

Sensitivity Analysis and Computational Uncertainty with Applications to Control of Nonlinear Parabolic Partial Differential Equations

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Abstract—In this paper we illustrate how sensitivities can be used to provide a practical precursor to dynamic transitions and numerical uncertainty in parameterized nonlinear parabolic partial differential equations. In particular, we focus on reaction-diffusion equations and provide numerical examples to illustrate the ideas and to suggest how one might use sensitivities to address computational uncertainty.

I. INTRODUCTION

It is well known that the long time behavior of a nonlinear dynamical system may not be captured even by convergent approximating methods and additional requirements must be placed on the scheme to ensure that the discretized equations capture the correct asymptotic behavior. This issue is particularly important when one is forced to use numerical methods to evaluate the asymptotic behavior of a closed-loop system when the model is defined by a nonlinear partial differential equation (PDE). In addition, using feedback to eliminate or delay transition in fluid flows often requires some type of mechanism to predict that a transition is about to occur. The recent papers [3], [4], [5], [21] and [22] provide considerable evidence that, for certain nonlinear systems that occur in fluid flows, sensitivity analysis can be used to indicate a transition is about to occur. In [4] and [5] it was shown that this information can be used to determine when to turn on a controller to prevent transition. In this paper we illustrate that similar sensitivity tools can also be used to provide insight into the asymptotic behavior of the closed-loop system. In particular, we show that time varying sensitivities can be used to determine when a numerical simulation is correctly predicting the longtime behavior of the response. In the cases considered here, the trigger of a transition can be a known parameter (wall roughness, etc.) or an un-modeled uncertainty in the problem data. This includes uncertainty in parameters, initial data, boundary conditions and forcing terms. These uncertainties in the problem data lead to uncertainty in the computed results and should be considered as part of a verification step. In addition, although we do not address this issue here, it has recently been observed that finite precision arithmetic and sensitivity to parameter uncertainty can lead to orders of magnitude errors in simulations of simple nonlinear convection-diffusion equations (see [1] and [3]). In this paper we focus on nonlinear reaction-diffusion equations to illustrate the problem and

method. However, we first present a simple ODE example to illustrate some of the basic ideas.

A. A Finite Dimensional Example

We consider a 3D system that is typical of those found in the papers [4], [5], [20], [21], [25], [26] and [27]. However, we focus on the role that small constant disturbances play in transition and illustrate how feedback can delay or eliminate transition in these cases. The system is governed by three ordinary differential equations and has the form

$$\dot{x}(t) = A(R)x(t) + \|x(t)\| Sx(t) + Bu(t) + Dq, \quad (1)$$

where $A(R) = [\frac{1}{R}A_0 + \mathcal{R}]$, $A_0 < 0$ is diagonal, \mathcal{R} is an upper triangular 3×3 matrix with 1's in the (1, 2) and (2, 3) positions and $S = -S^*$ is skew-adjoint. In particular, this 3 dimensional system is defined by

$$A_0 = \begin{bmatrix} -\alpha & 0 & 0 \\ 0 & -\beta & 0 \\ 0 & 0 & -\gamma \end{bmatrix}, \quad (2)$$

$$\mathcal{R} = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix}, \quad (3)$$

$$S = \begin{bmatrix} 0 & -b_1 & -b_2 \\ b_1 & 0 & b_3 \\ b_2 & -b_3 & 0 \end{bmatrix} \quad (4)$$

and

$$B = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}, D = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}, \quad (5)$$

where all constants are positive. Here, q is considered a “small” constant (un-modeled) disturbance. For the runs here we set $\alpha = 0.5$, $\beta = 0.75$, $\gamma = 1.0$, $b_1 = 1.0$, $b_2 = 0.5$ and $b_3 = 0.25$. The linear operator $A(R)$ is stable for all $R > 0$ and for the no disturbance case (i.e. when $q = 0$) the dynamical system is also dissipative. In particular, the nonlinear system (1)-(5) has a compact global attractor. The problem is sensitive to the parameter q and this sensitivity plays an important role in the transition process.

Let

$$s(t) \triangleq \frac{\partial x(t, q)}{\partial q} \Big|_{q=0} = \frac{\partial x(t, 0)}{\partial q} \quad (6)$$

denote the sensitivity of the solution $x(t) = x(t, q)$ at $q = 0$. It follows that the sensitivity $s(t)$ satisfies the linear differential equation

$$\dot{s}(t) = A(R)s(t) + \mathbf{F}(x(t))s(t) + D, \quad s(0) = 0, \quad (7)$$

where

$$\mathbf{F}(x) = \begin{cases} \|x\| S + Sxx^T / \|x\|, & x \neq 0 \\ 0, & x = 0 \end{cases}.$$

Consider the case where $x_0 = [9, 9, 9]^T \times 10^{-6}$ and $q = 5 \times 10^{-8}$. Figure 1 below contains the plots of the norms of solution $x(t, q)$ and the sensitivity $s(t)$ (top plot) for this system. Observe that the solution does not “transition” to the (chaotic) attractor until $t = 175$. However, in the neighborhood of $t = 50$ the sensitivity $s(t)$ satisfies $\|s(t)\| > 10^3$ while the norm of the solution $\|x(t)\|$ remains less than 10^{-6} well beyond $t = 150$. The vertical red line at $t = 50$ provides a precursor to the upcoming transition long before the transition is observable in the state. This precursor was used by Singler to determine when to switch on a capturing feedback controller which is then able to prevent the transition (see [20]).

Note: In general it is not always clear which parameters are most likely to provide the type of sensitivities and predictive information observed above. In this particular example we have a good understanding of what causes this type of “transition” because this model closely mimics what is observed in channel flow instabilities (see [5], [20] and [27]). The transition occurs because the initial data moves outside a basin of attraction as the parameter q varies. It is worth noting that the parameter in this case can represent un-modeled dynamics and disturbances, but some analysis of the dynamics is required to determine which parameters are important. This is not a new issue since one is always faced with the problem of determining “good” parameters to conduct bifurcation analysis and this is a similar problem. However, more research needs to be done to help provide a better understanding of this issue.

In the next section we use a similar technique to investigate the numerical simulation of the closed-loop behavior of a nonlinear parabolic PDE control system. However, in the PDE case the “sensitive” parameter is in the boundary condition which is typical in parabolic diffusion-convection-reaction equations (see [1], [3], [4], [5], [13], [20] and [21]).

II. THE CHAFFEE-INFANTE EQUATION

We consider a particular reaction-diffusion equation first studied by Chaffee and Infante in [9] and [10]. This model is a well understood dissipative dynamical system with a global attractor consisting of a finite number of fixed points and the corresponding unstable manifolds (see pages 301 - 306 in [18] for details). In particular, we focus on the partial differential equation defined on the interval $0 < x < \pi$ by

$$z_t(t, x) = z_{xx}(t, x) + \lambda(z(t, x) - [z(t, x)]^3), \quad (8)$$

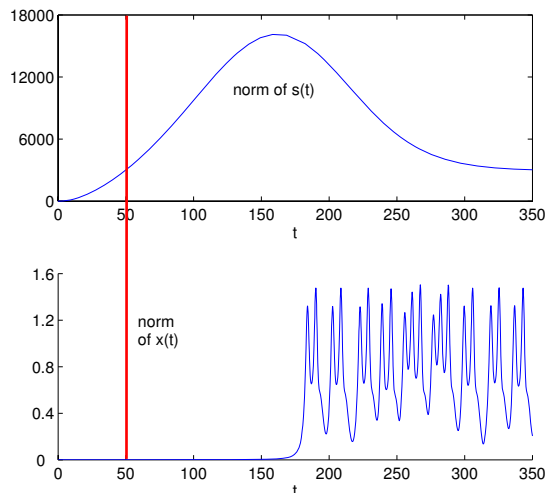


Fig. 1. Norm of $x(t)$ and $s(t)$

with initial condition

$$z(0, x) = \phi(x), \quad (9)$$

and Dirichlet boundary conditions

$$z(t, 0) = 0 = z(t, \pi). \quad (10)$$

Here $\lambda > 1$ and in this setting it is helpful to think of (8)-(10) as a closed-loop system that we wish to simulate. It is sufficient to consider the case where $\lambda = 4.1$ so that the following result holds (see page 303 in [18]).

Theorem 1 *If $\lambda = 4.1$, then the system (8)-(10) has five fixed points $\phi_0(\cdot) \equiv 0$, $\phi_1^+(\cdot)$, $\phi_1^-(\cdot)$, $\phi_2^+(\cdot)$ and $\phi_2^-(\cdot)$ in $L^2(0, \pi)$. The fixed points $\phi_0(\cdot) \equiv 0$, $\phi_2^+(\cdot)$ and $\phi_2^-(\cdot)$ are unstable and the attractor consists of the unstable manifolds for these fixed points along with the stable fixed points $\phi_1^+(\cdot)$ and $\phi_1^-(\cdot)$.*

Figure 2 provides a schematic picture of the global attractor. However, for certain initial conditions trajectories are pushed rapidly towards the unstable zero fixed point before “transitioning” to one of the stable fixed points $\phi_1^+(\cdot)$ or $\phi_1^-(\cdot)$. This is similar to the previous ODE example except for the fact that this system is not chaotic. However, if one uses standard simulation schemes to investigate the dynamic behavior of this system it is easy to obtain misleading results.

Consider the case where the initial function is given by $\phi(x) = 1.5 \sin(3x)$. Using the MatlabTM routine *PDEPE* to simulate (8)-(10) on the interval $0 < t < 8$, yields the solution shown in Figure 3.

It appears that by $t = 2$ the solution has “converged” to the zero steady state solution. However, since the theorem above tells us that this fixed point is unstable we know that this is unlikely. Indeed, if one continues to run the simulation to $t = 16$ we observe that the solution actually “transitions” to the stable fixed point $\phi_1^-(\cdot)$. This is shown in Figure 4 below.

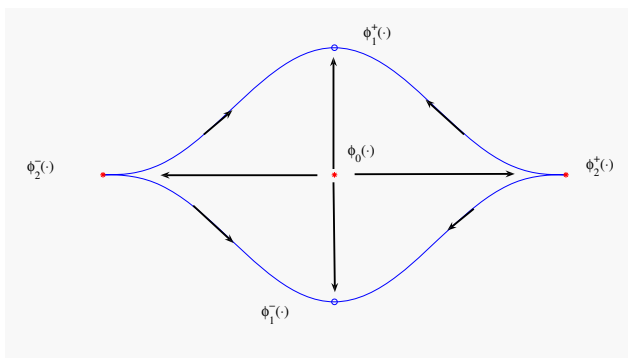


Fig. 2. Global Attractor for the Chaffee-Infante Equation

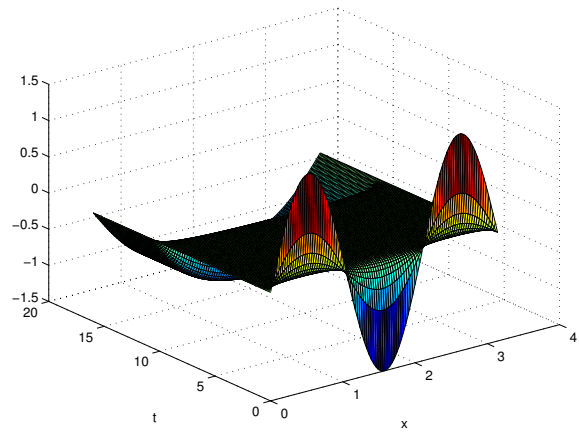


Fig. 4. $z(t, x)$ on $0 < t < 16$

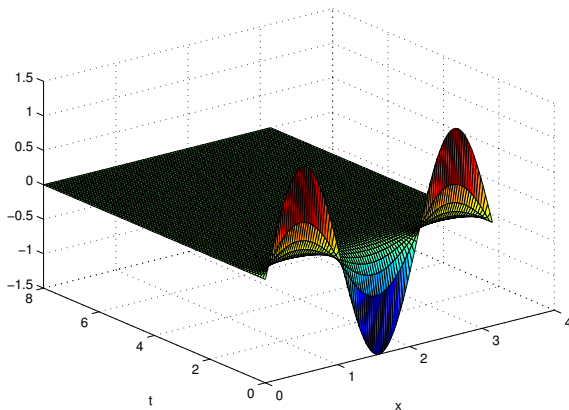


Fig. 3. $z(t, x)$ on $0 < t < 8$

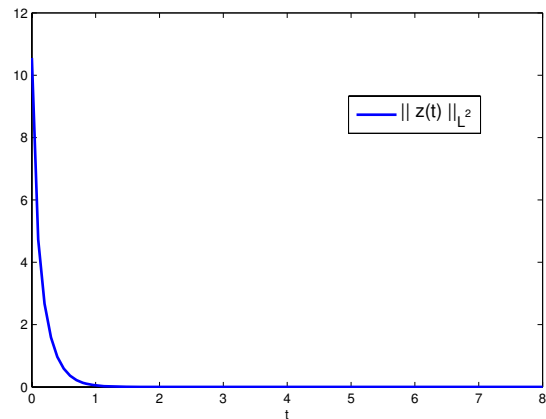


Fig. 5. L^2 norm of $z(t, \cdot)$ on $0 < t < 8$

This is also clearly demonstrated in Figure 5 and Figure 6 which contain the plots of the L^2 norms of the solution on the intervals $[0, 8]$ and $[0, 16]$, respectively.

In more complex problems one does not always have the type of qualitative information available for the Chaffee-Infante equation. As illustrated by this example, it is not always clear when a particular numerical solution is producing the proper asymptotic results. Even if the algorithm does **eventually** capture the correct limiting behavior, it is not obvious how long one must run the simulation to see this result. Therefore, it is important to devise numerical methods that can help predict when a simulation has or has not “converged” to the correct asymptotic behavior. Although this is a difficult problem for general systems, in certain cases sensitivity analysis can be helpful in dealing with this issue.

A. Boundary Sensitivity for the Chaffee-Infante Equation

Here we consider the sensitivity of the Chaffee-Infante equation with respect to the boundary condition. In particular, we replace the boundary condition (10) with the nonhomogeneous boundary condition

$$z(t, 0) = q = z(t, \pi), \tag{11}$$

where q is a “small” number. It is well known that reaction-convection-diffusion equations are highly sensitive

to changes in the boundary conditions (see [1], [2], [3], [5], [12], [13], [16] and [17]). Therefore, we focus on this sensitivity and define $s(t, x)$ by

$$s(t, x) \triangleq \frac{\partial z(t, x, q)}{\partial q} \Big|_{q=0} = \frac{\partial z(t, x, 0)}{\partial q},$$

where $z(t, x, q)$ is the solution to the Chaffee-Infante equation (8) with initial data (9) and nonhomogeneous boundary condition (11).

The sensitivity function $s(t, x)$ satisfies the linear boundary value problem on the interval $0 < x < \pi$ given by

$$s_t(t, x) = s_{xx}(t, x) + \lambda(s(t, x) - 3[z(t, x)]^2 s(t, x)), \tag{12}$$

with initial condition

$$s(0, x) = 0, \quad 0 < x < \pi, \tag{13}$$

and boundary conditions

$$s(t, 0) = s(t, \pi) = 1, \quad t > 0. \tag{14}$$

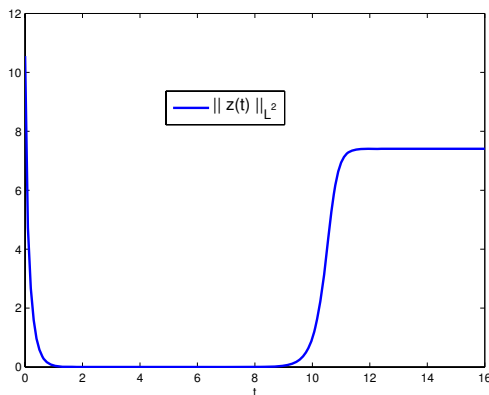


Fig. 6. L^2 norm of $z(t, \cdot)$ on $0 < t < 16$

This time varying sensitivity provides considerable insight into the long term behavior of the solution to the Chaffee-Infante equation. First note that if the solution $z(t, x) \rightarrow \hat{\phi}(x)$ and $\hat{\phi}(x)$ is a stable equilibrium state, then one would expect that the the sensitivity $s(t, x)$ would approach a steady state $\hat{s}(x)$ satisfying

$$0 = s''(x) + \lambda(s(x) - 3[\hat{\phi}(x)]^2 s(x)), \quad 0 < x < \pi,$$

with boundary conditions

$$s(0) = s(\pi) = 1.$$

In particular, one would have $\lim_{t \rightarrow +\infty} \|s(t, \cdot)\|_{L^2} \rightarrow c$ where c is a constant.

Figure 7 and Figure 8 below illustrate this point. Although the solution $z(t, x)$ shown in Figure 3 above appears to have “converged” to the fixed point $\phi_0(x) = 0$ by $t = 2$, and seemingly remains at zero for $2 < t < 8$, the sensitivity $s(t, x)$ plotted in Figure 7 is growing at an exponential rate on the entire interval $[0, 8]$. Moreover, when the solution transitions to the stable fixed point $\phi_1^-(\cdot)$ at $t \approx 9$ the sensitivity is maximized and then converges to a (small) steady state as expected. If one compares Figure (8) with Figure 6 above, then it is clear that this sensitivity provides insight into the transition.

The most important observation about the numerical results presented here is that even on the “short” time interval $0 < t < 8$, when the numerical solution $z(t, x)$ appears to have stabilized at zero, the sensitivity indicates otherwise. In particular, in Figure 9 and Figure 10 below we see the exponential growth of $s(t, x)$ on $[0, 8]$ and at $t \approx 7$ the norm of the sensitivity is of the order 10^9 . Thus, even on the short time interval $[0, 8]$ the sensitivity provides a clear indication that the solution $z(t, x)$ has not stabilized at a fixed point. As noted above, this insight can be used to turn on feedback controllers to prevent transition. Perhaps even more importantly, sensitivity analysis of this type can be used to help evaluate numerical simulations in problems where little is known about the actual asymptotic behavior of the system. We also note that the transition and the time to transition

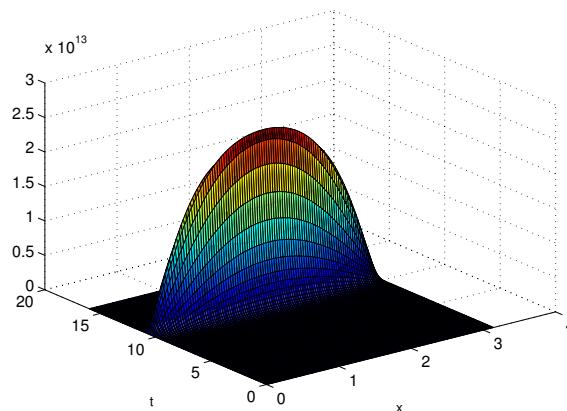


Fig. 7. $s(t, x)$ on $0 < t < 16$

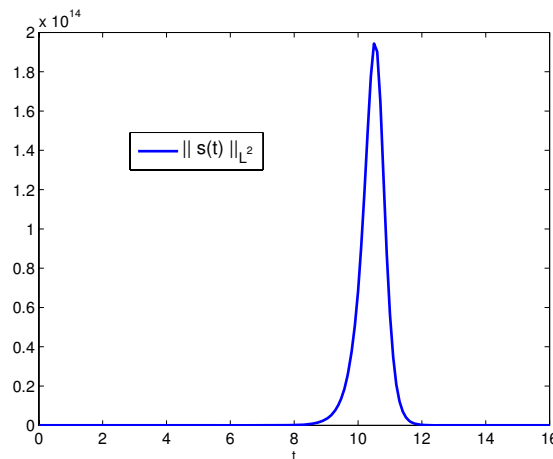
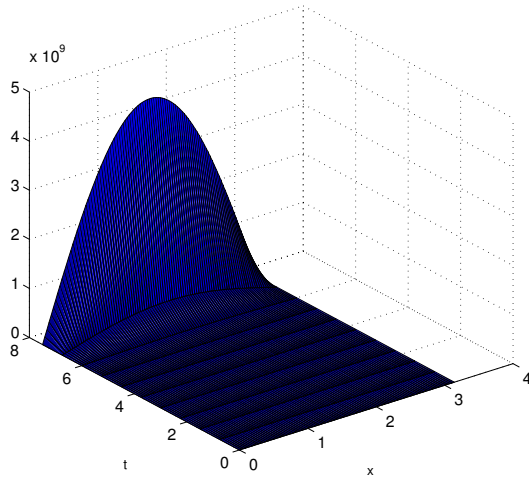
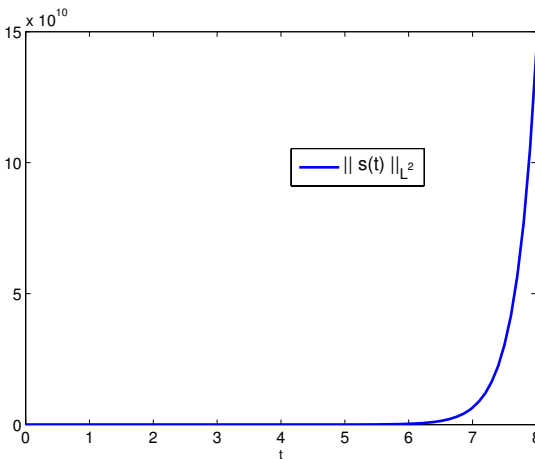


Fig. 8. L^2 norm of $s(t, \cdot)$ on $0 < t < 16$

is not a function of the particular spatial grid. These are properties of the partial differential equation. However, in order to check this we ran the problem on various meshes and observed the same quantitative behavior.

III. CONCLUSIONS AND FUTURE WORK

In this short paper we presented two examples to illustrate how time varying sensitivity analysis can be used for control and provide insight into the validation of numerical simulations in nonlinear systems. These ideas have also been applied to a wide variety of reaction-convection-diffusion systems and a complete paper will appear in the future. We note that many convection-diffusion problems such as Burgers’ equation, show extreme sensitivity to boundary perturbations and sensitivity analysis for these systems has provided amazing insight into the asymptotic behavior of numerical solutions (see [1], [2], [3], [5], [6], [7], [8], [12], [13], [14], [15], [11], [16], [17], [20], [21] and [22]). Problems of this type are infinitely sensitive to small parameter changes and can have a dramatic impact on the convergence

Fig. 9. $s(t, x)$ on $0 < t < 8$ Fig. 10. L^2 norm of $s(t, \cdot)$ on $0 < t < 8$

of optimal control and design algorithms.

We note that although the numerical results here provide considerable evidence that time varying sensitivities can play an important role in control design and analysis, considerable work needs to be done to place these ideas on a mathematically rigorous foundation. We have some theoretical results for parabolic dissipative systems similar to the Chafee-Infante equations. However, much work remains to be done to place these ideas on a sound theoretical basis. Finally, it is clear that in order to implement some of these ideas one needs to have some indication of which parameters (modeled or un-modeled) are important to use in the sensitivity analysis. We are currently looking into using Fisher information theory as a mechanism to identify these crucial parameters.

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