A computable realization of Ruelle’s formula for linear response of statistics in chaotic systems

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Abstract. We present a computable reformulation of Ruelle’s linear response formula for chaotic systems. The new formula, called Space-Split Sensitivity or S3, achieves an error convergence of the order $O(1/\sqrt{N})$ using $N$ phase points. The reformulation is based on splitting the overall sensitivity into that to stable and unstable components of the perturbation. The unstable contribution to the sensitivity is regularized using ergodic properties and the hyperbolic structure of the dynamics. Numerical examples of uniformly hyperbolic attractors are used to validate the S3 formula against a naïve finite-difference calculation; sensitivities match closely, with far fewer sample points required by S3.

Key words. sensitivity analysis, chaotic systems, linear response theory

AMS subject classifications. 68Q25, 68R10, 68U05

1. Introduction. Given a dynamical model, how much do the outputs change in response to small changes in input parameters? The computational aspect of this common question, which arises across science and engineering, entails the mature discipline of sensitivity analysis. Using numerical simulations or experimental observations of dynamical systems, the computed responses or sensitivities have enabled multidisciplinary design optimization, uncertainty quantification and parameter estimation in diverse non-chaotic models (see [28, 5] for recent surveys in aerodynamic systems). Sensitivity analysis in chaotic systems, however, still remains nascent. This is because traditional sensitivity computation is done through linear perturbation methods including tangent or adjoint equations, and automatic differentiation, but these are inherently unstable in chaotic systems [26, 32]. More sophisticated techniques are needed to calculate the long-term effects of parameter changes in chaotic systems. Some of them are being actively investigated as of this writing, and face challenges such as lack of convergence guarantees or prohibitive computational cost. In this work, we develop an alternative method for addressing some of these challenges. We propose a formula for differentiating statistical averages in chaotic systems to parameter perturbations, in a way that is amenable to computation. We postpone until section 2 the precise definition of the statistical response we aim to compute and the desired qualities of a computational solution.

Currently, the more sophisticated approaches to chaotic sensitivity computation include a) the ensemble sensitivity method b) shadowing-based approaches and c) perturbation methods on the transfer operator. The non-intrusive least squares shadowing (NILSS) method...
(see [3, 25], and [32] for the different versions of NILSS) computes a shadowing perturbation that remains bounded in a long time window under the tangent dynamics. However, the sensitivity computed by using the shadowing tangent solution is not guaranteed to be an unbiased estimate of the true sensitivity [4]. This is because while ergodic averages converge for almost every trajectory, there are measure zero subsets of the attractor (e.g. unstable periodic orbits [17]) on which they do not converge. We therefore seek an alternative that does not rely on computations along a single trajectory that is not guaranteed to be typical. The Lea-Allen-Haine ensemble sensitivity method [13] suggests a work-around to the exponentially diverging sensitivities computed by the conventional tangent/adjoint methods, by truncating the tangent/adjoint equations at a short time, and taking a sample of average of many such short-time sensitivities. But, although these sample averages converge in the infinite time limit, they are prohibitively expensive because the variance of tangent/adjoint solutions increases exponentially with time ([6]).

In a recent work, Crimmins and Froyland [12] have developed a new Fourier analytic method for constructing the Sinai-Ruelle-Bowen or SRB measures, the invariant probability distributions perturbations of which we are interested in, of uniformly hyperbolic dynamics on tori. They construct a matrix representation of perturbed transfer operators that are quasi-compact on certain anisotropic Banach spaces (see [16] for uniformly hyperbolic systems in particular, and [2] for a recent review). Using this matrix representation, the leading eigenvector, which is the SRB measure, is then approximated. Although equipped with a strong theoretical basis, this method would be overkill for our purpose, since we do not need to construct the SRB measure, but only compute the sensitivity of a given expectation with respect to it. Moreover, methods based on perturbations of the transfer operator such as [12, 23] typically have a computational cost that scales poorly with the problem dimension since they either involve Markov partitions (specific discretizations of the attractor) or need a number of basis functions to approximate the eigendistribution (the SRB measure) that scales with the dimension. Another recent method [20] computes sensitivities by solving an adjoint equation as a boundary value problem on periodic orbits, although questions surrounding the convergence of the computed sensitivity to the true sensitivity (like in the shadowing methods) must be investigated further.

The strategy developed in this paper, space-split sensitivity or S3, deviates from that of all the above-mentioned methods. However, like ensemble sensitivity methods, it builds upon Ruelle’s formula. While ensemble sensitivity suffers from the unbounded variance of the unstable contribution to the overall sensitivity, S3 splits the contributions and performs a finite-sample averaging of tangent equation solutions only for the stable contribution. The unstable contribution is manipulated through integration-by-parts and using the statistical stationarity (measure preservation) of the system to yield a computation that does not use unstable tangent solutions. Since both parts of the sensitivity are computed through sampling on generic flow trajectories, the problem of the computed sensitivities corresponding to atypical trajectories, which shadowing-based methods are vulnerable to, is averted. The paper is organized as follows. In the next section, we give the problem setting and state results from dynamical systems theory that are used in the derivation of S3. Our main results are stated in section 3, and the derivation of the S3 formula follows in section 4. An interpretation of the unstable contribution, as derived in S3, is presented in section 5, and some comments
on its computational details can be found in section 6. Numerical examples demonstrating a naive implementation of the S3 formula are reported in section 7, and the conclusions follow in section 8.

2. Problem statement. In this section, we define the output quantity of interest for S3 computation. Where they are used, we provide a brief description of concepts from ergodic theory and dynamical systems, in order to make it a self-contained presentation for computational scientists from different fields.

2.1. The primal dynamics. Our primal system is a $C^2$ diffeomorphism $\varphi^s$, on a $d$-dimensional compact manifold $M$, parameterized by a set of parameters $s$,

$$u_{n+1} = \varphi^s(u_n), \; n \in \mathbb{Z}, u_n \in M. \tag{2.1}$$

In a numerical simulation, $u_n \in M$ represents a solution state (a $d$-dimensional vector) at time $n$ and the transformation $\varphi^s$ can be thought of as advancing by one timestep. For simplicity, $s$ is assumed to be a scalar. Without loss of generality, we take $s = 0$ to be the reference value and the map $\varphi^0$ is simply written as $\varphi$, without the superscript. The state vector $u_n, n \in \mathbb{Z}^+$ is a function of the initial state $u_0$; explicitly, $u_n = \varphi_n(u_0)$, where the subscript $n \in \mathbb{Z}^+$ in $\varphi_n^s$ refers to an $n$-time composition of $\varphi^s$, and $\varphi_0^s$ is the identity map on $M$. We also use the notation $\varphi_{-n}, n \in \mathbb{Z}^+$ to denote the inverse transformation $(\varphi)^{-1}$ composed with itself $n$ times; that is, $\varphi_{-n}(u_n) = u_0$.

2.2. Ensemble and ergodic averages. We assume that the dynamics $\varphi^s$ preserves an ergodic, physical probability measure $\mu^s$ of an SRB-type (see [33] for an introduction to SRB measures), which gives us a statistical description of the dynamics. In particular, expectations with respect to $\mu^s$ can be observed as infinitely long time averages along trajectories: if $f \in L^1(\mu^s)$ is a scalar function, then $\lim_{N \to \infty} (1/N) \sum_{n=0}^{N-1} f(\varphi_n^s(u)) = \langle f, \mu^s \rangle$, $u$ Lebesgue-a.e on the basin of attraction. The superscript $s$ in $\mu^s$ emphasizes the dependence of the SRB measure on the parameter; simply $\mu$, without the superscript, refers to the SRB measure at $s = 0$. The ensemble average or the expectation of $f$ with respect to $\mu^s$, $\langle f, \mu^s \rangle$, is a distributional pairing of $f$ with $\mu^s$: the integral of $f$ on the phase space weighted by $\mu^s$. We sometimes use the shorter notation $\langle f \rangle^s$, and without the superscript at $s = 0$, to denote the same quantity. The infinite time average, called the ergodic average, is the more natural form of $\langle f \rangle^s$ from the computational/experimental standpoint, since it can be obtained by numerical evaluation/measurements of $f$ along trajectories. In practice the ergodic average is computed up to a large $N$ and this is used to approximate the ensemble average $\langle f \rangle^s$ – by ergodic average, we mean this long but finite time average, in the remainder of this work.

2.3. Quantity of interest. We are interested in determining the sensitivity of the ensemble average of an objective function $J \in C^2(M)$, $\langle J \rangle^s$, to $s$: $d_s \langle J \rangle^s = \langle J, \partial_s \mu^s \rangle$. The regularity of $J$, along with other assumptions on the dynamics which we detail where they appear, are such that the linear response formula of Ruelle [29, 31] is satisfied. The objective function $J$ can also explicitly depend on $s$, and assuming that $J$ is continuously differentiable with respect to $s$, the quantity of interest $d_s \langle J \rangle^s = \langle \partial_s J, \mu^s \rangle + \langle J, \partial_s \mu^s \rangle$. As we will see however, in a chaotic system, the mathematical or algorithmic difficulty lies in computing the derivative of the SRB measure in the second term, and not in the first, which can be computed as an
ergodic average, assuming the function \( \partial_s J(u, s) \) is known. Thus from now on we ignore the first term and develop an algorithm for \( \langle J, \partial_s \mu^s \rangle \), which is nontrivial to compute – we describe precisely why, in the next section.

2.4. Ruelle’s formula and its computational inefficiency. To introduce Ruelle’s formula, let the matrix-valued function \( D \varphi : M \to GL(d) \)\(^2\) give us the Jacobian matrix of the transformation \( \varphi \). Here \( D \) refers to the derivative with respect to phase space; so, the Jacobian at \( u \), \( D \varphi(u) \), is a map from the tangent space of \( M \) at \( u \), denoted as \( T_u M \), to \( T_{\varphi(u)} M \). We now introduce a more succinct notation for the tangent operator in the following definition.

**Definition 2.1.** The tangent operator \( T(u, n) : T_u M \to T_{\varphi_n(u)} M \) is a linear operator (a matrix) for each \( n \in \mathbb{Z} \) and is defined as the derivative of \( \varphi_n \) with respect to the state vector \( u \), evaluated at \( u \). By this definition, it can be written as Jacobian matrix products, as follows,

\[
T(u, n) := \begin{cases} 
D \varphi(\varphi_{n-1}(u)) \cdots D \varphi(u), & n > 0 \\
(D \varphi(\varphi_n(u)))^{-1} \cdots (D \varphi(\varphi^{-1}(u)))^{-1}, & n < 0 \\
\text{Id}, & n = 0.
\end{cases}
\]

From the linear response theory that was rigorously developed by Ruelle [29, 31], we have the following formula for the sensitivity of interest,

\[
\left. \frac{d\langle J \rangle^s}{ds} \right|_{s=0} = \sum_{n=0}^{\infty} \langle D(J \circ \varphi_n(\cdot)) \cdot X(\cdot), \mu \rangle,
\]

where \( X(u) := \partial_s \varphi^s(\varphi^{-1}(u)) \) denotes the vector field corresponding to parameter perturbation. Here \( DJ \) refers to the derivative of \( J \) with respect to the phase space. For brevity, we adopt the subscript notation also with scalar and vector fields, as explained below:

1. if \( f : M \to \mathbb{R} \) is a scalar field, \( f_n \) is used to denote the function \( f \circ \varphi_n \).
2. The derivative of \( f_n = f \circ \varphi_n \), evaluated at a \( \mu \)-typical point \( u \), is denoted as \( Df_n(u) := D(f \circ \varphi_n)(u) \). On the other hand, \( (Df)_n \) refers to the derivative of \( f \) evaluated at \( u_n = \varphi_n(u) \), where again \( u \) is a \( \mu \)-typical point.
3. if \( V \) is a vector field, then \( V_n(u) \in T_{\varphi_n(u)} M \) denotes its value at \( u_n \): \( V_n(u) := V(u_n) \). Using this notation, the integrand in the \( n \)-th summand of Ruelle’s formula (Eq. 2.2) can be written as \( D(J \circ \varphi_n) \cdot X = DJ_n \cdot X \). Note that \( DJ_n \cdot X = (DJ)_n \cdot T(\cdot, n)X \), is the instantaneous sensitivity of \( J_n = J \circ \varphi_n \) to an infinitesimal perturbation to \( u \) along \( X(u) \). So, the \( n \)-th summand is the ensemble sensitivity of the function \( J_n \). In a chaotic system, the integrand exhibits exponential growth \( \mu \)-a.e. The reason is that, by the definition of chaos, the norm of an infinitesimal perturbation to a \( \mu \)-a.e. initial condition \( u \), along a direction \( X(u) \), asymptotically grows exponentially with time, for almost every \( X(u) \). More clearly, at \( u \) \( \mu \)-a.e., for almost every tangent vector \( X(u) \in T_u M \), where \( \|\cdot\| \) indicates the Euclidean norm in \( \mathbb{R}^d \),

\[
\limsup_{n \to \infty} \frac{\log \| T(u, n)X(u) \|}{n} > 0.
\]

For a generic \( J \), \( |D(J \circ \varphi_n) \cdot X| \) (\( |\cdot| \) denotes the Euclidean norm on \( \mathbb{R} \)) shows the same asymptotic trend as \( \| T(u, n)X(u) \| \), that is, the integrand in Ruelle’s formula, denoted as

\(^2GL(d) \) is the set of all invertible matrices of dimension \( d \times d \).
$L_n(u) := (DJ)_n \cdot T(u, n) X(u)$ grows exponentially in norm, with $n$, at almost every $u$. This makes Ruelle’s formula inefficient to evaluate directly, because the number of samples required to accurately obtain the $n$th term in the series, grows rapidly with $n$. It is worth noting that despite the pointwise exponential growth, since Ruelle’s formula converges, i.e., the series in Eq. 2.2 converges, the ensemble averages $\langle L_n \rangle$ tend to 0 as $n \to \infty$, due to cancellations in phase space.

The pointwise exponential growth of the sensitivities is however manifest in the variance of the direct approximation of the formula, which has been shown to be computationally intractable in practical examples [6, 13]. Specifically, evaluating the series upto $N$, the variance of $\sum_{n=0}^{N} L_n$, grows exponentially with $N$, at almost every $u$. As illustrated by previous numerical results [6, 13], this leads to the least mean squared error achievable at a given computational cost, to reduce poorly with the cost, usually much worse than in a typical Monte Carlo simulation.

3. Main contributions. The main contribution of this paper is a reformulation of Ruelle’s formula (Eq. 2.2) into a different ensemble average that provably converges like a typical Monte Carlo computation. That is, the error in the $N$-term ergodic average approximation of the alternative ensemble average asymptotically declines as $O(1/\sqrt{N})$. The reformulation relies on the following result, which we also prove: the effect of an unstable perturbation on the ensemble average of an objective function is captured by its time correlation with a certain, bounded function. The formal statement is as follows.

**Theorem 3.1.** Given an unstable covariant Lyapunov vector $V^i$, $1 \leq i \leq d_u$, there exist bounded scalar functions $g^i$ such that for any $J \in C^2(M)$,

$$\sum_{n=0}^{\infty} \langle D(J \circ \varphi_n) \cdot V^i, \mu \rangle = \sum_{n=0}^{\infty} \langle J \circ \varphi_n g^i, \mu \rangle.$$  \hfill (3.1)

While the proof is delayed until subsection 4.4, here we mention the foremost implication of the above theorem for computation. Since the explanation in 2.4 applies to any unstable perturbation field, the left hand side of 3.1 does not yield a Monte Carlo computation. On the other hand, the ergodic average approximation of the right hand side does. That is, the rate of convergence would be $-1/2$, independent of the system dimension, for the right hand side. Moreover, since the right hand side enables an ergodic average approximation, a discretization of the phase space, which is impractical in high-dimensional systems, is not required.

The main result of this paper, a computable realization of Ruelle’s formula, follows as a corollary to Theorem 3.1, and can be stated as follows:

**Corollary 3.2.** In uniformly hyperbolic systems, Ruelle’s formula in Eq. 2.2 is equivalent to the following sum of two exponentially converging series,

$$\frac{d(J)^s}{ds} \bigg|_{s=0} = \sum_{n=0}^{\infty} \langle D(J \circ \varphi_n) \cdot X^s, \mu \rangle + \sum_{n=0}^{\infty} \langle J \circ \varphi_n g, \mu \rangle,$$  \hfill (3.2)

where $g \in L^\infty(\mu)$, and $X = X^u + X^s$ is the decomposition of $X$ along the unstable and stable Oseledets spaces respectively.
The regularized expression that is Eq. 3.2, is referred to as the space-split sensitivity or S3 formula. We briefly explain how Corollary 3.2 is obtained, and direct the reader to section 4 for a complete presentation. We first split Ruelle’s formula (Eq. 2.2) into two terms by decomposing the vector field $X$ into its unstable and stable components. The first term in Eq. 3.2 directly results from this splitting. As shown in subsection 4.2, it leads to an efficient Monte Carlo computation and hence is left unchanged. The other term however, which contains the contribution from the unstable perturbation $X^n$, needs modification. First, it is further split into $d_u$ terms by writing $X^n$ in the basis of the unstable covariant Lyapunov vectors or CLVs, $V^i, 1 \leq i \leq d_u$. Assuming that each of the $d_u$ series is well-defined, each is modified by using Theorem 3.1.

Before we proceed with the derivation of Eq. 3.2, we close this section by discussing the advantages offered by the new formula in Eq. 3.2. The first advantage is of course the Monte Carlo convergence of the new formula, while no such guaranteed problem-independent convergence rate can be ascribed to the direct evaluation of the original formula in Eq. 2.2. Secondly, the S3 algorithm, an efficient implementation of Eq. 3.2 the details of which are deferred to a future work, only uses information obtained along trajectories, and therefore does not exhibit a direct scaling with the problem dimension. Thirdly, since Eq. 3.2 is an equivalent restatement of Ruelle’s formula, the convergence of Eq. 3.2 to the true sensitivity is immediate from the convergence of Ruelle’s formula [29].

4. Derivation of the S3 formula. Our goal is to find an alternative representation of the formula 2.2 that can be easily computed. For this, we begin by splitting the parameter perturbation vector $X$ into its stable and unstable components, along stable and unstable Oseledets spaces, denoted by $E^s$ and $E^u$ respectively. The motivation for splitting $X$ becomes clear when we define the subspaces. The reader is referred to Chapter 4 of [1] for a detailed exposition of Oseledets multiplicative ergodic theorem (MET); here we use the two-sided version of the theorem for the cocycle $T$, with the assumptions explained below. Oseledets MET gives us a direct sum decomposition (the so-called Oseledets splitting) $T_0 M = E^1(u) \oplus \cdots \oplus E^d(u)$, $u$ $\mu$-a.e., into subspaces of different asymptotic exponential growth. The subspaces $E^i(u)$, assumed here to be one-dimensional, have the following properties:

1. covariance property: for each $i = 1, 2, \cdots, d$, $T(u, 1)E^i(u) = E^i(\varphi(u))$.
2. exponential growth/decay: there exist real numbers $\lambda_i$, $i = 1, \cdots, d$ such that $v \in E^i(u) \neq 0 \in \mathbb{R}^d$ implies that $\lim_{n \to \pm \infty} \frac{1}{n} \log \|T(u, n)v\| = \lambda_i$.

The asymptotic rates $\lambda_i$, which are called the Lyapunov exponents (LEs), are assumed to be, for simplicity, nonzero and distinct, and indexed in decreasing order, i.e., $\lambda_1 > \lambda_2 > \cdots > \lambda_d$. Suppose $d_u$ is the number of positive LEs. The unstable subspace $E^u$ is defined as $E^u := \oplus_{i=1}^{d_u} E^i(u)$. As noted in subsection 2.4, a chaotic system by definition has $d_u > 0$, and a nontrivial unstable subspace, consisting of nonzero vectors at $\mu$-a.e. phase point. The stable subspace is defined as $E^s := \oplus_{i=d_u+1}^{d} E^i$.

4.1. Ruelle’s formula split along Oseledets spaces. The unit vectors along $E^i$ are denoted as $V^i$ and are also called the covariant Lyapunov vectors (CLVs). Suppose $X$ in the CLV basis (span of the $V^i$s) can be expressed as $X(u) := \sum_{i=1}^{d} a_i(u) V^i(u)$. We write $X^u$ and $X^s$ to represent the decomposition of $X$ along $E^u$ and $E^s$ respectively, i.e., $X^u(u) = \sum_{i=1}^{d_u} a_i(u) V^i(u)$.
and \( X^s(u) = \sum_{i=d_u+1}^{d} a^i(u)V^i(u) \). Then, we can rewrite Ruelle’s formula (Eq. 2.2) as,

\[
\frac{d(J)^s}{ds}_{s=0} = \sum_{n=0}^{\infty} \langle D(J \circ \varphi_n) \cdot X^s, \mu \rangle + \sum_{n=0}^{\infty} \langle D(J \circ \varphi_n) \cdot X^u, \mu \rangle.
\]

The first term on the right hand side of the split formula (Eq. 4.1) will henceforth be referred to as the stable contribution (denoted using the subscript “stable”) and the second term as the unstable contribution (denoted using the subscript “unstable”) to the overall sensitivity.

The motivation for the split is that the stable contribution can now be computed as if the system were not chaotic, using a stable tangent equation that is developed below.

### 4.2. Derivation of the stable contribution

The stable contribution can be written as

\[
(J, \partial_s \mu^s |_{s=0})_{\text{stable}} = \sum_{n=0}^{\infty} \langle D(J \circ \varphi_n) \cdot X^s, \mu \rangle = \sum_{n=0}^{\infty} \langle (DJ)_n \cdot T(\cdot, n)X^s, \mu \rangle.
\]

Now we develop a stable iterative procedure for the above expression, that satisfies our constraint of a Monte Carlo convergence, under the assumption of uniform hyperbolicity – a simplifying assumption on the dynamics that gives uniform rates of decay of perturbations along \( E^s \) and \( E^u \) forward and backward in time respectively. To wit, in a uniformly hyperbolic system, there exist constants \( C, \lambda > 0 \) such that \( \|T(u, n)X^s(u)\| \leq Ce^{-\lambda n}\|X^s(u)\| \), for all \( n \in \mathbb{Z}^+ \) and for \( u \) \( \mu \)-a.e. Such a uniform decay also applies backward in time to perturbations along \( E^u \), i.e., \( \|T(u, -n)X^u(u)\| \leq Ce^{-\lambda n}\|X^u(u)\| \), for all \( n \in \mathbb{Z}^+ \), and for \( u \mu \)-a.e., with the same constants \( C, \lambda > 0 \). Under the assumption that \( \varphi \) is uniformly hyperbolic on \( M \), and the assumption that \( \|DJ\|, \|X^s\| \in L^\infty(\mu) \), at \( \mu \) almost every \( u \), \( \|DJ(\varphi_n(u)) \cdot T(u, n)X^s(u)\| \leq Ce^{-\lambda n}\|DJ\|_\infty\|X^s\|_\infty \), where \( \|f\|_\infty := \inf \{ \alpha : \mu \{ u \in M : |f(u)| > \alpha \} = 0 \} \) for a scalar function \( f : M \to \mathbb{R} \); when \( V \) is a vector field, \( \|V\|_\infty \) is defined similarly with \( |f(u)| \) replaced with \( \|V(u)\| \). In other words, the \( L^\infty \)-norm of the integrand in Eq. 4.2 is exponentially decreasing with \( n \).

### 4.3. Computation of the stable contribution

As a result of the exponentially decaying summation, truncation at a small number of terms provides a good approximation. We suggest the following method that uses a tangent equation, to compute the stable contribution in practice, since a tangent solver is usually available. We introduce the stable tangent equation, named so for using only the stable component of the perturbation but otherwise resembling a conventional tangent equation,

\[
\zeta_i^s = D\varphi(u_{i-1})\zeta_{i-1}^s + X_i^s, \quad i = 0, 1, \cdots, N - 1
\]

\[
\zeta_{-1}^s = 0 \in \mathbb{R}^d.
\]

We can show that using the solutions of the above stable tangent equation, the stable contribution can be approximated as,

\[
(J, \partial_s \mu^s |_{s=0})_{\text{stable}} \approx \frac{1}{N} \sum_{n=0}^{N-1} DJ(u_n) \cdot \zeta_n^s.
\]

In Proposition 9.1, we show, under the assumption of uniform hyperbolicity, that the error in the above approximation decays as \( \mathcal{O}(1/\sqrt{N}) \).
4.4. The unstable contribution: an ansatz. In this section, we derive a regularized expression for the unstable contribution defined in Eq. 4.1. Denoting the components of $X$ along the $i$th CLV by the scalar field $a^i$, we can write $X^u := \sum_{i=1}^{d_u} a^i V^i$. Thus, the unstable contribution from Eq. 4.1 can be written as,

\begin{equation}
\langle J, \partial_a \mu^a \rangle_{s=0}^{\text{unstable}} = \sum_{n=0}^{\infty} \sum_{i=1}^{d_u} \langle D(J \circ \varphi_n) \cdot a^i V^i, \mu \rangle,
\end{equation}

with the underlying assumption that the series in Eq. 4.5 converges for each $i \leq d_u$. We first informally motivate the ensuing derivation of a mollified expression for Eq. 4.5. The integrand can be viewed as a linear functional $l_n : E^u(u) \to \mathbb{R}$, evaluated at $V^i(u)$, and defined by $l_n(V(u)) := a^i(u)(DJ)_n \cdot T(u, n)V(u)$, $V(u) \in E^u(u)$. Recall that although $l_n$ may be bounded for a finite $n$, the bound is an exponentially increasing function making the evaluation of $\langle l_n(V^i) \rangle$ computationally infeasible. In particular, at $\mu$-a.e. $u$, there exists an $N(u)$ such that $l_n(V(u)) \leq \|a^i\|_\infty \|DJ\|_\infty c e^{\lambda_1 n} \|V(u)\|$, for all $n \geq N(u)$. On the other hand, due to the convergence of Ruelle’s formula, the ensemble average $\langle l_n(V^i) \rangle$ declines asymptotically at least when $V = V^i$, $i \leq d_u$. Since we ultimately want to compute $\langle l_n(V^i) \rangle$ as opposed to the pointwise values of $l_n(V^i)$, we propose the following ansatz for the unstable contribution, for some $Y^{i,n} \in E^{u*}$, the dual of $E^u$,

\begin{equation}
\langle J, \partial_a \mu^a \rangle_{s=0}^{\text{unstable}} = \sum_{n=0}^{\infty} \sum_{i=1}^{d_u} \langle V^i \cdot Y^{i,n}, \mu \rangle.
\end{equation}

In particular, we require that the vector field $Y^{i,n}$ is bounded for all $n$ and additionally such that $\left| \sum_{i=1}^{d_u} (Y^{i,n} \cdot V^i) \right|$ exponentially decreases with $n$. Then, if the central limit theorem holds for the integrand above, the heuristic expression in Eq. 4.6 leads to a desired Monte Carlo algorithm via ergodic averaging. Essentially, the ansatz chosen to satisfy our computational constraints suggests a vector field $Y^{i,n}$ that captures the overall sensitivity of $J_n$ to perturbations along $V^i$. It is important that the pointwise values of $l_n(V^i)$ are not matched. The reason is, whenever for a finite $n$ depending on $u$, $l_n$ is a bounded linear functional on $E^u(u)$, the uniqueness of $Y^{i,n}(u) \in E^{u*}(u)$ from Riesz representation theorem gives $Y^{i,n}(u) = a^i(u)DJ_n(u)$. As a result, $Y^{i,n}$ does not satisfy our requirement anymore and the original problem of large variances of ergodic averages has not been solved. Thus, we may require that $l_n(V^i(u))$ not equal $V^i(u) \cdot Y^{i,n}(u)$ at each $u$ and only that $\langle l_n(V^i) \rangle = \langle V^i \cdot Y^{i,n} \rangle$, at each $n$.

4.4.1. Reformulation of the unstable contribution. In this section, beginning with the original expression in Eq. 4.1, we derive a new expression for the unstable contribution, holding Eq. 4.6 as a motivation. From Eq. 4.1, fixing an $i \leq d_u$, and isolating the $n$-th summand,

\begin{equation}
\langle a^i D(J \circ \varphi_n) \cdot V^i, \mu \rangle = \langle D(a^i J \circ \varphi_n) \cdot V^i, \mu \rangle - \langle (J \circ \varphi_n) Da^i \cdot V^i, \mu \rangle.
\end{equation}

First, assuming each $a^i$ is differentiable along $E^i$, Eq. 4.7 is valid. Moreover, the second term is a time correlation at time $n$, between the functions $J$ and $Da^i \cdot V^i$. If both these functions
are assumed to be continuous, then the correlation between them decays exponentially in time \[10\]. That is, the second term would approach its mean exponentially fast, for some \(\gamma \in (0, 1)\):  
\[
\langle (J \circ \varphi_n) Da^i \cdot V^i, \mu \rangle - \langle J, \mu \rangle \langle Da^i \cdot V^i, \mu \rangle \sim O(\gamma^n). 
\]

In fact, if \(X\) is assumed to be smooth, \(\sum_{i=1}^{d_n} \langle Da^i \cdot V^i \rangle = 0\) (this result is proved in Theorem 3.1(b) of \[29\]). It then follows that \(\langle J \circ \varphi_n \sum_{i=1}^{d_n} Da^i \cdot V^i \rangle\) exponentially decreases in \(n\), and hence the vector field \(Y_{1:n} := -J \circ \varphi_n Da^i\) potentially forms a part of \(Y_{i:n}\). The restatement in Eq. 4.7 therefore confines the problematic derivative to the first term in Eq. 4.7. We can now focus our attention on the first term to obtain the remainder of \(Y_{i:n}\). Applying measure preservation of \(\varphi\) on the first term, we obtain, for some \(k \in \mathbb{N}\),

\[
\langle D(\alpha^J \circ \varphi_n) \cdot V^i, \mu \rangle = \langle (D(\alpha^J_{n+k}))(k) \cdot V^i_k, \mu \rangle, 
\]

where we have adopted the succinct notation \(J_k\) to denote the function \(J \circ \varphi_k\); we neglect writing the subscript when \(k = 0\). The motivation for using measure preservation forward in time becomes clear in the subsequent steps. Some intuitive reasoning can be immediately made however: \(Y_{i:n}\) is a vector field that captures the ensemble average of the directional derivative of \(J_n := J \circ \varphi_n\), without matching the pointwise derivatives. As a next step, we use the covariance of \(V^i\) to express the integrand in Eq. 4.9 as a linear functional on \(V^i(u)\) since we want to obtain part of \(Y_{i:n}(u)\). Putting \(k = 1\),

\[
\langle D(\alpha^J_n) \cdot V^i, \mu \rangle = \langle (D(\alpha^J_{n+1}))_1 \cdot \frac{T(u,1)V^i}{z^i}, \mu \rangle = \langle D(\alpha^J_{n+1}) \cdot \frac{V^i}{z^i}, \mu \rangle, 
\]

where we have introduced \(z^i(u) := \|T(u,1)V^i(u)\|\), and used the chain rule to go from the second expression to the third. Note that \(\langle \log |z^i|, \mu \rangle = \lambda_i\), and in a uniformly hyperbolic system \(\|z^i\|_\infty > e^{\lambda}/C\). In order to take full advantage of the downscaling offered by the \(z^i\), we again rewrite the integrand in the following way that is valid because \(z^i\) is differentiable along \(E^i\):

\[
\langle D(\alpha^J_n) \cdot V^i, \mu \rangle = \langle (D(\alpha^J_{n+1}/z^i) \cdot V^i, \mu \rangle - \langle J_{n+1} a^i_1 D(1/z^i) \cdot V^i, \mu \rangle. 
\]

One advantage of rewriting is immediately clear – an infinite sum of the second term over \(n\), to obtain the unstable contribution, is well-posed. This is because, similar to the second term in Eq. 4.7, this term is in the form of a time correlation. The other advantage in Eq. 4.11 is that it can be used iteratively to evaluate the left hand side, making the integrand asymptotically smaller in norm. We now develop such an iterative procedure by first noticing that Eq. 4.11 is valid for any bounded function \(J\). Indeed since \(\|a^J_{n+1} \|/ \|a^i z^i\|_\infty \leq \|J\|_\infty \|1/z^i\|_\infty \leq C e^{-\lambda} \|J\|_\infty\), \((a^J_{n+1} a^i z^i)\) is also a bounded function and thus can replace \(J_n\) on the left hand side of Eq. 4.11. Doing this replacement we obtain,

\[
\langle D(a^J_{n+1}/z^i) \cdot V^i, \mu \rangle = \langle D(a^J_{n+2}/(z^i_1 z^i)) \cdot V^i, \mu \rangle - \langle a^J_{n+2} D(1/z^i) \cdot V^i, \mu \rangle. 
\]
Note that \( (z^i u) = \|T(u, 2)V^i(u)\| \); for notational convenience we introduce the scalar function \( y^{ik} = \|T(u, k)V^i(u)\| = \prod_{j=1}^{k-1} z^i_j, k \in \mathbb{N} \). Now Eq. 4.11 can be used as a base for recursion by substituting for the first term on its right hand side using Eq. 4.12. Thus Eq. 4.11 becomes,

\[
\langle D(a^i J_n) \cdot V^i, \mu \rangle = \langle D\left(\frac{a^i J_{n+2}}{y^{i,2}}\right) \cdot V^i, \mu \rangle - \sum_{k=1}^{\infty} \langle \frac{a^i J_{n+k} z^i_k}{y^{i,k}} D(1/z^i) \cdot V^i, \mu \rangle.
\]

Now the recursion can be continued by obtaining an expression for the first term on the right hand side of Eq. 4.13, by using \( (a^i J_{n+2})/(a^i y^{i,2}) \) in place of \( J_n \) and so on. We obtain the following expression in the infinite limit of applying this recursion,

\[
\langle D(a^i J_n) \cdot V^i, \mu \rangle = \lim_{k \to \infty} \langle D(a^i J_{n+k}/y^{i,k}) \cdot V^i, \mu \rangle - \sum_{k=1}^{\infty} \langle \frac{a^i J_{n+k} z^i_k}{y^{i,k}} D(1/z^i) \cdot V^i, \mu \rangle.
\]

In lemma 9.2, we show that the limit in the first term in Eq. 4.14 is 0. In fact, the result that is proved is that for a sequence of bounded functions \( f_n \) which goes to 0 pointwise almost everywhere, the sequence of ensemble averages of directional derivatives along the unstable directions also converges to 0. On applying measure preservation to each summand in the second term of Eq. 4.14, we obtain a series of time correlations of a function \( J \) with another bounded function, so that Eq. 4.14 becomes,

\[
\langle D(a^i J_n) \cdot V^i, \mu \rangle = -\sum_{k=1}^{\infty} \langle \frac{a^i J_n z^i_k}{y^{i,k}} (1/z^i)_{-k} \cdot V^i_{-k}, \mu \rangle.
\]

The second term in the equation above is a converging series because the \( L^\infty \) norms of the integrands are exponentially decreasing with \( k \). More clearly, we have at \( \mu \)-a.e. \( u \) that

\[
\left| \frac{a^i J_n z^i_k}{y^{i,k}} (1/z^i)_{-k} \cdot V^i_{-k} \right| \leq \|a^i\|_\infty \|J\|_\infty \|D(1/z^i) \cdot V^i\|_\infty \frac{z^i_k}{y^{i,k}} \leq C' e^{-\lambda(k-1)},
\]

and hence

\[
\left\| \frac{a^i J_n z^i_k}{y^{i,k}} (1/z^i)_{-k} \cdot V^i_{-k} \right\|_\infty \leq C' e^{-\lambda(k-1)}.
\]

Thus by dominated convergence applied to the sequence \( g_j, j = 1, 2, \cdots \) of bounded functions,

\[
g_j := -\sum_{k=1}^{j} \frac{z^i_k}{y^{i,k}} (1/z^i)_{-k} \cdot V^i_{-k},
\]

we obtain that \( g^i := \lim_{j \to \infty} g_j^i \) is also a bounded function and that Eq. 4.14 becomes,

\[
\langle D(a^i J_n) \cdot V^i, \mu \rangle = -\langle a^i J_n \sum_{k=1}^{\infty} \frac{z^i_k}{y^{i,k}} (1/z^i)_{-k} \cdot V^i_{-k}, \mu \rangle = \langle a^i J_n g^i, \mu \rangle.
\]
By assumption, the summation over $n$ of the left hand side of Eq. 4.17 converges. This implies, since the series on the right hand side must also converge, that $\lim_{n \to \infty} \langle a^i J_n g^i, \mu \rangle = 0$. On the other hand, this limit must be equal to $\langle J, \mu \rangle \langle a^i g^i, \mu \rangle$ since time correlations must decay to 0 on hyperbolic attractors. Thus, we have $\langle a^i g^i, \mu \rangle = 0$ since this is true for any bounded function $J$ that satisfies the assumption that the series $\sum_{n=0}^{\infty} \langle D(a^1 J_n) \cdot V^i, \mu \rangle$ converges. The derivation of Eq. 4.17 and showing that $g^i \in L^\infty$ complete the proof of Theorem 3.1. Finally, note that the ansatz from section 4.4 is also valid. To see this, take

$$Y_2^{i,n} = - \sum_{k=1}^{\infty} \left( \frac{a^i_k J_{n+k} z^i_k}{y^i_k} \right) D(1/z^i),$$

and set $Y_i^{i,n} = Y_1^{i,n} + Y_2^{i,n}$.

### 4.5. Computation of the unstable contribution.

To complete the derivation of a regularized unstable contribution, we can rewrite the first term in Eq. 4.7 by using the expression derived in Eq. 4.17. Thus, we obtain the following regularized unstable contribution,

$$\langle J, \partial_s \mu^i |_{s=0} \rangle_{\text{unstable}} = \sum_{n=0}^{\infty} \left( \langle J_n \sum_{i=1}^{d_u} a^i g^i, \mu \rangle - \sum_{i=1}^{d_u} \langle J_n D a^i \cdot V^i, \mu \rangle \right)$$

$$= \sum_{n=0}^{\infty} \langle J_n \sum_{i=1}^{d_u} (a^i g^i - Da^i \cdot V^i), \mu \rangle.$$

In order to compute the unstable contribution in the form above, we resort to ergodic approximation of the ensemble average. Since we expect the time correlation between the bounded function $g := \sum_{i=1}^{d_u} a^i g^i - Da^i \cdot V^i$ and $J$ to decay exponentially in a uniformly hyperbolic system, the summation over $n$ would converge (to within machine precision of the true unstable contribution) with a small number of terms, when compared to $N$, the trajectory length used for an ergodic average approximation of each term. Thus, the computational time for the unstable contribution is roughly equal to that for evaluating $g$ along $N$ points. The function $g^i$ is naturally in the form of an iteration and thus can be obtained along a trajectory, by solving the following set of $d_u$ scalar equations, $1 \leq i \leq d_u$, setting $\beta_{-1} = 0$,

$$\beta_{k+1}^i = \frac{\beta_k^i}{z_k^i} + D(1/z_k^i) \cdot V_k^i, \quad k = 0, 1, \cdots.$$

The solutions $\beta_k^i$, $K \in \mathbb{Z}^+$, approximate the scalar function $g^i$, asymptotically. That is, for large $K$, $g^i(\varphi_K(u)) \approx -\beta_K^i$. Using this approximation of $g^i$ and a finite difference approximation of $Da^i \cdot V^i$, we can obtain the function $g$ along a primal trajectory starting from a $\mu$-typical phase point $u$. Then, the numerical approximation of the unstable contribution is the following ergodic average,

$$\frac{d \langle J \rangle}{ds}_{\text{unstable}} \approx \frac{1}{N} \sum_{n=0}^{M} \sum_{i=0}^{N-1} J(u_{n+i}) g(u_i).$$

Ignoring the numerical errors in the computation of $g$, Lemma 9.3 shows that the error in the approximation above decays as $O(1/\sqrt{N})$. This completes the proof of Corollary 3.2.
5. Interpretation of the unstable contribution. In the previous section, we rewrote each term of Ruelle’s formula, which represents the ensemble average of an unstable derivative, \( \langle DJ_n \cdot X^n \rangle \), as a time correlation integral \( \langle J_n g, \mu \rangle \) where \( g \) was a bounded distribution that we obtained through an iterative procedure. In this section, we provide physical intuition for \( g \) by relating it to the change in the SRB measure due to a perturbation along \( X^u \).

We start with the simple case in which the SRB measure is absolutely continuous with respect to Lebesgue measure on the whole manifold \( M \). For the derivation of an S3 formula that assumes the existence of a density on the whole manifold, see [8]. Examples of systems where this is true include expanding dynamics on compact attractors that have no stable submanifolds. In these cases, the volume element \( d\mu = \rho \ d\mu \), where \( d\mu = |dx_1 \cdot dx_d| \) is the standard volume element, for some smooth function \( \rho : M \rightarrow \mathbb{R}^+ \). Then, integration by parts of each term of the unstable contribution according to Ruelle’s formula, can be performed as follows,

\[
\langle DJ_n \cdot X^n, \mu \rangle = \int_M \text{div}(DJ_n(\varphi_n)X^n) \rho \ d\mu - \int_M J_n \varphi_n \text{div}X^n \rho \ d\mu \\
(5.1) \quad = \int_M \rho \text{div}(J_n \varphi_n X^n) \ d\mu - \int_M (J_n \varphi_n) \left( \frac{D\rho}{\rho} \cdot X^n + \text{div}(X^n) \right) \rho \ d\mu.
\]

By Stokes theorem, the first term in Eq. 5.1 is a boundary integral that gives the flux of the vector field \( X^u \) at the boundary of \( M \), which is 0. Thus, in this case, the function \( g \equiv -(D\rho \cdot X^u/\rho + \text{div}(X^n)) \). Hence, \( g\rho = -\text{div}(\rho X^u) \). Roughly speaking, Eq. 5.1 captures the average of the function \( J_n \) multiplied by the change in the probability distribution. Hence, this definition of \( \rho g \) matches our intuition since locally, the perturbation \( X^u \) stretches the standard volume \( (d\mu) \) by \( g\rho = -\text{div}(\rho X^u) \). Moreover, as derived in section 4, it is easy to see that \( \langle g, \mu \rangle = \int g\rho \ d\mu = 0 \).

Now consider the more general case where the SRB measure is not absolutely continuous on the whole manifold. Although the derivation of Eq. 5.1 is not valid, an interpretation of the unstable contribution can be made using a similar argument. First we choose a measurable partition, say \( \xi \), such that each partition element \( \xi(u) \) that contains \( u \) lies within the local unstable manifold at \( u \). Since conditional measures of SRB measures along unstable manifolds are absolutely continuous, (see [21, 11] for constructions of measurable partitions and disintegration of SRB measures), we can write the conditional measure of \( \mu \) on \( \xi(u) \) as \( \rho_u(w) \ d\mu \) for some function \( \rho_u \), where \( d\mu = |dx_1 \cdot dx_{d_u}| \) is the standard Euclidean volume element in \( d_u \) dimensions. In coordinates, at any \( w \in \xi(u) \), \( X^u(w) \) can be written as \( X^u(w) = \sum_{k=1}^{d_u} v^k(w) \partial_{x_k} \), for some scalar functions \( v^k \). Using such a disintegration of the SRB measure, each term of the unstable contribution will then have the following form, taking \( a^i = 1 \) for simplicity,

\[
(5.2) \quad \langle DJ_n \cdot \varphi_n X^n, \mu \rangle = \int_{M/\xi} \int_{\xi(u)} \sum_{k=1}^{d_u} v^k(w) \frac{\partial J_n \varphi_n}{\partial x_k} \rho_u(w) \ d\mu dw \ d\hat{\mu},
\]

where \( \hat{\mu} \) is the factor measure defined as the pushforward of \( \mu \) under the projection map \( \pi : M \rightarrow \xi \), which maps a phase point \( u \) to \( \xi(u) \), hence: \( \hat{\mu} = \mu \circ \pi^{-1} \) [11]. From this point, we can treat the \( d_u \)-dimensional inner integral analogously to the previous case of the expanding
map. In particular, we can apply integration by parts to the inner integral, and analogous to Eq. 5.1, we obtain,
\[
\langle D(J \circ \varphi_n) \cdot X^u, \mu \rangle = -\int_{M/\xi} \int_{\xi(u)} J \circ \varphi_n \left( \sum_{k=1}^{d_u} v_k \frac{\partial \rho_u}{\partial x_k} \right) dw \, d\hat{\mu} \\
- \int_{M/\xi} \int_{\xi(u)} J \circ \varphi_n \sum_{k=1}^{d_u} \frac{\partial v_k}{\partial x_k} \rho_u(w) \, dw \, d\hat{\mu}.
\]
(5.3)

Here, again we obtain an integral representing a flux term on the boundaries of \( \xi(u) \), the integral over \( u \) of which is 0, due to cancellations [31]. Then, comparing with Eq. 4.18, we can see that
\[
g \rho_u \equiv -\sum_{k=1}^{d_u} \left( v_k \frac{\partial \rho_u}{\partial x_k} + \frac{\partial v_k}{\partial x_k} \rho_u \right) = -\sum_{k=1}^{d_u} \frac{\partial v_k}{\partial x_k} \rho_u,
\]
which is again a divergence of \( \rho_u X^u \) on pieces of unstable manifolds. While this provides an intuitive interpretation of \( g \), it does not lead to a straightforward computation since the densities on the unstable manifolds, denoted \( \rho_u \) above, are unknown. This justifies resorting to an iterative procedure that we did in section 4, since the formula in 4.18 only makes use of known quantities computed along trajectories. The other primary motive that Eq. 4.18 fulfills is that the algorithm must not involve discretization of the phase space, but remain a Monte Carlo method of computing integrals, which have convergence rates that are independent of the dimension of the phase space.

6. Comments on S3 computation. Revisiting the sketch of the proof in section 3, the first term of Eq. 3.2 appears as is from the split Ruelle’s formula in Eq. 4.1. Piecing together all the work carried out in subsection 4.4, an exponentially converging, regularized expression for the unstable contribution, the second term of Eq. 4.1, is crystallized into Eq. 4.18. Putting these two contributions together in Eq. 4.1 completes the proof of Corollary 3.2. Moreover, the error in the ergodic approximation of Eq. 4.18 decays as \( \mathcal{O}(1/\sqrt{N}) \) using an \( N \)-term ergodic average: this follows from Lemma 9.3. Thus, combining this result with Proposition 9.1, the overall S3 formula has an error that decays as a typical Monte Carlo integration, as we sought.

We now briefly discuss a na"ıve implementation of the S3 formula, postponing an efficient algorithmic implementation (see [7] for a superficial report in the case \( d_u = 1 \)) to a future work. Using a generic initial condition \( u \) sampled according to \( \mu \) on the attractor, a primal trajectory of length \( N \), chosen large enough for convergence of ergodic averages, is obtained from the solution of Eq. 2.1. Along the primal trajectory, we use Ginelli et al.’s algorithm (see [15] for the algorithm and [27] for more details and a new convergence proof) to obtain \( V^i_n, 0 \leq n \leq N - 1, 1 \leq i \leq d_u \). Additionally, we also apply Ginelli et al.’s algorithm to the adjoint cocycle (dual of \( T \)) to obtain a set of adjoint CLVs, also normalized at each \( u \), and denoted as \( W^i_n, 0 \leq n \leq N - 1, 1 \leq i \leq d_u \). Note that since \( E^u(u) \perp E^{u^*}(u) \), \( X^s \cdot W^i = (X - X^u) \cdot W^i = 0 \). This fact is used in order to obtain the stable and unstable components \( X^u_n \) and \( X^s_n \) along a trajectory.

To realize the stable contribution in practice, the iterative equation referred to as the stable tangent equation (Eq. 4.3) is used, as suggested in subsection 4.3. For the unstable
contribution, Eq. 4.18 is computed as an ergodic average. For the computation of each $g^i$, Eq. 4.19 is used as suggested in subsection 4.5. In the numerical examples discussed below, we use both analytical expressions and approximate finite difference calculations to obtain $z^i$ and $D(1/z^i) \cdot V^i$, along trajectories. An algorithm for computation of derivatives of scalar functions along CLVs will be discussed in a future work, along with an adjoint (reverse-mode) algorithm for S3, in the interests of serving a high-dimensional parameter space.

Before we close this section, we comment on the uniform hyperbolicity assumption. Firstly, note that the assumption has been used to obtain the desired error convergence of both the stable and unstable contribution; the split of Ruelle’s formula itself does not require uniform hyperbolicity. In particular, in the stable contribution, we used the uniform rates of contraction of stable vectors, in Proposition 9.1. In the unstable contribution derivation (i.e., in proving Theorem 3.1), and in fact in Ruelle’s linear response formula itself, we use the existence of an SRB measure, which is guaranteed on a compact uniformly hyperbolic attractor. To obtain the error convergence of the unstable contribution, we used exponential decay of correlations and the CLT, which only hold on a hyperbolic attractor, for Hölder continuous functions of some positive Hölder exponent. (see [22] and section 6 of [33]). While the function $J$ is in $C^2$ and hence in a Hölder class, we have only shown boundedness of $g^i$, but assumed exponential decay of correlations with $J$. However, if the two functions satisfy the finite first moment condition of Chernov (see Corollary 1.7 of [10]), the assumption of CLT and exponential decay of correlations would be valid. Moreover, besides these caveats, the assumption of uniform hyperbolicity itself could appear restrictive enough to affect the applicability of our results to high-dimensional dynamical systems encountered in practice. In this regard, it is worth mentioning that in a widely accepted hypothesis due to Gallovotti and Cohen ([14], see also [30] for more comments on this hypothesis), many fluid systems, and more generally, statistical mechanical models, behave as if they were uniformly hyperbolic. Several recent studies also provide supportive evidence, wherein numerical methods that, strictly speaking, assume some hyperbolicity for their derivation and convergence, work well in high-dimensional real-life models (see [9] for an example from climate dynamics and [24] for a turbulent fluid flow simulation).

7. Numerical examples.

7.1. Smale-Williams solenoid map. The Smale-Williams solenoid map is a classic example of low-dimensional hyperbolic dynamics. It is a three-dimensional map given by

$$
\varphi^*(u) = \left[ s_1 + \frac{r - s_1}{4} + \frac{\cos(\theta)}{2}, 2\theta + \frac{s_2}{4} \sin(2\pi\theta), \frac{z}{4} + \frac{\sin(\theta)}{2} \right]^T,
$$

where $u := [r, \theta, z]^T$ in cylindrical coordinates. The attractor is a subset of the solid torus at the reference values of $s_1 = 1.4$ and $s_2 = 0$. The probability distribution on the attractor is an SRB distribution [29, 33] that has a density on the unstable manifolds. In this map, $r$ and $z$ directions form a basis for the stable subspace at each point (and the orthogonal $\theta$ direction forms a basis for the adjoint unstable subspace). Applying a perturbation to $s_1$ causes a stable perturbation, i.e., the unstable contribution is zero, since it affects only the $r$ coordinate. On the other hand, perturbing $s_2$ leads to a nonzero unstable contribution. A set of nodal basis functions along $r$ and $\theta$ is chosen to be the objective function. We use a naïve implementation of the S3 algorithm presented in section 6. In order to validate the S3 computation, we compare the
Figure 1. Comparison of the sensitivities computed with S3 to finite-difference for the solenoid map in Section 7.1. (a) $J$ is a set of two-variable nodal basis functions along $r$ and $\theta$ axes. (b) $J_\theta$ is a set of nodal basis functions along $\theta$ axis.

Figure 2. Comparison of the sensitivities of the nodal basis functions along the $\theta$ and $\phi$ axes to the parameter $s_2$ obtained for the Kuznetsov-Plykin attractor using (a) finite difference and (b) the S3 algorithm.

Sensitivities ($d\langle J \rangle/ds_2$) with finite-difference results generated using 10 billion Monte Carlo samples on the attractor. The sensitivities to the parameter $s_2$ are shown in Figure 1(a). In Figure 1(b), the objective function is a set of nodal basis functions along the $\theta$ direction. From Figures 1(a,b), we see close agreement between the sensitivities computed with (a more general version of) S3 and, finite-difference results, thus validating both the stable and unstable parts of the S3 algorithm.
7.2. Kuznetsov-Plykin map. As a second test case for S3, we consider the Kuznetsov-Plykin map as defined by [19], which describes a sequence of rotations and translations on the surface of the three-dimensional unit sphere. The two parameters we choose to vary are \( s_1 := \epsilon \) and \( s_2 := \mu \), which are defined by [19]. The map is given by \( \varphi_{n+1}^s(u) = f_{1-1} \circ f_{1,1}^s(u) \) where \( u = [x_1, x_2, x_3]^T \in \mathbb{R}^3 \). For the function \( f_{1,1}^s \), and further details regarding the hyperbolicity of the system, the reader is referred to [19]. The probability distribution on the attractor again is again of SRB type, with the existence of a density along the unstable manifolds. We again use a naïve implementation of the S3 formula to compute the sensitivities as in the case of the solenoid map in Section 7.1. The objective function \( J \) is a set of nodal basis functions along the \( \theta \) and \( \phi \) spherical coordinate axes. The finite-difference sensitivities were computed with the central difference around the reference value of \( s_2 = 1 \) by means of 10 billion independent samples on the attractor. The results from S3 agree well with finite-difference sensitivities as shown in Figure 2.

8. Conclusions. We have presented a tangent space-split sensitivity formula to compute the derivatives of statistics to system parameters in chaotic dynamical systems. The algorithm to implement the formula requires the computation of a basis for the tangent and adjoint unstable subspaces along a long trajectory. The stable contribution to the overall sensitivity can be efficiently computed by a conventional tangent/adjoint computation just as in nonchaotic systems. The unstable contribution has been rederived to be expressed as an ergodic average that yields a Monte Carlo convergence. The numerical examples described in Section 7 satisfy the simplifying assumptions of uniform hyperbolicity that were made in the derivation. They show close agreement with finite-difference results, serving as a proof-of-concept for the new formulation. In order to make the new formulation applicable to a high-dimensional problem, more work is needed toward an efficient implementation, particularly for the terms in Eq. 4.19.

9. Appendix.

Proposition 9.1. The error in an \( N \)-term ergodic approximation using the stable tangent equation 4.3, of the stable contribution, decays as \( \mathcal{O}(1/\sqrt{N}) \). That is,

\[
\epsilon_N := \left| \frac{d(J)}{ds} \bigg|_{s_{\text{stable}}} - \frac{1}{N} \sum_{n=0}^{N-1} \mathbf{D}J(u_n) \cdot \zeta_n^s \right| \leq \epsilon^s/\sqrt{N}, \epsilon^s > 0.
\]

Proof. It is easy to check that \( \zeta_n^s := \sum_{i=0}^n \mathcal{T}(u_i, n-i)X_i^s \) satisfies Eq. 4.3. So the approximation to the stable contribution can be written, for some \( M \leq N-1 \) as, where \( \sum_i = 0 \) if \( i > j \),

\[
\frac{1}{N} \sum_{n=0}^{N-1} \sum_{i=0}^{n} \mathbf{D}J(u_n) \cdot \mathcal{T}(u_i, n-i)X_i^s = \frac{1}{N} \sum_{n=0}^{N-1} \sum_{i=n-M}^{n} \mathbf{D}J(u_n) \cdot \mathcal{T}(u_i, n-i)X_i^s \\
- \frac{1}{N} \sum_{n=0}^{M-1} \sum_{i=n-M}^{n-1} \mathbf{D}J(u_n) \cdot \mathcal{T}(u_i, n-i)X_i^s + \frac{1}{N} \sum_{n=M+1}^{N-1} \sum_{i=0}^{n-M-1} \mathbf{D}J(u_n) \cdot \mathcal{T}(u_i, n-i)X_i^s.
\]
Thus,

\[ e_N \leq \left| \frac{1}{N} \sum_{n=0}^{M-1} \sum_{i=1}^{M-n} DJ(u_n) \cdot T(u_{−i}, n + i)X^u_i \right| + \left| \frac{1}{N} \sum_{n=M+1}^{N-1} \sum_{i=0}^{n-M-1} DJ(u_n) \cdot T(u_i, n - i)X^s_i \right| + \left| \frac{d(J)}{ds}_{\text{stable}} - \frac{1}{N} \sum_{n=0}^{N-1} \sum_{i=n-M}^n DJ(u_n) \cdot T(u_i, n - i)X^s_i \right|. \]

Under the uniform hyperbolicity assumption, we know that \( \|T(u, n)X^s(u)\| \leq Ce^{-\lambda n} \). Moreover, we assume that \( \|DJ\|, \|X^s\| \) are bounded functions. Hence, where \( \gamma := \sum_{i=0}^\infty e^{-\lambda i} \),

\[
\begin{align*}
\epsilon_N & \leq \frac{C\gamma^2 \|DJ\|_\infty \|X^s\|_\infty}{N} + \frac{C'\gamma e^{-\lambda(M+1)}(N - (M + 1)) \|DJ\|_\infty \|X^s\|_\infty}{N} \\
& \quad + \left| \frac{d(J)}{ds}_{\text{stable}} - \frac{1}{N} \sum_{n=0}^{N-1} \sum_{i=n-M}^n DJ(u_n) \cdot T(u_i, n - i)X^s_i \right|.
\end{align*}
\]

(9.1)

To obtain an upper bound for the third term, again we use the uniform hyperbolicity assumption. So, the integrand in the right summand of the stable contribution (Eq. 4.1) satisfies \( \|(DJ)_n \cdot T(\cdot, n)X^s(\cdot)\|_\infty \leq C \|DJ\|_\infty \|X^s\|_\infty e^{-\lambda n} \). Hence \( \sum_{n=0}^M (DJ)_n \cdot T(\cdot, n)X^s(\cdot) \|_\infty \leq C \|DJ\|_\infty \|X^s\|_\infty \gamma \), for any \( M \) and by dominated convergence, \( \sum_{n=0}^\infty (DJ)_n \cdot T(\cdot, n)X^s(\cdot) \in L^1(\mu) \), and the stable contribution can be written as,

\[
\frac{d(J)}{ds}_{\text{stable}} = \sum_{i=0}^\infty (DJ)_i \cdot T(\cdot, i)X^s(\cdot, \mu).
\]

Thus the third term in Eq. 9.1 has the following bound,

\[
\left| \frac{d(J)}{ds}_{\text{stable}} - \frac{1}{N} \sum_{n=0}^{N-1} \sum_{i=n-M}^n DJ(u_n) \cdot T(u_i, n - i)X^s_i \right| \\
\leq \left| \sum_{i=0}^M (DJ)_i \cdot T(\cdot, i)X^s(\cdot, \mu) - \frac{1}{N} \sum_{n=0}^{N-1} \sum_{i=n-M}^n DJ(u_n) \cdot T(u_i, n - i)X^s_i \right| \\
+ C\gamma \|DJ\|_\infty \|X^s\|_\infty e^{-\lambda M},
\]

(9.2)

where the second term on the right hand side of Eq. 9.2 again uses uniform hyperbolicity. Applying measure preservation in each of the integrals in the first term of Eq. 9.2,

\[
\left| \frac{d(J)}{ds}_{\text{stable}} - \frac{1}{N} \sum_{n=0}^{N-1} \sum_{i=n-M}^n DJ(u_n) \cdot T(u_i, n - i)X^s_i \right| \\
\leq \left| \sum_{i=0}^M DJ \cdot T(\cdot, i)X^s(\cdot, \mu) - \frac{1}{N} \sum_{n=0}^{N-1} \sum_{i=n-M}^n DJ(u_n) \cdot T(u_i, n - i)X^s_i \right| \\
+ C\gamma \|DJ\|_\infty \|X^s\|_\infty e^{-\lambda M}.
\]

(9.3)
The integrand in 9.3 is continuous on $M$ since $\mathcal{T}(u, n) : E^s(u) \to E^s(u_n)$ is a continuous map and, $DJ(u) : T_u M \to \mathbb{R}$ and $X^s : M \to E^s$ are continuous by assumption. Then we expect that $\sum_{i=0}^N DJ \cdot \mathcal{T}(\varphi_{-i}, i)X^s_{E_i}$ obeys the central limit theorem [10]. Using this in Eq. 9.3, Eq. 9.1, gives, letting $M \to N - 1,$

$$e_N \leq C\gamma^2 \frac{\|DJ\|_{\infty} \|X^s\|_{\infty}}{N} + \frac{\var[\sum_{i=0}^N DJ \cdot X^s]}{\sqrt{N}} + C\gamma \|DJ\|_{\infty} \|X^s\|_{\infty} e^{-\lambda(N-1)} \in O(1/\sqrt{N}).$$

Lemma 9.2. If the pointwise limit of a sequence of bounded functions $\{f_n\}_{n=0}^\infty \subset L^1(\mu)$ vanishes, i.e., $\lim_{n \to \infty} f_n(u) = 0, u \mu - a.e.$, then the sequence $\langle Df_n \cdot V, \mu \rangle$ converges to 0, when $V$ is an unstable vector field differentiable along $E^u$.

Proof. Let $\xi$ be a measurable partition of $M$ such that for $\mu$-a.e. $u$, the element of the partition containing $u$, denoted $\xi(u)$, is contained in a local unstable manifold of $u$, i.e., $\xi(u) \subset W^u(u)$. We assume a $\xi$ constructed according to Ledrappier-Young’s Lemma 3.1.1 [21], and also use the Lyapunov-adapted coordinates introduced there. In a neighborhood of each $u$, let $\Phi_u : M \to [-\delta, \delta]^d \oplus [-\delta, \delta]^d$, be the adapted coordinate system such that $E^u(u), E^s(u)$ are identified with $\mathbb{R}^d, \mathbb{R}^d$ respectively. Ledrappier-Young prove the existence of a measurable function $\delta$ depending on $u$ in order for $\xi$ to be a measurable partition of $M$; note however that in our more specific case of a uniformly hyperbolic compact attractor, we can choose a $\delta$ independently of $u$ (see section 6.2 of [18]).

Furthermore, the image of $W^u(u)$ under $\Phi_u$ is a neighborhood of the origin in $\mathbb{R}^d$, i.e., the last $d_u$ coordinates of $\Phi_u(W^u(u))$ are 0. Let the image of $\xi(u)$ under this map be $B_u \subset [-\delta, \delta]^d_u$. If $x_1, \ldots, x_{d_u}$ are Euclidean coordinate functions in $\mathbb{R}^{d_u}$, the pushforward of $V|\xi(u)(w) \in E^s(w)$ through $\Phi_u$ can be expressed as $V(w) = \sum_{k=1}^{d_u} v_k(x) \partial x_k, w \in \xi(u),$ and $x = \Phi_u(w)$, for differentiable functions $v_k : B_u \to \mathbb{R}$. Since $\xi(u)$ is a measurable partition, we can apply disintegration of $\mu$ on $\xi$, which gives for some measurable set $E$ that $\mu(E) = \int_{\xi} \int_{\xi(u)} 1_E(w) d\mu_{\xi(u)}(w) d\mu(\xi(u))$ [11, 33]. Here the conditional measures of $\mu$ on $\xi(u)$ are denoted as $\mu_{\xi(u)}$ and the factor measure on the quotient space $M/\xi$ is denoted as $\hat{\mu}$. Given that $\mu$ is an SRB measure of $\varphi$, the conditional measure $\mu_{\xi(u)}$ is absolutely continuous with respect to $d_u$-dimensional volume measure, at $\mu$ almost every $u$; let the corresponding probability density function be denoted by $\rho_u : B_u \to \mathbb{R}^+$. Using this setup, each term of the sequence of our interest is, where $dx = |dx_1 \cdots dx_{d_u}|$ is the standard $d_u$-dimensional volume element, and $\hat{f}_n := f_n \circ \Phi_u$.

$$\langle Df_n \cdot V, \mu \rangle = \int_{M/\xi} \int_{B_u} \sum_{k=1}^{d_u} v_k(x) \frac{\partial \hat{f}_n}{\partial x_k}(x) \rho_u(x) \ dx \ d\hat{\mu}. \tag{9.5}$$

Rewriting the integrand we obtain,

$$\langle Df_n \cdot V, \mu \rangle = \int_{M/\xi} \int_{B_u} \sum_{k=1}^{d_u} \frac{\partial}{\partial x_k} (\hat{f}_n v_k \rho_u) \ dx \ d\hat{\mu}$$

$$- \int_{M/\xi} \int_{B_u} \sum_{k=1}^{d_u} \frac{\partial (\rho_u v_k)}{\partial x_k} \ dx \ d\hat{\mu}. \tag{9.6}$$
The first term goes to zero at each $n$ due to cancellations along the boundaries of $B_u$ at different $u$ [31]. To see this, choose a finite cover $\bigcup_{i \leq r} \xi(u_i) \supset M$ and take a partition of unity supported on each $B_u = \Phi_u(\xi(u_i))$ so that the integrals on the boundaries of $B_u$ are 0. Using dominated convergence, the second term converges to 0 as $n \to \infty$ at $u$ almost every $u$. Hence $\lim_{n \to \infty} \langle D f_n \cdot V, \mu \rangle = 0$.

Lemma 9.3. The approximate formula Eq. 4.20 for the unstable contribution has an error that decays as $O(1/\sqrt{N})$: $e_{N,M} := \left| \langle J, \partial_n \mu \rangle_{\text{unstable}} - \frac{1}{N} \sum_{i=0}^{N-1} J(u_{n+i})g(u_i) \right| \leq c^u/\sqrt{N}$, as $M \to N$, for some $c^u > 0$.

Proof. Suppose that the central limit theorem applies to the function $\sum_{n=0}^{M} J \circ \varphi_n g$. Then, we can say that, for a sufficiently large $N$,

\begin{equation}
\left| \frac{1}{N} \sum_{i=0}^{N-1} \sum_{n=0}^{M} J(u_{n+i})g(u_i) - \langle \sum_{n=0}^{M} J \circ \varphi_n g, \mu \rangle \right| \leq \frac{c_1}{\sqrt{N}}.
\end{equation}

Further assuming that the decay of correlations between $J \circ \varphi_n$ and $g$ is exponentially fast, we have, for every $n \in \mathbb{Z}^+$,

\begin{equation}
|\langle J \circ \varphi_n g, \mu \rangle - \langle J \rangle| \leq c_2 \gamma^n, \quad 0 \leq \gamma < 1.
\end{equation}

Since we have already shown in the main text (subsection 4.5) that $\langle g \rangle = 0$, Eq. 9.8 gives $|\langle J \circ \varphi_n g, \mu \rangle| \leq c_2 \gamma^n$. Thus, considering the sequence of functions $h_m := \sum_{n=0}^{m} J \circ \varphi_n g$,

\begin{equation}
|\langle h_m, \mu \rangle| \leq c_2 \sum_{n=0}^{m} \gamma^n \leq c_2/(1 - \gamma).
\end{equation}

Thus, $\{h_m\} \in L^1(\mu)$ and $\|h_m\|_1 \leq c_2/(1 - \gamma)$, and so by dominated convergence theorem, we have that, $\sum_{n=0}^{\infty} \langle J \circ \varphi_n g, \mu \rangle = \langle \sum_{n=0}^{\infty} J \circ \varphi_n g, \mu \rangle$. Then, again using Eq. 9.8, we have

\begin{equation}
\left| \sum_{n=0}^{\infty} \langle J \circ \varphi_n g, \mu \rangle - \sum_{n=0}^{M} \langle J \circ \varphi_n g, \mu \rangle \right| \leq c_2 \gamma^M/(1 - \gamma).
\end{equation}

Finally,

\begin{equation}
\epsilon_{N,M} \leq \frac{1}{N} \sum_{i=0}^{N-1} \sum_{n=0}^{M} J(u_{n+i})g(u_i) - \langle \sum_{n=0}^{M} J \circ \varphi_n g, \mu \rangle + \sum_{n=0}^{\infty} \langle J \circ \varphi_n g, \mu \rangle - \langle \sum_{n=0}^{M} J \circ \varphi_n g, \mu \rangle
\end{equation}

which using Eq. 9.7 and Eq. 9.10 gives,

\begin{equation}
\epsilon_{N,M} \leq c_2 \gamma^M/(1 - \gamma) + \frac{c_1}{\sqrt{N}}.
\end{equation}

Taking the limit $M \to N$, this results in $\epsilon_{N,N} \in O(1/\sqrt{N})$. 

\end{proof}
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REFERENCES

[1] L. Arnold, The Multiplicative Ergodic Theorem on Bundles and Manifolds, Springer Berlin Heidelberg, Berlin, Heidelberg, 1998, pp. 163–199, https://doi.org/10.1007/978-3-662-12878-7_4, https://doi.org/10.1007/978-3-662-12878-7_4.

[2] V. Baladi, Dynamical zeta functions and dynamical determinants for hyperbolic maps, Springer, 2018, https://doi.org/10.1007/978-3-319-77661-3.

[3] P. J. Blonigan, Adjoint sensitivity analysis of chaotic dynamical systems with non-intrusive least squares shadowing, Journal of Computational Physics, 348 (2017), pp. 803–826, https://doi.org/10.1016/j.jcp.2017.08.002.

[4] P. J. Blonigan and Q. Wang, Probability density adjoint for sensitivity analysis of the mean of chaos, Journal of Computational Physics, 270 (2014), pp. 660 – 686, https://doi.org/https://doi.org/10.1016/j.jcp.2017.08.002.

[5] J. Capecelatro, D. J. Bodony, and J. B. Freund, Adjoint-based sensitivity and ignition threshold mapping in a turbulent mixing layer, Combustion Theory and Modelling, (2018), pp. 1–33, https://doi.org/10.2514/6.2017-0846.

[6] N. Chandramoorthy, P. Fernandez, C. Talnikar, and Q. Wang, Feasibility analysis of ensemble sensitivity computation in turbulent flows, AIAA Journal, 57 (2019), pp. 4514–4526, https://doi.org/10.2514/1.J058127, https://doi.org/10.2514/1.J058127, https://arxiv.org/abs/10.2514/1.J058127.

[7] N. Chandramoorthy and Q. Wang, Sensitivity computation of statistically stationary quantities in turbulent flows, in AIAA Aviation 2019 Forum, https://doi.org/10.2514/6.2019-3426, https://arc.aiaa.org/doi/abs/10.2514/6.2019-3426.

[8] N. Chandramoorthy, Z.-N. Wang, Q. Wang, and P. Tucker, Toward computing sensitivities of average quantities in turbulent flows, Center for Turbulence Research Summer Program 2018, (2018), https://arxiv.org/abs/1902.11112.

[9] M. D. Chekroun, J. D. Neelin, D. Kondrashov, J. C. McWilliams, and M. Ghil, Rough parameter dependence in climate models and the role of ruelle-pollicott resonances, Proceedings of the National Academy of Sciences, 111 (2014), pp. 1684–1690, https://doi.org/10.1073/pnas.1321816111.

[10] N. I. Chernov, Limit theorems and markov approximations for chaotic dynamical systems, Probability Theory and Related Fields, 101 (1995), pp. 321–362, https://doi.org/10.1007/BF01200500, https://doi.org/10.1007/BF01200500.

[11] V. Climenhaga and A. Katok, Measure theory through dynamical eyes, 2012, https://arxiv.org/abs/1208.4550.

[12] C. Grebogi, E. Ott, and J. A. Yorke, Unstable periodic orbits and the dimensions of multifractal chaotic attractors, Phys. Rev. A, 37 (1988), pp. 1711–1724, https://doi.org/10.1103/PhysRevA.37.1711, https://link.aps.org/doi/10.1103/PhysRevA.37.1711.
[18] A. Katok and B. Hasselblatt, *Introduction to the modern theory of dynamical systems*, vol. 54, Cambridge University Press, 1997, https://doi.org/10.1017/CBO9780511809187.

[19] S. P. Kuznetsov, *Plykin-type attractor in nonautonomous coupled oscillators*, Chaos: An Interdisciplinary Journal of Nonlinear Science, 19 (2009), p. 013114, https://doi.org/10.1063/1.3072777, https://aip.scitation.org/doi/10.1063/1.3072777, https://arxiv.org/abs/https://doi.org/10.1063/1.3072777.

[20] D. Lasagna, *Sensitivity analysis of chaotic systems using unstable periodic orbits*, SIAM Journal on Applied Dynamical Systems, 17 (2018), pp. 547–580, https://doi.org/10.1137/17M114354X, https://arxiv.org/abs/https://doi.org/10.1137/17M114354X.

[21] F. Ledrappier and L.-S. Young, *The metric entropy of diffeomorphisms: Part I: Characterization of measures satisfying Pesin’s entropy formula*, Annals of Mathematics, (1985), pp. 509–539.

[22] C. Liverani, *Central limit theorem for deterministic systems*, in International Conference on Dynamical Systems (Montevideo, 1995), vol. 362, 1996, pp. 56–75.

[23] V. Lucarini, *Response operators for Markov processes in a finite state space: Radius of convergence and link to the response theory for axiom a systems*, Journal of Statistical Physics, 162 (2016), pp. 312–333, https://doi.org/10.1007/s10955-015-1409-4, https://doi.org/10.1007/s10955-015-1409-4.

[24] A. Ni, *Hyperbolicity, shadowing directions and sensitivity analysis of a turbulent three-dimensional flow*, Journal of Fluid Mechanics, 863 (2019), p. 644669, https://doi.org/10.1017/jfm.2018.986.

[25] A. Ni and C. Talnikar, *Adjoint sensitivity analysis on chaotic dynamical systems by non-intrusive least squares adjoint shadowing (nilsas)*, Journal of Computational Physics, 395 (2019), pp. 690 – 709, https://doi.org/10.1016/j.jcp.2019.06.035, http://www.sciencedirect.com/science/article/pii/S0021999119304437.

[26] A. Ni and Q. Wang, *Sensitivity analysis on chaotic dynamical systems by non-intrusive least squares shadowing (nilss)*, Journal of Computational Physics, 347 (2017), pp. 56–77, https://doi.org/10.1016/j.jcp.2017.06.033.

[27] F. Noethen, *A projector-based convergence proof of the Ginelli algorithm for covariant Lyapunov vectors*, Physica D: Nonlinear Phenomena, 396 (2019), pp. 18 – 34, https://doi.org/10.1016/j.physd.2019.02.012, http://www.sciencedirect.com/science/article/pii/S0167278919302549.

[28] J. E. Peter and R. P. Dwight, *Numerical sensitivity analysis for aerodynamic optimization: A survey of approaches*, Computers & Fluids, 39 (2010), pp. 373–391, https://doi.org/10.1016/j.compfluid.2009.09.013.

[29] D. Ruelle, *Differentiation of srb states*, Communications in Mathematical Physics, 187 (1997), pp. 227–241, https://doi.org/10.1007/s002200050134.

[30] D. Ruelle, *General linear response formula in statistical mechanics, and the fluctuation-dissipation theorem far from equilibrium*, Physics Letters A, 245 (1998), pp. 220 – 224, https://doi.org/https://doi.org/10.1016/S0375-9601(98)00419-8, http://www.sciencedirect.com/science/article/pii/S0375960198004198.

[31] D. Ruelle, *Differentiation of srb states: correction and complements*, Communications in Mathematical Physics, 234 (2003), pp. 185–190, https://doi.org/10.1007/s00220-002-0779-2.

[32] Q. Wang, *Convergence of the least squares shadowing method for computing derivative of ergodic averages*, SIAM Journal on Numerical Analysis, 52 (2014), pp. 156–170, https://doi.org/10.1137/130917665.

[33] L.-S. Young, *Statistical properties of dynamical systems with some hyperbolicity*, Annals of Mathematics, 147 (1998), pp. 585–650, https://doi.org/10.2307/120960.