SAND21XX-XXXXR
LDRD PROJECT NUMBER: 227154
LDRD PROJECT TITLE: Computational Response Theory for Dynamics
PROJECT TEAM MEMBERS: Andrew Steyer (PI)

ABSTRACT:

Quantifying the sensitivity - how a quantity of interest (QoI) varies with respect to a parameter – and response – the representation of a QoI as a function of a parameter - of a computer model of a parametric dynamical system is an important and challenging problem. Traditional methods fail in this context since sensitive dependence on initial conditions implies that the sensitivity and response of a QoI may be ill-conditioned or not well-defined. If a chaotic model has an ergodic attractor, then ergodic averages of QoIs are well-defined quantities and their sensitivity can be used to characterize model sensitivity. The response theorem gives sufficient conditions such that the local forward sensitivity – the derivative with respect to a given parameter - of an ergodic average of a QoI is well-defined. We describe a method based on ergodic and response theory for computing the sensitivity and response of a given QoI with respect to a given parameter in a chaotic model with an ergodic and hyperbolic attractor. This method does not require computation of ensembles of the model with perturbed parameter values. The method is demonstrated and some of the computations are validated on the Lorenz 63 and Lorenz 96 models.

INTRODUCTION AND EXECUTIVE SUMMARY OF RESULTS:

Understanding the response of a quantity of interest (QoI) (the representation of the QoI as function of a given parameter) and its local forward sensitivity (the derivative of the QoI with respect to a parameter) is critical in computer models of dynamical systems. Henceforth, we use whenever we shall use sensitivity and local forward sensitivity interchangeably. Traditional methods for computing sensitivities struggle in chaotic models, where sensitive dependence on initial conditions leads to ill-conditioning and associated convergence and stability issues. This has lead to the development of various modern methods for computing sensitivities of QoIs in chaotic models. Modern approaches characterize the sensitivity of a QoI in a chaotic model by determining the sensitivity of its ergodic time average which is well-defined and well-conditioned so long as the model has a hyperbolic ergodic attractor. The two main approaches are based on shadowing of dynamical systems (see e.g. shadowing (Ni and Wang, 2017), (Ni et al., 2019), (Chater et al. 2017) and see (Palmer, 2000) for an introduction to shadowing) and response theory (see e.g. (Abramov and Majda, 2007), (Eyink et al. 2004), (Lea et al. 2000), (Sliwiak and Wang, 2022) and see (Ruelle, 2009) for an introduction to response theory). Approaches based on shadowing typically compute shadowing trajectories via some minimization or zero-finding procedure and then approximate sensitivities in terms of an unperturbed trajectory and a shadow trajectory. Approaches based on response theory typically

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approximate the sensitivity using the linear response formula or some approximation or derivation of it.

The R&D undertaken is this work is to develop an algorithm to approximate the response and sensitivity based on ergodic and response theory. Our approach is different from the literature in that, rather than relying on approximating an expression of the sensitivity in terms of the linear response formula, we approximate the sensitivity directly using approximations of ergodic integrals. To approximate these integrals, we use a box-covering algorithm that represents the attractor as a union of nearly disjoint (except on a set of Lebesgue measure zero) generalized rectangles that enable the development of accurate and efficient quadrature rules for functions defined on an attractor. These accurate quadrature rules are then used to compute the response – the representation of an ergodic average of a QoI as a function of a parameter – from which sensitivities can be obtained using standard methods based on finite differences. The algorithms we develop and associated results (see the proceeding two sections) demonstrate that we have been successful in developing methods that can compute the response and sensitivity of low-dimensional chaotic models. We are able (see Figures 1-2 that present the results of our experiments) to accurately reconstruct the response function of several QoIs for the Lorenz 63 and Lorenz 96 models and can validate the ergodic average calculations. Implementations for our algorithms can be found at https://gitlab-ex.sandia.gov/asteyer/crtfd. Below, we present some theory necessary to develop algorithms and present the results of experiments in the proceeding two sections.

We now briefly review the linear response and ergodic theory that is necessary for the development of our methods. Let d and p be positive integers and let $\|\cdot\|$ be some norm on $\mathbb{R}^d$. Let $\varphi \in C^2(\mathbb{R}^d \times O, \mathbb{R}^d)$ where $O \subseteq \mathbb{R}^p$ is an open set such that $\varphi_a \coloneqq \varphi(\cdot, a)$ is a diffeomorphism for each $a \in O$. Denote by $D_u\varphi$ and $D_a\varphi$ the derivative of $\varphi = \varphi(u, a)$ with respect to u and a, respectively. Consider the following discrete-time dynamical system:

$$u_{m+1} = \varphi(u_{m+1}, a), \qquad u_m \in \mathbb{R}^d, a \in O. \qquad \text{(Eq 1)}$$

Let $u = u(m; u_0, a)$ denote the solution of (Eq 1) with initial condition $u(0; u_0, a) = u_0$. We assume throughout the remainder of this paper that for some $a_0 \in O$ there exists a compact set $C(a_0) \subset \mathbb{R}^d$ that is *invariant*:

$$u_0 \in C \Longrightarrow u(m; u_0, a_0) \in C \quad \forall m \in \mathbb{Z}, \qquad \text{(Eq 2)}$$

attractive: there exists an open set $U \subseteq \mathbb{R}^d$ with $C \subset U$ so that:

$$v_0 \in U \Longrightarrow \lim_{m \to \infty} \sup \| u_0 - u(m; v_0, a_0) \| = 0, \qquad \text{(Eq 3)}$$

and *hyperbolic*: there exists $K_1, K_2, \lambda_1, \lambda_2 > 0$ and subspaces $E^s \oplus E^u = \mathbb{R}^d$ so that

$$\| [D_u\varphi(u_0, a_0)]^k \xi \| \leq K_1 \lambda_1^k, \;\; \xi \in E^s, \qquad \text{(Eq 4)}$$
$$\| [D_u\varphi(u_0, a_0)]^{-k} \xi \| \leq K_2 \lambda_2^k, \;\; \xi \in E^u.$$

Basic results on the theory of hyperbolic sets (see e.g. (Palmer, 2000)) imply that for all $a \in O$ is sufficiently near to a_0, there is a unique compact set $C(a)$ that is invariant, attractive, and hyperbolic with respect to (Eq 1) and such that $C(a)$ is close to $C(a_0)$ in the C^1-topology. This is the theoretical basis for our sensitivity and response algorithms.

If (Eq 1) is chaotic and $Q \in C^0(C, \mathbb{R})$, then it is challenging to determine the sensitivity of $Q\big(u(\cdot; u_0, a)\big)$ since sensitive dependence on initial conditions implies that $u(m; u_0, a_0)$ and $u(m; u_0, a)$ will decorrelate as $m \to \infty$ regardless of how close a is to a_0. We therefore take the traditional approach of characterizing QoIs of chaotic systems in terms of their time-averages, which are typically well-behaved under the assumptions (Eq 2)-(Eq 4) taken above. For each $u_0 \in C$ and $a \in O$ we define the following time-averaged quantities:

$$J(u_0, a) = \limsup_{m \to \infty} \frac{1}{m} \sum_{j=0}^{m} Q\big(u(j; u_0, a)\big). \tag{Eq 5}$$

The assumptions on $C(a_0)$ imply (see Theorem 1 of (Young, 2002)) that for all $a \in O$ sufficiently close to a_0, there exists a unique φ_a-invariant probability measure μ_a, referred to as the SRB measure of $C(a)$, such that the following holds for any $Q \in C^0(C, \mathbb{R})$:

$$J(u_0, a) = \int_{x \in C(a)} Q(x) d\mu_a \quad \text{for a.e. } u_0 \in C. \tag{Eq 6}$$

(Eq 6) implies that $C(a)$ is an ergodic attractor. Without loss of generality, ergodicity of $C(a)$ implies that we can write $J = J(u_0, a) = J(a)$. We refer to the function $a \mapsto J(a)$, locally defined for $a \approx a_0$, as the response of (Eq 1) near a_0. The SRB measure μ_a is said to be *mixing* if the following limit holds for sets $A, B \subseteq C$ that are Borel measurable with respect to μ_a:

$$\lim_{m \to \infty} \mu_a(\varphi_a^{-m}(A) \cap B) = \mu_a(A)\mu_a(B).$$

If J is differentiable in a neighborhood of $a_0 \in O$, then we define the linear response R of J as:

$$R(a) := J(a_0) + J'(a_0)a \tag{Eq 7}$$

which is of course defined for all a sufficiently close to a_0. We refer to the derivative of $J'(a_0)$ as the sensitivity of Q at a_0. Linear response theory (LRT) characterizes the change of the ergodic averages $J = J(a)$ in terms of the linear approximation of (Eq 7). The main result of LRT is the following theorem, proved in (Ruelle, 1997) and (Jiang, 2012), giving sufficient conditions such that R is well-defined and J is differentiable with respect to the parameter a:

Theorem 1. Assume that $\varphi_{a_0} \in C^3(C(a_0), C(a_0))$ and that the SRB measure μ_{a_0} is mixing. Then $J = J(a)$ is differentiable in a neighborhood of a_0.

Under the assumptions of Theorem 1, an expression for $J'(a_0)$ is proved in (Ruelle, 1997) and (Jiang, 2012). We do not make use of the formula is this paper due to issues related to stably and accurately computing the divergence terms associated with the stable and unstable subspaces required by this expression. In the next section we describe algorithms based on the above theory that we use to compute ergodic averages, sensitivities, and response.

DETAILED DESCRIPTION OF RESEARCH AND DEVELOPMENT AND METHODOLOGY:.

Recall that the response J of a QoI Q of (Eq 1) is without loss of generality represented as:

$$J(a) = \int_{x \in C(a)} Q(x) d\mu_a \quad \text{for all } a \approx a_0.$$

We can therefore approximate $J'(a_0)$ by taking finite differences of integrals of the form $\int_{x \in C(a)} Q(x) d\mu_a$. The main advantage of using the space integral expression for J rather than the time-average defining J is that by using the space average we can avoid the serial bottleneck of time-stepping. This is discussed in more detail after Algorithm 2.

To compute the space integral representation of J we develop algorithms based on box-covering methods which we now describe below. A generalized rectangle (GR) centered at $c = (c_1, \ldots, c_d)^T \in \mathbb{R}^d$ with side-lengths $r = (r_1, \ldots, r_d)^T \in \mathbb{R}^d$ is defined by

$$R(c,r) = \{y = (y_1, \ldots, y_d)^T \in \mathbb{R}^d : |c_j - y_j| \le r_j, j = 1, \ldots, d\}$$

A box-covering $B(a)$ of the attractor $C(a)$ is a collection of GRs such that every pairwise intersection of elements of $B(a)$ has Lebesgue measure zero and $C(a) \subseteq B(a)$. We now present an algorithm based on subdivision for computing a box-covering of $C(a)$ from a set of points $E(a)$ contained in a neighborhood of $C(a)$.

Algorithm 1

Inputs: initial set of points $E(a)$ contained in a small neighborhood of $C(a)$ and a number $\kappa < |E(a)|$ that defines termination criterion.

Step 1. Let $R(c,r)$ be a GR such that $E(a) \subseteq R(c,r)$ and let $B = \{R(c,r)\}$

Step 2. Set $k = |E(a)|$

Step 3. While $k \ge \kappa$

For $j = 1, \ldots, d$

(i) For each $R \in B$ let $R = R_1 \cup R_2$ where R_1 and R_2 are the two GRs that result from dividing R into two rectangles with respect to the j^{th} coordinate.

(ii) $B = B \backslash \{R\}$.

(iii) If $R_l \cap E(a) \neq \emptyset$, then $B = B \cup \{R_l\}$ for $l = 1,2$.

(iv) $k = |E(a)|/|B|$.

End For

End While

Outputs: Box-covering $B(a)$ of $C(a)$.

The results of (Dellnitz and Hohmann, 1997) imply convergence of the output box-covering $B(a)$ in Algorithm 1 to $C(a)$, in the sense $B(a)$ contains $C(a)$ and the size of the GRs comprising $B(a)$ goes to zero as $\kappa \to \infty$. The convergence depends on the constants defining the hyperbolicity of $C(a)$. Our implementation of Algorithm 1 is a modification of the implementation of Molteno's box-counting algorithm (Molteno, 1993) in DynamicalSystems.jl (Datseris, 2018). Implementations for our algorithms can be found at https://gitlab-ex.sandia.gov/asteyer/crtfd

Using a box-covering of $C(a)$, we can approximate $J = J(a)$ with a simple quadrature rule as follows. Let B be a box-covering of $C(a)$. We then approximate:

$$J(a) = \int_{x \in C(a)} Q(x) d\mu_a = \sum_{D \in B} \int_{b \in D} Q(x) d\mu_a \approx \sum_{D \in B} Q(d)|D|, \quad d \in D. \qquad \text{(Eq 8)}$$

Here we take $|D|$ to represent the Lebesgue measure of the GR D. The approximation in (Eq 8) is validated in the Results and Discussion section. Using Algorithm 1 and (Eq 8) we develop the following algorithm to compute the sensitivity and response.

Algorithm 2. Inputs: initial parameter value $a_0 \in \mathbb{R}^p$; set of parameters $A \subset \mathbb{R}^p$ that are all near a_0; box-covering termination criterion κ; QoI Q.

Step 1. Compute an initial ensemble $U(a_0)$ of (Eq 1) whose elements are contained in a small neighborhood of $C(a_0)$.

Step 2. Compute a box-covering $B(a_0)$ of $C(a_0)$ with Algorithm 1 using $E(a_0) = U(a_0)$ with termination criterion κ.

Step 3. Compute $J(a_0)$ using (Eq 8).

Step 4. For each $a \in A$:

- (i) Set $U(a) \leftarrow U(a_0)$.
- (ii) Iteratively compute $U(a) \leftarrow \varphi(U(a), a)$ until $U(a)$ is contained in a small. neighborhood of $C(a)$.
- (iii) Compute a box-cover $B(a)$ of $C(a)$.
- (iv) Compute $J(a)$ using (Eq 8).

Step 5. (optional) Compute sensitivities using finite differences.

Outputs: Approximation to $J(a)$ for each $a \in A \cup \{a_0\}$ and (optionally) $J'(a)$ for each $a \in A \cup \{a_0\}$.

The implementation of Algorithm 2 only requires time-stepping to compute the initial ensemble $U(a_0)$. Once this initial ensemble is formed we can obtain box-coverings of $C(a)$ for $a \approx a_0$ by by parallel iterations of φ_a applied to the initial ensemble $U(a_0)$. This requires few iterations due to exponentially fast convergence of points near the attractor $C(a)$. Therefore, our Algorithm 2 can be efficiently implemented without running time-stepping ensembles of perturbed parameter values.

RESULTS AND DISCUSSION:

In this section we present the results of some experiments of our implantation of Algorithms 1-2 (implentations can be found at https://gitlab-ex.sandia.gov/asteyer/crtfd). We present results for two models: the Lorenz 63 (Lorenz, 1963) model and Lorenz 96 (Lorenz, 1996) models which are widely used as low-dimensional testbeds for numerical methods applied to chaotic problems. The Lorenz 63 model is defined by the following three-dimensional differential equation:

$$\dot{x} = \sigma(y - x) \quad \text{(Eq 9)}$$
$$\dot{y} = x(\rho - z) - y$$
$$\dot{z} = xy - \beta z.$$

The three parameters of the Lorenz 1963 models have the following standard parameter values $\rho = 28, \sigma = 10, \beta = 8/3$ that are known to lead to chaotic behavior in numerical discretizations of (Eq 9). We refer to these values as the standard parameter values for Lorenz 63. The parameter ρ is taken to be the parameter that we vary in our experiments ($\rho = a$ and $a_0 = 28$). We make use of the following QoIs for our tests of the Lorenz 63 system:

$$Q631(x, y, z) = z, \qquad Q632(x, y, z) = (x^2 + y^2 + z^2)/2 \quad \text{(Eq 11)}$$

The Lorenz 96 model is defined by the following d-dimensional differential equation:

$$\dot{u}_j = (u_{j+1} - u_{j-2})u_j + F, \quad j = 1, \ldots, d. \quad \text{(Eq 12)}$$

The standard value for the forcing parameter is $F = 8$ and is known to lead to chaotic behavior in numerical discretizations of (Eq 12). We refer to $F = 8$ as the standard parameter value of Lorenz 1996. The parameter F is taken to be the parameter that we vary in our experiments ($F = a$ and $a_0 = 8$) and we set $d = 20$. We use the following QoIs for our tests of the Lorenz 1996 system:

$$Q961(u_1, \ldots, u_d) = u_d, \qquad Q962(x, y, z) = (u_1^2 + \cdots u_d^2)/2 \quad \text{(Eq 13)}$$

To obtain discrete-time models of the form of (Eq 1) we discretize (Eq Y1) and (Eq Y2) with the standard fourth order RK4 time-integration method with a fixed time-step of $\Delta t = 10^{-2}$. We remark here that results for computed sensitivities are dependent on both the time-stepping algorithm and on the time-step used – we leave detailed investigation of this for future work.

We first validate the box-covering algorithm (Algorithm 1) and the quadrature rule that approximates the spatial integral from the right-hand side of (Eq 6). To accomplish this we define two quantities (where Q denotes any continuous QoI, $B(a)$ represents some box-covering of $C(a)$, and d_D represents some value contained in $D \in B(a)$):

$$TA(m, Q, u_0) = \frac{1}{m}\sum_{j=0}^{m} Q(u(j; u_0, a_0)), \qquad SA(B) = \sum_{D\in B} Q(d_D)|D|, \qquad \text{(Eq Y4)}$$

Ergodicity implies that $TA(m, q, u_0)$ and $SA(B)$ should be nearly equal for a randomly chosen $u_0 \in C(a)$, m sufficiently large, and box-covering with $\sup_{D\in B} |D|$ sufficiently small. To show this is the case, first we randomly select 100 initial conditions $u_0 \in C(a)$ and compute an ensemble of trajectories on $C(a)$. Next, we use Algorithm 1 with $E(a)$ given by the union of the points of all the ensemble trajectories and using $\kappa = 10$ to compute the box-covering $B(a)$ of $C(a)$. Finally, we compute the maximum of $|TA(m, Q, u_0) - \text{SA(B)}|$ over all initial conditions u_0 from the ensemble for increasing values of m and using $Q \in \{Q631, Q632, Q961, Q962\}$. In Figure 1 we show the results of a validation experiment for the Lorenz 63 and Lorenz 96 models. The standard parameter values are used for both models. It is clear from these figures that with increasing time (equivalently m since time is given by $m\Delta t$) the difference between the time-average and space-average goes to zero for each of the randomly chosen initial conditions and each of the tested QoIs. This serves as validation that these models are ergodic and therefore that we can obtain the correct values for the sensitivities by taking finite differences of the spatial integrals approximated as $SA(B)$.

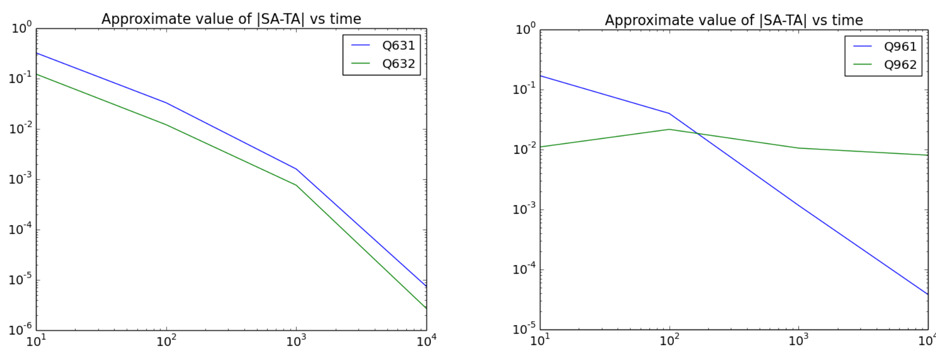

Figure 1. Approximate value of the maximum of |TA(m,Q,u_0)-SA(B(a)| for an ensemble with 100 elements with randomly chosen initial conditions on vs time ($m\Delta t$) *for Lorenz 63 (left) and Lorenz 96 (right) for the QoIs defined in (Eq 11) and (Eq 13).*

Our second main result is the computation of the response from Algorithm 2. An ensemble of 100 initial conditions is run to compute $U(a_0)$ where a_0 is the standard parameter values of Lorenz 63 or Lorenz 96. We use $A = \{a_0 - 10^{-2}, a_0 + 10^{-2}\}$ with the value of $\kappa = 10$ for the stopping criterion for the box-covering algorithms in both models and 20 iterations of φ_a are applied to the initial ensemble to ensure $U(a)$ is contained in a small neighborhood of $C(a)$. After this, Algorithm 2 is reapplied using the perturbed parameter values $a_0 \leftarrow a_0 \pm 10^{-2}$ as the new initial parameter values and new perturbed parameter values $A = \{a_0 \pm 10^{-2}\}$, but we avoid computing an initial ensemble by using the earlier computed sets $U(a)$ from the previous run. The results (Figure 2) show that we obtain approximations to $J(a)$ for values of a quite far from

a_0. Sensitivities can be obtained from simple finite-differencing methods from the compute values of $J(a)$.

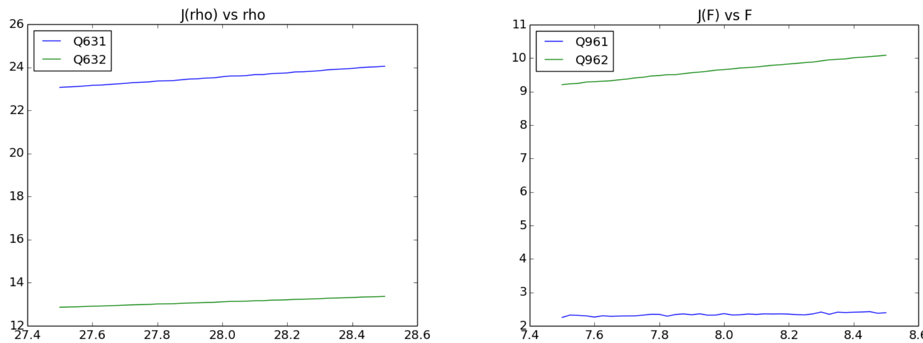

Figure 2. Approximate value $J(a)$ vs time where $a = \rho$ for Lorenz 63 (left) and $a = F$ for Lorenz 96.

ANTICIPATED OUTCOMES AND IMPACTS: This should be > 700 words (no upper limit) without any addendum materials. If the impact is well articulated in the Addendum section, then the word count can be reduced to >300 words. The impact should include a description of next step(s), summary of publications and anticipated publications, conference presentations, potential new R&D deriving from what was learned, IP development, potential impact and path forward for NNSA and DOE, etc.

The main direct impact of this project is to contribute to the foundational knowledge base for methods to compute sensitivities and response in chaotic models in the CIS Mathematics, Algorithms, and Simulation (MAS) Core Research Area. This knowledge resulted in the development of new algorithms to compute sensitivity and response (Algorithm 2) as well as an algorithm (Algorithm 2) to validate ergodicity in low-dimensional chaotic models. Concretely, this work and new knowledge resulted in a software package (implementation located at https://gitlab-ex.sandia.gov/asteyer/crtfd) and an invited presentation A box-covering method for computing forward sensitivities in low-dimensional chaotic models" at the KU Computational and Applied Math Seminar (April 2022). This work has enhanced basic algorithms and capabilities for computing forward sensitivities in chaotic models.

Secondarily, the knowledge gained from this project has lead to staff development to prepare future proposals and contributions. This can be leveraged for LDRD, ASCR, Early Career, or AI/ML for Science and Security proposals. This knowledge has already had some limited impact since aspects of the LDRD Idea 23-0308 "Geometric Deep Learning Framework for Physics-Informed Reduced Order Modeling" were motivated by what was learned in this project. Next steps after this project would be presenting this work at various conferences and seminars, preparing a peer-reviewed publication, and potentially developing a full LDRD proposal or early career proposal based on this work.

This work has also pointed to new research directions. First, there are several important aspects to consider including how to develop higher order quadrature rules to compute the spatial ergodic average and how the time-discretization affects Algorithms 1-2. Second and more importantly, it remains to be shown how to efficiently compute box-coverings of attractors of high-dimensional problems that arise in applied problems since box-covering algorithms scale badly with dimension. For problems that have low-dimensional attractors (such as fluid and plasma problems) embedded in a high dimensional space, it should be possible to efficiently apply a box-covering method using a representation of the embedding that preserves geometric properties of the attractor (this motivated some aspects of the LDRD Idea 23-0308).

CONCLUSION:

Computing the sensitivity and response of chaotic dynamical systems remains a challenging and important problem with implications for models arising in climate, fluid dynamics, plasma modeling, and structural mechanics. In this report we have derived a new algorithm for computing the response and sensitivity of low-dimensional chaotic models based on ergodic and response theory. Results from experiments indicate that these methods are promising, and that additional R&D effort is needed to develop similar algorithms that can efficiently compute response and sensitivity for high-dimensional problems.

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ADDENDUM:

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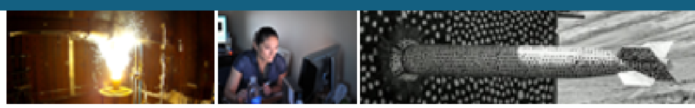
LDRD Ending Project Review Computational Response Theory for Dynamics, Project 227154



PI: Andrew Steyer/Org. 1442 PM: Jim Stewart/1400

Andrew Steyer

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PURPOSE, GOALS AND APPROACH

Purpose: Develop methods and algorithms based on linear response and ergodic theory to compute forward sensitivities and uncertainties in chaotic models where there is presently a lack of general purpose methods that are accurate/efficient/robust.

Goals: Develop methods to compute forward sensitivities and uncertainties more efficiently than existing methods.

Approach: Use methods and techniques from linear response and ergodic theory to develop robust methods based on rigorous mathematical theory.

PI's PROJECT LEGACY

3

Summary:

- Investigated use of linear response formula and ergodic theory to compute forward sensitivities.
- Developed method and software to compute forward sensitivities of low-dimensional chaotic models using ergodic spatial averages computed from a box-covering approximation of the attractor, implementation found at https://gitlab-ex.sandia.gov/asteyer/crtfd).
- Above method was validated for Lorenz 63 and 96 models by comparing time- and space-averages.
- Determined potential to leverage modern ideas (machine learning, autodiff) to more accurately and efficiently compute forward sensitivities.

Key aspects and results:

- Found that direct application of linear response formula for dynamical systems with a hyperbolic attractor requires: (1) evaluation of an expensive integral (2) computing some representation of the attractor.
- Found that ergodic theory can be accurately computed and used to approximate forward sensitivities.
- Challenging to get convergence of methods that directly approximate the linear response integrals.
- Remains to be seen: can ergodic-theory based methods be developed that are more efficient than existing approaches?

Impact:

- Some aspects of the LDRD idea 23-0308 "Geometric Deep Learning Framework for Physics-Informed Reduced Order Modeling" were motivated by what was learned in this project.
- Knowledge: Limitations of linear response formula implies focus needs to be on efficient methods to compute representations of attractors, use of ergodic theory to compute forward sensitivities with some accuracy.
- Next 1-2 fiscal years: more proposals (LDRD, ASCR, early career) related to the knowledge that was learned.

PROJECT OUTPUTS

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- Knowledge and methods related to computing sensitivities in chaotic models with linear response and ergodic theory that can be leveraged for future LDRD, ASCR, Early Career, or AI/ML for Science and Security proposals.
- Software: https://gitlab-ex.sandia.gov/asteyer/crtfd.
- Presentation:
  - "A box-covering method for computing forward sensitivities in low-dimensional chaotic models" at the KU Computational and Applied Math Seminar (April 2022).

LABORATORY DIRECTED
RESEARCH & DEVELOPMENT
WHERE INNOVATION BEGINS

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CAPABILITIES DEVELOPMENT

- Knowledge and expertise in linear response and ergodic theory and computing sensitivities in chaotic models.
- Validation method for computing ergodic averages in low-dimensional models.
- New algorithm to compute forward sensitivities with box-covering method.
- Software: https://gitlab-ex.sandia.gov/asteyer/crtfd.
- Ideas for future proposals (LDRD, ASCR, Early Career, AI/ML for Science and Security proposals).

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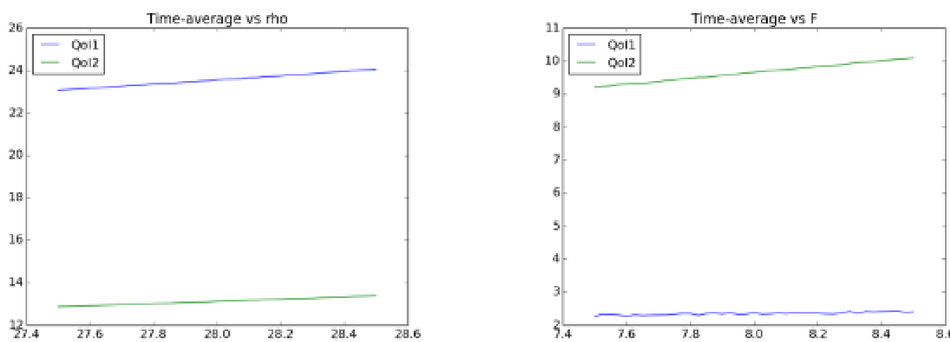
Sensitivity and response for Lorenz models



Results for the Lorenz 63/96 models integrated with RK4 using $\Delta t = 10^{-2}$ with a final time of 10^4. (Left) Response of Lorenz 63 with respect to changes in ρ for $\rho \approx 28$. (Right) Response of Lorenz 96 with respect to changes in F for F$\approx$ 8. Sensitivities are computed by using second-order centered differences of spatial averages obtained from a box-covering algorithm of the attractor.

Lorenz 63 (3D, 3 parameters)

$$\begin{cases} \dot{x} = \sigma(y - x) \\ \dot{y} = x(\rho - z) - y \\ \dot{z} = xy - \beta z \end{cases}$$

Lorenz 96 (arbitrary dimension, one parameter)

$$\dot{u}_j = (u_{j+1} - u_{j-2})u_j + F, \qquad j = 1, \dots, 20$$

$QoI1$ - (resp. $QoI1\big((x,y,z)\big) = z$ and $QoI1(u) = u_N$)
$QoI2$ - (resp. $QoI2\big((x,y,z)\big) = (x^2 + y^2 + z^2)/2$ and . $QoI2(u) = u^T u/2$)

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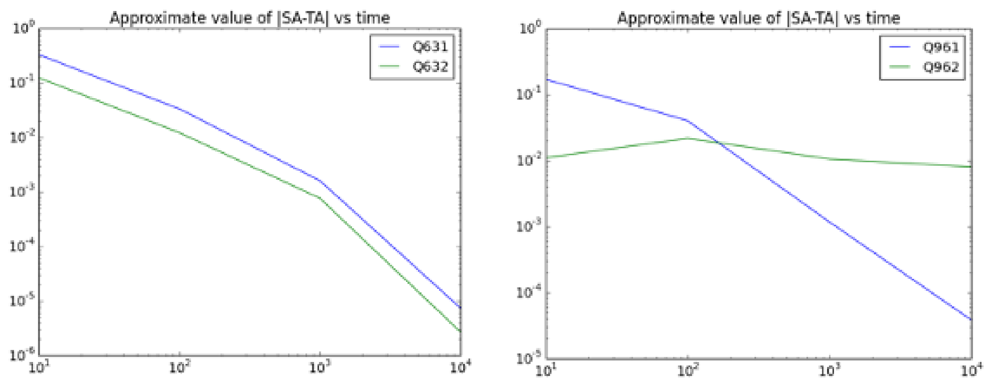
Validation Algorithm: does time-average equal space-average a.e.?

"Time average" $= \text{TA(T)} = \frac{1}{T}\int_0^T Q\big(u(t;u_0)\big)dt,$ "Space average" $= SA(B) = \int_{x\in A} Q(x)d\mu(x)$

- are these equal regardless of initial condition?



Approximate value |SA-TA| vs time for Lorenz 63 (left) and Lorenz 96 (right) for an ensemble with 100 elements with randomly chosen initial conditions on the attractor. Spatial average computed using a box-covering of the attractor.

$Q631\big((x,y,z)\big) = z$ and $Q961(u) = u_N$

$Q632\big((x,y,z)\big) = (x^2+y^2+z^2)/2$ and $Q962(u) = u^T u/2$

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IA/PM PROJECT LEGACY

Important Lesson: Efficiently computing sensitivities of chaotic models using the linear response formula requires computing structures related to the attractor.

Key results useful to current/future projects:

- Presentation: "A box covering method for computing forward sensitivities in low-dimensional chaotic models" at University of Kansas Computational and Applied Math Seminar (April 2022).
- Algorithm to validate numerical approximation of ergodic averages in low-dimensional models.

IA contribution:

- Contributed to foundational knowledge base in the CIS Mathematics, Algorithms, and Simulation (MAS) Core Research Area.
- Enhanced capabilities for computing forward sensitivities in chaotic models.
- Staff development to help prepare you for future proposals, including LDRD and ASCR.

LABORATORY DIRECTED
RESEARCH & DEVELOPMENT
WHERE INNOVATION BEGINS

Computational response theory for dynamics

PI: Andrew Steyer, PM: Jim Stewart

Project goal(s)

Investigate use of linear response and ergodic theory to compute forward sensitivities and uncertainties in low-dimensional chaotic models.

Develops methods and algorithms based on this investigation.

Compare these methods against the current state-of-the-science.

Technical Accomplishments

Implemented and validated methods for computing ergodic averages of the Lorenz 63/96 models.

Developed new algorithms to compute forward sensitivities in low-dimensional models and demonstrated these methods on Lorenz 63/96 models.

Mission impact

Developed expertise and knowledge base in linear response and ergodic theory for computing forward sensitivities.

New algorithm for computing forward sensitivities in low-dimensional models.

Staff development for future LDRD, ASCR, Early Career proposals.

Legacy

Springboard for new LDRD idea(s) for FY24 as well as other project proposals such for ASCR, early career, or AI/ML for Science and Security.

Presentation: "A box covering method for computing forward sensitivities in low-dimensional chaotic models" at University of Kansas Computational and Applied Math Seminar (April 2022).