Journal of Computational Physics 354 (2018) 447–475

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Multiple shooting shadowing for sensitivity analysis of chaotic dynamical systems

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ARTICLE INFO

Article history:
Received 6 October 2016
Received in revised form 7 April 2017
Accepted 20 October 2017

Keywords:
Sensitivity analysis
Adjoint
Chaos
Shadowing

ABSTRACT

Sensitivity analysis methods are important tools for research and design with simulations. Many important simulations exhibit chaotic dynamics, including scale-resolving turbulent fluid flow simulations. Unfortunately, conventional sensitivity analysis methods are unable to compute useful gradient information for long-time-averaged quantities in chaotic dynamical systems. Sensitivity analysis with least squares shadowing (LSS) can compute useful gradient information for a number of chaotic systems, including simulations of chaotic vortex shedding and homogeneous isotropic turbulence. However, this gradient information comes at a very high computational cost. This paper presents multiple shooting shadowing (MSS), a more computationally efficient shadowing approach than the original LSS approach. Through an analysis of the convergence rate of MSS, it is shown that MSS can have lower memory usage and run time than LSS.

1. Introduction

Computational methods for sensitivity analysis are invaluable tools for research and design in many engineering and scientific fields. These methods compute derivatives of outputs with respect to inputs in computer simulations. In applications with large amounts of parameters and only a few important outputs, adjoint-based sensitivity analysis is especially efficient [1]. In aircraft design, for example, the number of geometric parameters that define the outer mold line is typically very large, but engineers may only be interested in a few outputs, such as the lift-to-drag ratio. As a result, the adjoint method of sensitivity analysis has proven to be very successful for aircraft design with gradient-based optimization [2–4]. The adjoint method has also been an essential tool for adaptive grid methods for solving partial differential equations (PDE's) [5], error estimation [6], and flow control problems [7]. Finally, some techniques for uncertainty quantification can benefit immensely from sensitivity information [8,9].

Unfortunately, conventional sensitivity analysis methods, including the adjoint method, can break down when applied to chaotic systems. This occurs for sensitivities of long-time-averaged quantities of interest to design inputs. In this context "long-time" refers to time averaging horizons much larger than the physical time scales associated with the chaotic system being considered. This is problematic, as many key scientific and engineering quantities of interest in chaotic systems are long-time-averaged quantities, such as the time-averaged lift or drag coefficient of a flight vehicle in a high-lift configuration or the average heat transfer to a turbine blade.

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https://doi.org/10.1016/j.jcp.2017.10.032
0021-9991/

To carry out efficient design and analysis of chaotic systems and fluid flows, a new sensitivity analysis method is needed. One promising new approach is Least Squares Shadowing (LSS) [10–13]. The most common implementation of LSS in the literature is called transcription LSS. Transcription LSS involves solving a globally coupled space-time problem, which can be computationally intensive [10]. The study of LSS for chaotic vortex shedding by Blonigan et al. [14] shows that transcription LSS is very costly in memory usage and operation count for a relatively small simulation. Similar issues with computational cost were encountered in a study of transcription LSS for a direct numerical simulation (DNS) of homogeneous isotropic turbulence [15].

This paper presents an alternative way to pose the minimization statement to compute the shadowing direction or the adjoint shadowing direction. This formulation, multiple shooting shadowing (MSS), addresses the high computational cost of LSS. It is shown that MSS can reduce the memory requirements and the run time required to compute sensitivities of chaotic systems, making LSS sensitivity analysis more tractable for large chaotic dynamical systems such as turbulent fluid flow simulations. The convergence properties of MSS are presented in great detail, along with some approaches to control the convergence rate of MSS.

This paper is organized as follows: section 2 discusses how conventional sensitivity analysis approaches break down for chaotic systems and the past work done to avoid this break down. Section 3 provides an overview of the formulation of transcription LSS. Section 4 introduces the MSS minimization statement and section 5 discusses how MSS can be implemented. Next, section 6 shows MSS results for a chaotic dynamical system and a chaotic partial differential equation (PDE). Section 7 discusses the convergence properties of MSS. Finally, section 8 summarizes this thesis and discusses some future research directions.

2. Sensitivity analysis of a chaotic dynamical system

The first question to be asked is if sensitivities are in fact well defined for chaotic systems. It is believed that many, but not every, chaotic system has differentiable time averaged quantities $\overline{J}$. Specifically, chaotic systems classified as uniformly hyperbolic or quasi-hyperbolic have differentiable time averaged quantities, but non-hyperbolic systems do not. These classes are discussed in greater detail below.

A uniformly hyperbolic attractor is a strange attractor with a tangent space that can be decomposed into stable, neutrally stable, and unstable subspaces at every point in phase space [16]. In other words, the Lyapunov covariant vectors make up a basis for phase space at all points on an attractor. Ruelle's linear response theorem states that hyperbolic attractors have mean quantities that respond differentiably to small perturbations to their parameters [17]. Therefore, sensitivities are well defined for chaotic systems with hyperbolic attractors. A well studied example of a hyperbolic attractor is the Plykin attractor [18]. The equations governing the Plykin attractor were designed to have hyperbolic properties, which are rare in practice.

Although uniformly hyperbolic attractors are rare, many important properties of hyperbolic systems, including Ruelle's linear response theorem, can also be shown to hold for the far more common non-uniformly hyperbolic or quasi-hyperbolic attractors [17,19,20]. One example of a quasi-hyperbolic attractor is the Lorenz attractor [21]. At the origin of phase space, the Lyapunov covariant vectors for the positive and negative exponent are parallel, so hyperbolicity does not apply. However, this point is an unstable saddle point and almost all phase space trajectories do not pass through it. Because of this the Lorenz attractor appears to have the properties of a hyperbolic attractor, most importantly differentiable mean quantities [22,10].

Other chaotic dynamical systems have non-hyperbolic attractors. In these non-hyperbolic systems the time averaged quantities are usually not differentiable or even continuous as the parameters vary. In fact, long-time-averages for non-hyperbolic systems may have nontrivial dependence on the initial condition (i.e. the system is not ergodic), which leads to time averaged quantities that are not well-defined.

Fortunately, Gallavotti and Cohen's chaotic hypothesis conjectures that larger systems behave more like hyperbolic systems than non-hyperbolic systems [23,24]. That is, larger systems should have differentiable infinite time-averaged quantities. Additionally, a study by Albers and Sprott found that larger chaotic systems tend to have smoothly varying topology changes in the attractor as system parameters are varying [25]. Long-time-averaged quantities do not necessarily vary smoothly across sudden topology changes like bifurcations. Therefore, the chaotic hypothesis and the work by Albers and Sprott suggest there are well defined sensitivities to be computed for a large range of chaotic systems, especially if these systems have a large number of degrees of freedom (DoF). This is encouraging considering the large numbers of DoF's in simulations such as those of chaotic and turbulent fluid flows.

Additionally, there is some evidence that the chaotic hypothesis applies to simulations of turbulent fluid flows. Grid convergence studies have been done in many cases to ensure that the discretization of the governing equations is sufficiently detailed. For example, Kim et al. used a direct numerical simulation (DNS) to compute turbulent statistics such as the mean velocity profile of a turbulent channel flow with a coarse and a fine spatial discretization [26] to check if their fine discretization was fine enough. The statistics were the same for the coarse and fine discretizations, which shows that long-time-averaged quantities of the DNS respond smoothly to perturbations in the spatial discretization, as predicted by the chaotic hypothesis. Similar results of grid convergence studies for other DNS and Large Eddy Simulation (LES) results [27,28] also support the chaotic hypothesis, making it very likely that sensitivities of long-time-averaged quantities are well defined for high-fidelity turbulent flow simulations.