compute $\mathbf{G} = -\mathbf{I}_n^* + \sum_{i=1}^{d} \mathbf{B}^{(i)}\mathbf{D}_i \in M_{n^d \times N}$.

Set $\mathbf{G}^* = \mathbf{G}^T\mathbf{G} \in M_{N \times N}$.

Compute smoother $\mathbf{Q} = \mathbf{I}_N + \sum_{i=1}^{d} (\mathbf{B}^{(i)}\mathbf{D}_i)^T(\mathbf{B}^{(i)}\mathbf{D}_i) \in M_{N \times N}$.

With $f_0\colon [0,X]^d \to \mathbb{R}$ an initial guess function, set $v_0 = (f_0(x_j)) \in \mathbb{R}^N$.

Set counter $k = 0$.

II. Iterate Until Convergence:

Increment k.

Compute $v_k^* = \mathbf{G}^* v_k$.

Solve $\mathbf{Q}\chi_k = v_k^*$ for Sobolev gradient $\chi_k \in \mathbb{R}^N$.

Compute optimal stepsize $\delta_k = (v_k^* \cdot \chi_k)/|\mathbf{G}\chi_k|^2$.

Step $v_{k+1} = v_k - \delta_k \chi_k$.

Break if $|\delta_k \chi_k| <$ tolerance.

Notes on code: The inverse of what is called 'smoother' this psuedo-code is a preconditioner. At first a tolerance is specified. The computation is stopped when residual error is below this tolerance. This is conventional discrete steepest descent except that the preconditioner comes from Sobolev gradient theory [5]. We start with the least squares objective function (10) and derive its conventional gradient in (11). We multiply the conventional gradient by the preconditioner derived from the Sobolev metric (12), yielding what we call our Sobolev gradient. The optimal step size is, given our

Sobolev, entirely conventional. This gradient, multiplied by the calculated step size is then subtracted from the previous approximation, yielding the next approximation.

Observe that there are several different schemes for creating the difference matrices $\mathbf{D}_i$, even of slightly varying dimensions. There would be different ways to evaluate B to create the matrices $\mathbf{B}^{(i)}$ as well. More significantly mathematically, there are different smoothers $\mathbf{Q}$ that can be used as well. The optimal choice for a smoother is not well understood. We have tried $\mathbf{Q} = \mathbf{I}_N + \sum_{i=1}^{d} \mathbf{D}_i^T \mathbf{D}_i$, $\mathbf{Q} = \sum_{i=1}^{d} \mathbf{D}_i^T \mathbf{D}_i$, and $\mathbf{Q} = \sum_{i=1}^{d} (\mathbf{B}^{(i)}\mathbf{D}_i)^T (\mathbf{B}^{(i)}\mathbf{D}_i)$, and found cases where one smoother significantly outperforms the others.

Note that the smoother indicated above varies from step to step, giving a variable metric Sobolev descent method. The choice of weights using B_i, $i = 1, \dots N$, has the following effect: Near critical points, that is, places where B_i, $i = 1, \dots N$, are all nearly zero, the smoother tends to allow great freedom in the descent process to alter the previous estimate. The resolution of an estimate to an eigenfunction near a critical point is potentially difficult, but freedom allowed by our choice of weights benefits such calculations. Refer to Figure 2 to see an accurate resolution between the critical points 0 and 1. Reference [5] has a discussion of gradients calculated with weighted Sobolev gradients.

Direct method

In this subsection a variant of the above is given for cases in which zeros of a conventional generator is known. It has been observed that zeros of a conventional generator can be related to points of particular interest in eigenfunctions of the corresponding Lie generator.

To utilize knowledge of zeros of a conventional generator B, we offer the following: The approach of numerically approximating by $v \in \mathbb{R}^N$ an eigenfunction of A corresponding to an eigenvalue one supplements the n^d equations given by

$$\left(-\mathbf{I}_n^* + \sum_{i=1}^{d} \mathbf{B}^{(i)} \mathbf{D}_i \right) v = 0$$

with $(n+1)^d - n^d$ more constraints, and then rely on existing linear solvers to finish the job. This idea has some strong and interesting advantages, as well as some puzzling and distinct disadvantages. The general idea is to specify values of f (approximated by $v \in \mathbb{R}^N$) on a codimension-one set $S \subset [0, X]^d$ that is transverse to trajectories of the system. Then, the values of f would be determined all along the trajectories, which cover all or part of $[0, X]^d$. If $x \in S$, and u is the solution to $u' = B(u)$, $u(0) = x$, then the value of f on the whole trajectory is given by

$$f(u(t, x)) = f(x) e^t, \qquad 0 < t < m(x).$$

In practice in using this second method, it might be necessary to overdetermine the system by specifying a value of zero for f at singular points or along singular sets in addition to specifying f to be nonzero somewhere. When this is done, the resulting system has more equations than unknowns, and the '\' operator in *Matlab* automatically finds a least squares solution.

We have had success with this second approach as long as we had some knowledge of where the B vanishes and where it was sensible to enforce a non-zero value for the solution. When it works, it is certainly much, much faster than the iterative approach. This option might be very important if one plans to attack a huge system, even on a massively parallel computational platform.

7. Closing comments

For the first item in Introduction, something besides finite differences is almost certainly indicated. A substantially smaller computational space might be used with a good choice of bases functions in a finite element or wavelet setting. There is a great deal known about use of such bases that can be considered for use on present problems.

In regard to the second item, once dimensions pass three, graphical representation of solutions becomes challenging. Fortunately, in the computational community, there are many years of experience by some very creative people in dealing with such problems. As one proceeds to larger systems, such past examples of creativity needs to be tapped.

In Section 4, there are some simple problems for which closed form solutions exist. These can be compared to corresponding numerical computations. Such examples may lead to theoretical results by means of inequalities which reduce large scale problems to ones in which closed form or other tractable, non-computational methods prevail.

An obstacle to efficient computation on current massively parallel computers is the relative slowness of inter-processor communications. Fortunately, there seems to be 'blowing in the wind' a new generation of machines with greatly improved communication. With such machines substantially larger eigenvalue problems might be made.

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