ABSTRACT. For discrete time systems, we show that the derivative of the (measure) transfer operator with respect to the system parameters is a divergence. Then, for physical measures of hyperbolic chaotic systems, we derive an equivariant divergence formula for the unstable derivative of transfer operators. This formula and hence the derivative of physical measures can be sampled by only $2u + 1$ recursive relations on one orbit, where $u$ is the unstable dimension. The numerical implementation of this formula in [39] is neither cursed by dimensionality nor the butterfly effect.

**Keywords.** transfer operator, unstable divergence, SRB measures, linear response, fast response algorithm.

1. **Introduction**

1.1. **Literature review.**

The transfer operator, also known as the Ruelle-Perron-Frobenius operator, describes how the density of a measure is evolved by a map, and is frequently used to study the behavior of dynamical systems. The transfer operator was historically used for expanding maps because it makes the density smoother. The anisotropic Banach space of Gouëzel, Liverani, and Baladi extends the operator theory to hyperbolic maps, which has both expanding and contracting directions [26, 27, 5]. The unique eigenvector corresponding to the largest eigenvalue, 1, is the physical measure, or the SRB measure; it encodes the long-time statistics of the system, and is typically singular with respect to the Lebesgue measure.

The derivative of the transfer operator with respect to system parameters is useful in several settings, especially in the linear response, which is the derivative of the physical measure [44, 15, 4, 21]. The operator formula is particularly attractive in numerical computations because it is not affected by the exponential growth of unstable vectors.

When the phase space is high-dimensional, the cost of resolving the phase space is cursed by dimensionality (see appendix A), and it is typically much more efficient to sample the measure by an orbit. It is natural to ask if the derivative operator and hence the linear response can also be sampled by an orbit; this is impossible for the entire derivative operator, which is typically singular for physical measures, and is
not pointwisely defined. Similarly, the two most well-known linear response formulas, the ensemble formula and the operator formula, are not well-defined pointwisely.

However, we typically only need the transfer operator to handle the unstable perturbations, which turns out to be pointwisely well-defined. There were pioneering works concerning pointwise formulas of the unstable part of the linear response, though they were not very clearly related to the perturbation of unstable transfer operators. Ruelle mentioned how to derive a pointwise defined formula for the unstable divergence, but no explicit formulas were given [45, lemma 2]. Gouëzel and Liverani gave an explicit pointwise formula via a cohomologous potential function, but the differentiation is in the stable subspace, which typically has very high dimension [27, proposition 8.1]. It is also difficult to obtain coordinate-independent formulas.

In this paper, we derive a new divergence formula for the unstable perturbation of unstable transfer operators on physical measures, which naturally handles the unstable part of the linear response. Compared to previous works, our formula has a more direct physical meaning, simpler derivation, and is coordinate independent. More importantly, our formulas are recursive: to evaluate the formula, we only need to track the evolution of $2\mathbf{u} + 1$ vectors or covectors. Furthermore, the number of recursive relations we involve is minimal.

Our work bridges two previously competing approaches for computing the linear response, the orbit/ensemble approach and the measure/operator approach. That is, we should add up the orbit change caused by stable/shadowing perturbations and the measure change caused by unstable perturbations; both changes are sampled by an orbit. Our work may be viewed as the generalization of the well-known MCMC (Markov Chain Monte Carlo) method for sampling derivatives of transfer operators and physical measures.

Our work is also inspired by our recent numerical algorithm, the fast response algorithm, for computing the linear response on a sample orbit [37]. This paper generalizes the previous results to derivative operators using a new and intuitive proof by transfer operators. Our generalization is crucial for the study of transient perturbations and the development of the fast adjoint response algorithms, whose cost is almost independent of the number of parameters. The fast adjoint response algorithm generalizes the well-known backpropagation method to hyperbolic chaotic neural networks, where gradient explosion and vanishing are abundant [39].

1.2. Main results.

Section 2 proves theorem 1, that is, when the measure has a smooth density, the transfer operator $\tilde{\mathcal{L}}$ of a perturbation diffeomorphism $\tilde{f}$ is a divergence. This is the mass continuity equation on Riemannian manifold. It can be proved simply by an integration by parts, but we shall also give a pointwise proof which is more useful on submanifolds.

Theorem 1 (mass continuity equation). For a measure with fixed smooth density $h$, and any $\tilde{f}$ such that $\delta \tilde{f} = X$, then

$$\frac{\delta \tilde{\mathcal{L}} h}{h} = \frac{\text{div}(hX)}{h} =: \text{div}_h X.$$

For physical measures of hyperbolic attractors, section 3 proves theorem 2, which is a new formula for the transfer operator $\delta \tilde{\mathcal{L}}^u$ of the unstable perturbation $X^u$ on
the conditional measure $\sigma$ on unstable manifolds. Appendix B gives another proof of this formula using a previous result [37]. The main significance is that this formula is pointwisely defined and it involves only $(2u + 1)$ recursive relations on an orbit. This number should be close to the fewest possible, since we need at least $u$ modes to capture all the unstable perturbative behaviors of a chaotic system.

**Theorem 2** (equivariant divergence formula).

\[
\text{div}^u \sigma X^u := -\frac{\delta \tilde{L}^u \sigma}{\sigma} = \text{div}^u X + (S(\text{div}^u f_\ast)) X.
\]

Here $\text{div}^u$ is the contraction by the unit unstable hypercube and its co-hypercube in the adjoint unstable subspace, so $\text{div}^u f_\ast$ is a covector. $S$ is the adjoint shadowing operator and $\omega := S(\text{div}^u f_\ast)$ is the only bounded covector field such that $\omega = f^* \omega + \text{div}^u f_\ast$. Note that $X^u$ is not differentiable, so $\text{div}^u X^u$, the unstable submanifold divergence under conditional measure $\sigma$, is defined via the equivalence in the smooth situation in theorem 1. Hence, we can not directly use theorem 1, since it involves exploding intermediate quantities.

Section 4 shows how to use the equivariant divergence formula to compute the linear response recursively on an orbit. We do not reprove the linear response, the focus is to sample on an orbit. In high-dimensional phase spaces, sampling by an orbit is much more efficient than finite element methods, whose cost is estimated in appendix A on a simple example.

The numerical implementation of our formulas is in [39]; the so-called fast adjoint response algorithm is very efficient in high dimensional phase spaces; it is also robust in stochastic noise and some nonuniform hyperbolicity. Its cost is cursed by neither the dimensionality nor the butterfly effect, and the cost is almost independent of the number of parameters.

2. **DIVERGENCE FORMULA OF DERIVATIVE OPERATOR**

We first assume that the measure on which we apply the transfer operator is smooth ($C^\infty$) and apriorily known. For this simple case, we can choose from many sampling schemes for the underlying measure, then integrate our divergence formula to get the derivative operator. Some sampling methods, such MCMC, sample by an orbit; but an orbit is not necessary here.

2.1. **A functional proof.**

We denote the background $M$-dimensional Riemannian manifold by $\mathcal{M}$. Let the perturbation $\tilde{f}$ be a smooth diffeomorphism on $\mathbb{R}^M$ smoothly parameterized by $\gamma$, with $|f|_{\gamma=0}$ being the identity map. More specifically, we assume the map $\gamma \mapsto \tilde{f}$ is $C^r$ from $\mathbb{R}$ to $C^r$ for any large $r$. For a fixed measures with a smooth density function $h$, the transfer operator $\tilde{L}$ gives the new density function after pushing forward by $\tilde{f}$. More specifically, $\tilde{L}$ of $\tilde{f}$ is defined by the duality

\[
\int h \cdot (\Phi \circ \tilde{f}) =: \int \tilde{L} h \cdot \Phi,
\]

where $\Phi$ is any smooth observable function. Note that $\tilde{L}$ operates on the entire density function, and $L h(x) := (L h)(x)$. In this paper, all integrals are taken with respect to the Lebesgue measure, except when another measure is explicitly mentioned.
We are interested in how perturbations in $\gamma$ would affect $\tilde{L}$. Define
\[ \delta(\cdot) := \frac{\partial(\cdot)}{\partial \gamma} \bigg|_{\gamma=0}. \]
We emphasize that when a function has more than one variables, $\delta$ is the partial derivative. Define the perturbation vector field $X$ as
\[ X := \delta \tilde{f}. \]
For this paper, we only consider the derivatives at $\gamma = 0$. Hence, we can freely assume the value of $\partial \tilde{f}/\partial \gamma$ for any $\gamma \neq 0$, so long as it is smooth and its value at $\gamma = 0$ is $X$. Without loss of generality, we may assume that $\tilde{f}$ is the flow of $X$. If so, and regarding $\gamma$ as ‘time’, then theorem 1 is exactly the mass continuity equation on Riemannian manifold.

We define $\text{div}_h$ as the divergence under the measure $h$,
\[ \text{div}_h X := \text{div}(hX) = \text{div}(X) + \frac{X(h)}{h}. \]
For two measures $h'$ and $h''$, if $h' \propto h''$, that is, $h' = Ch''$ for a constant $C > 0$, then $\text{div}_{h'} = \text{div}_{h''}$.

**Proof.** (theorem 1) Differentiate equation (1), notice that $\delta(\Phi \circ \tilde{f}) = \delta \tilde{f}(\Phi) = X(\Phi)$, where $X(\cdot)$ is to differentiate a function in the direction of $X$, we have
\[ \int \delta \tilde{L}h \cdot \Phi = \int h \cdot \delta(\Phi \circ \tilde{f}) = \int h \cdot X(\Phi). \]
We call the left hand side the operator formula, and the right side the Koopman formula for the perturbation.

First assume that $h$ is compactly supported, then there is no boundary term for integration-by-parts, and we have
\[ \int \delta \tilde{L}h \cdot \Phi = \int h \cdot X(\Phi) = -\int \text{div}(hX) \cdot \Phi. \]
Since this holds for any $\Phi$, it must be $\delta \tilde{L}h = -\text{div}(hX)$. When $h$ is not compactly supported, just apply a smooth cutoff function. □

**2.2. A pointwise proof.**

This section derives $\delta \tilde{L}$ using the pointwise definitions of $\tilde{L}$, which is useful later when we consider perturbations on the conditional measure on unstable manifolds. Note that $\tilde{L}$ is equivalently defined by a pointwise expression,
\[ \tilde{L}h(x) := \frac{h}{|\tilde{f}_s|}(y) \quad \text{where} \quad y := \tilde{f}^{-1}x. \]
Here the point $x$ is fixed, and $y$ varies according to $\gamma$. $|\tilde{f}_s|$ is the Jacobian determinant, or the norm as an operator on $M$-vectors,
\[ |\tilde{f}_s| := \frac{|\tilde{f}_s e|}{|e|}, \quad \text{where} \quad e = e_1 \wedge \cdots \wedge e_M. \]
Here $e_i$'s are smooth 1-vector fields; $e$ is a smooth $M$-vector field, which is basically an $M$-dimensional hyper-cube field, and $|\cdot|$ is its volume. Here $\tilde{f}_s$ is the Jacobian matrix. Note that $|\tilde{f}_s|$ is independent of the choice of basis, and we expect this independence to hold throughout our derivation.
The volume of $M$-vectors, $|\cdot|$, is a tensor norm induced by the Riemannian metric, 

$$|e| := \langle e, e \rangle^{0.5}.$$ 

For two 1-vectors, $\langle \cdot, \cdot \rangle$ is the typical Riemannian metric. For simple $M$-vectors, 

$$\langle e, r \rangle := \det \langle e_i, r_j \rangle,$$

where $e = e_1 \wedge \cdots \wedge e_u$, $r = r_1 \wedge \cdots \wedge r_u$, $e_i, r_j \in T \mathcal{M}$. When the operands are summations of simple $M$-vectors, the inner-product is the corresponding sum.

Applying $\delta$ on both side of equation (3), notice that $h$ is fixed, also that $|\tilde{f}_*| = 1$ when $\gamma = 0$, we have

$$\delta L h = \delta y(h) - h \frac{d}{d\gamma}(|\tilde{f}_*|(y)).$$

Here $\delta y = -X$, and we use it to differentiate $h$ in the coordinate variable. Note that $\frac{d}{d\gamma}$ is the total derivative: $\tilde{f}$ has two direct parameters $y$ and $\gamma$, $y$ implicitly depends on $\gamma$. Substituting the following lemma into equation (4), we get a pointwise proof of theorem 1.

**Lemma 1.** $\frac{d}{d\gamma}(|\tilde{f}_*|(y)) = \text{div } X$, where $X := \delta \tilde{f}$.

**Proof.** By the chain rule, the total derivative is

$$\frac{d}{d\gamma}(|\tilde{f}_*|(y)) = \delta |\tilde{f}_*|(x) + \delta y(|\tilde{f}_*|(x)).$$

Since $|\tilde{f}_*| \equiv 1$ at $\gamma = 0$, the second term is zero. The first term $\delta |\tilde{f}_*|$ is the partial derivative with respect to $\gamma$ while fixing $x$. For any $u$-vector $e$ at $x$, by the Leibniz rule,

$$\delta |\tilde{f}_*| = \frac{\delta \langle \tilde{f}_* e, \tilde{f}_* e \rangle^{0.5}}{|e|} = \frac{1}{2|\tilde{f}_* e||e|} \sum_{i=1}^{M} 2 \langle \tilde{f}_* e_1 \wedge \cdots \wedge \delta \tilde{f}_* e_i \wedge \cdots \wedge \tilde{f}_* e_M, \tilde{f}_* e \rangle$$

$$= \frac{1}{|e|^2} \sum_{i=1}^{M} \langle e_1 \wedge \cdots \wedge \delta \tilde{f}_* e_i \wedge \cdots \wedge e_M, e \rangle = \sum_{i=1}^{M} \varepsilon^i \delta \tilde{f}_* e_i,$$

where $\varepsilon^i$ is the $i$-th covector in the dual basis of $\{e_i\}_{i=1}^{M}$.

We use $\nabla_{e_i}$ to denote the partial (Riemannian) derivative in the location variable in the direction of $e_i$. Then $\tilde{f}_* e_i = \nabla_{e_i} \tilde{f}$. We can change the order of the derivative in the location and the derivative in the parameter, hence

$$\delta \tilde{f}_* e_i = \frac{\partial}{\partial \gamma} \nabla_{e_i} \tilde{f} = \nabla_{e_i} \frac{\partial}{\partial \gamma} \tilde{f} = \nabla_{e_i} X.$$ 

Hence, we see that $\delta |\tilde{f}_*$ is the contraction of $\nabla X$: this is another definition of the divergence, which is independent of the choice of the basis $\{e_i\}_{i=1}^{M}$. □

3. **Equivariant divergence formula for the unstable perturbation of transfer operator**

Many important measures typically live in high dimensions, such as physical measures of chaotic systems. Efficient handling of such measures requires sampling by an orbit, since it is very expensive to resolve a high-dimensional phase space by
finite elements, for which we give a rough cost estimation in appendix A. But \( \delta \tilde{L} \) is not even pointwisely defined for typical physical measures. However, we only need the derivative operator to handle the unstable perturbations; the stable perturbations are typically computed by the Koopman formula on the right of equation (2).

In this section, we derive the equivariant divergence formula of the unstable perturbation operator on the unstable manifold. The formula is pointwisely defined, moreover, it is in the form of a few recursive relations on one orbit. As shown in figure 1, we first write the derivative operator as the derivative of the ratio between two volumes. Then we can obtain an expansion formula, which can be summarized into a recursive relation using the adjoint shadowing lemma.

3.1. Notations.

We assume the dynamical system of the \( C^\infty \) diffeomorphism \( f \) has a mixing axiom \( A \) attractor. There is a continuous \( f_* \)-equivariant splitting of the tangent vector space into stable and unstable subspaces, \( V^s \oplus V^u \), such that there are constants \( C > 0, 0 < \lambda < 1 \), and

\[
\max_{x \in K} |f_*^n|V^u(x)|, |f_*^n|V^s(x)| \leq C\lambda^n \quad \text{for } n \geq 0,
\]

where \( f_* \) is the Jacobian matrix. Define oblique projection operators \( P^u \) and \( P^s \), such that

\[
X = P^u X + P^s X, \quad X^u := P^u X \in V^u, \quad X^s := P^s X \in V^s.
\]

The stable and unstable manifolds, \( V^s \) and \( V^u \), are submanifolds tangential to the equivariant subspaces. We also use \( u \) to denote the unstable dimension. Under our assumptions, the physical measure, defined as the limit of an orbit, is also SRB, which is smooth on the unstable manifold.

We introduce some general notations to be used. We use subscripts \( i \) and \( j \) to label directions, and use subscripts \( m, n, k \) to label steps. Denote

\[
e_k(x) := e(f^k x).
\]

Let \( \{e_i\}_{i=1}^M \) be a basis vector field of \( \mathbb{R}^M \) such that \( \text{span}\{e_i\}_{i=1}^u = V^u \); we further require that

\[
|e| = 1, \quad \text{where } e := e_1 \wedge \cdots \wedge e_u.
\]

Let \( \{\varepsilon^i\}_{i=1}^M \) be the dual basis covector field of \( \{e_i\}_{i=1}^M \), that is,

\[
\varepsilon^i e_j = \begin{cases} 1, & \text{if } i = j; \\ 0, & \text{otherwise}. \end{cases}
\]

We further require that

\[
\varepsilon(e) = 1, \quad \text{where } \varepsilon := \varepsilon^1 \wedge \cdots \wedge e^u.
\]

In other words, \( \varepsilon \) takes out the unstable component of \( u \)-vectors.

We use \( \nabla_Y X \) to denote the (Riemann) derivative of the vector field \( X \) along the direction of \( Y \). \( \nabla_Y f_* \), the derivative of the Jacobian, is the Hessian matrix, such that

\[
\nabla_{f_* Y}(f_* X) = (\nabla_Y f_*) X + f_* \nabla_Y X.
\]
This is essentially the Leibniz rule. Note that \((\nabla_Y f_*) X = (\nabla_X f_*) Y\). Denote 
\[
\nabla_x X := \sum_{i=1}^u e_1 \wedge \cdots \wedge \nabla_{e_i} X \wedge \cdots \wedge e_u, \quad \nabla_X e := \sum_{i=1}^u e_1 \wedge \cdots \wedge \nabla_X e_i \wedge \cdots \wedge e_u.
\]

One of the slots of \(\nabla (\cdot) f_*(\cdot)\) can take a \(u\)-vector, in which case 
\[
(\nabla_X f_*) e := \sum_{i=1} f_{e_i} e_1 \wedge \cdots \wedge (\nabla_{e_i} f_*) X \wedge \cdots \wedge f_* e_u,
\]
\[
\nabla f_* e X := \sum_{i=1} f_{e_i} X \wedge \cdots \wedge f_* e_i \wedge \cdots \wedge e_u.
\]

There are two different divergences on an unstable manifold, which coincide only if \(u = M\). The first divergence is taken within the unstable submanifold, 
\[
div^u X^u := \langle \nabla e X, e \rangle.
\]

We call this the submanifold unstable divergence, or \(u\)-divergence.

The second kind of unstable divergence might be more essential for hyperbolic systems. Define the equivariant unstable divergence, or \(v\)-divergence, as 
\[
div^v X^u := \varepsilon \nabla e X^u.
\]

We define the \(v\)-divergence of the Jacobian matrix \(f_*\), 
\[
div^v f_* := \frac{\varepsilon_1 \nabla e f_*}{|f_* e|}, \quad \quad \text{(div}^v f_*) X := \frac{\varepsilon_1 (\nabla e f_*) X}{|f_* e|}, \quad \text{where} \quad \varepsilon_1(x) := \varepsilon(f x).
\]

Note that \(\text{div}^v f_*\) is a Holder continuous covector field on the attractor.

### 3.2. One volume ratio for the entire unstable perturbation operator.

We define the unstable perturbation on the unstable manifold as the composition of a perturbation of \(\tilde{f}\) and a projection along stable manifolds. As illustrated in figure 1, fix \(x\), let \(\mathcal{V}^u(x)\) be the unstable manifold through \(x\); for any \(\gamma\), \(\mathcal{V}^{u\gamma} := \{\tilde{f}(z) : z \in \mathcal{V}^u\}\) is a \(u\)-dimensional manifold. For any \(z \in \mathcal{V}^{u\gamma}\), denote the stable manifold that goes through it by \(\mathcal{V}^s(z)\). Define \(\xi(z)\) as the unique intersection point of \(\mathcal{V}^s(z)\) and \(\mathcal{V}^u(x)\).

Since \(\delta \tilde{f} = X\) is the perturbation and \(\xi\) is the projection along stable directions, \(\delta(\xi \tilde{f}) = X^u\). Note that \(\delta\) is partial derivative.

**Figure 1.** Definitions. Here \(y + X\gamma\) means to start from \(y\) and flow along the direction of \(X\) for a length of \(\gamma\). Roughly speaking, 
\[
\tilde{L}^u \sigma/\sigma(x) = (l_2 + l_1)/l_1 = (l_2' + l_1')/l_1',
\]
where \(l_1, l_2\) are lengths of dotted lines.
We define $\tilde{L}^u$ as the transfer operator of $\xi \tilde{f} : \mathcal{V}^u \to \mathcal{V}^u$. Since $\delta(\xi \tilde{f}) = X^u$, $\delta \tilde{L}^u$ is the perturbation by $X^u$. Denote the conditional measure at $\gamma = 0$ by $\sigma$, fix a point $x$, we want to compute $\delta \tilde{L}^u \sigma(x)$. Let $y = (\xi \tilde{f})^{-1} x$, by the pointwise definition of $\tilde{L}^u$,

$$\tilde{L}^u \sigma(x) = \frac{\sigma}{|\xi_s f_s|} \circ \tilde{f}^{-1}(x) = \frac{\sigma(y)}{\sigma(x) |f_s(y)| |\xi_s(fy)|}.$$

Roughly speaking, we dissect the perturbation by $X^u$ into the perturbation of $X$ subtracting the perturbation of $X^s$.

**Lemma 2** (A volume ratio). Let $e_{-k}$ be the unit $u$-vector field on $\mathcal{V}^u(x_{-k})$,

$$\frac{\tilde{L}^u \sigma}{\sigma}(x) = \lim_{k \to \infty} \frac{|f_{x}^{2k} e_{-k}(x_{-k})|}{|f_{x}^{k} e_{-k}(y_{-k})|}.$$

**Proof.** First, we find an expression for $\sigma$ by considering how the Lebesgue measure on $\mathcal{V}^u(x_{-k})$ is evolved. The mass contained in the cube $e_{-k}$ is preserved via pushforwards, but the volume increased to $f_{x}^{k} e_{-k}$. Hence the density

$$\sigma \propto \lim_{k \to \infty} \frac{1}{|f_{x}^{k} e_{-k}|}.$$

We use the proportional sign to indicate that the conditional measure is determined up to a constant coefficient. Let $x_{-k} := f^{-k} x$,

$$\frac{\tilde{L}^u \sigma}{\sigma}(x) = \lim_{k \to \infty} \frac{|f_{x}^{k} e_{-k}(x_{-k})|}{|f_{x}^{k} e_{-k}(y_{-k})|} = \lim_{k \to \infty} \frac{|f_{x}^{k} e_{-k}(x_{-k})|}{|f_{x}^{k} e_{-k}(y_{-k})|}.$$

Both $f_{x}^{k} e_{-k}(x_{-k})$ and $\xi_s f_{x}^{k} e_{-k}(y_{-k})$ are in $\wedge^u \mathcal{V}^u(x)$, which is a one-dimensional subspace. Hence, their ratio does not change via pushforwards, and

$$\frac{\tilde{L}^u \sigma}{\sigma}(x) = \lim_{k \to \infty} \frac{|f_{x}^{2k} e_{-k}(x_{-k})|}{|f_{x}^{k} e_{-k}(y_{-k})|}.$$

Since $\xi$ is the projection along the stable direction, $\lim_{k \to \infty} f^{k} \xi = \lim_{k \to \infty} f^{k}$. Hence, intuitively,

$$\lim_{k \to \infty} f^{k} \xi = \lim_{k \to \infty} f^{k}.$$

This intuitive statement is proved as a corollary of the absolute continuity of the holonomy map [6, theorem 4.4.1]. Hence

$$\frac{\tilde{L}^u \sigma}{\sigma}(x) = \lim_{k \to \infty} \frac{|f_{x}^{2k} e_{-k}(x_{-k})|}{|f_{x}^{k} e_{-k}(y_{-k})|}.$$

\[\square\]

**Lemma 3** (Expanded equivariant divergence formula).

$$-\frac{\delta \tilde{L}^u \sigma}{\sigma} = \div^u X - \sum_{m=1}^{\infty} (\div^v f_{s})_{-m} f_{s}^{-m} X^u + \sum_{n=0}^{\infty} (\div^u f_{s})_{n} f_{s}^{n} X^s.$$

**Proof.** Formally differentiate above expressions,

$$-\frac{\delta \tilde{L}^u \sigma}{\sigma}(x) = \lim_{k \to \infty} \frac{d}{d\gamma} |f_{x}^{k} f_{s} f_{s}^{k} e_{-k}(y_{-k})| = \lim_{k \to \infty} \frac{\left(\frac{d}{d\gamma} f_{x}^{k} f_{s} f_{s}^{k} e_{-k}(y_{-k}), f_{x}^{2k} e_{-k}\right)}{|f_{x}^{2k} e_{-k}|^2},$$

where

$$\frac{d}{d\gamma} f_{x}^{k} f_{s} f_{s}^{k} e_{-k} = \sum_{i=1}^{u} f_{x}^{k} f_{s} f_{s}^{k} e_{-k,1} \wedge \cdots \wedge \frac{d}{d\gamma} f_{x}^{k} f_{s} f_{s}^{k} e_{-k,i} \wedge \cdots \wedge f_{x}^{k} f_{s} f_{s}^{k} e_{-k,u}.$$
Here \( e_{-k,i} = e_i(y_{-k}) \). We emphasize that \( \frac{d}{d\gamma} \) is the total derivative: \( \tilde{f} \) has two direct parameters \( y \) and \( \gamma \); \( \hat{f} \) has only one variable \( y \), and \( y \) depends on \( \gamma \). Recursively apply the Leibniz rule, note that \( \tilde{f}_s = I_d \) when \( \gamma = 0 \), we get

\[
- \frac{\delta \tilde{L} u |\sigma(x)|}{\sigma} = \lim_{k \to \infty} \frac{\langle f_s^k (\frac{d}{d\gamma}) \tilde{f}_s, f_s^k e_{-k} \rangle}{|f_s^k e_{-k}|^2} + \frac{\langle f_s^k \nabla_{-f_s^{n-k} X_u} e_{-k}, f_s^{2k} e_{-k} \rangle}{|f_s^{2k} e_{-k}|^2}
\]

\[
+ \sum_{n=0}^{k-1} \frac{\langle f_s^{2k-n-1} (\nabla_{-f_s^{n-k} X_u} f_s) f_s^n e_{-k}, f_s^{2k} e_{-k} \rangle}{|f_s^{2k} e_{-k}|^2} + \frac{\langle f_s^{k-n-1} (\nabla f_s^* X^* f_s) f_s^{n+k} e_{-k}, f_s^{2k} e_{-k} \rangle}{|f_s^{2k} e_{-k}|^2}.
\]

The convergence as \( k \to \infty \) is uniform for a small range of \( |\gamma| \), justifying the formal differentiation.

The second term on the right of this equation is zero, since

\[
\lim_{k \to \infty} f_s^{-k} X u = 0.
\]

Then we resolve \( d\tilde{f}_s / d\gamma \) in the first term. For fixed \( e \),

\[
\left( \frac{d}{d\gamma} \tilde{f}_s \right) e = \frac{d}{d\gamma} \nabla_{e} \tilde{f}(y, \gamma) = \nabla_{\delta y} \nabla_{e} \tilde{f} + \frac{\partial}{\partial \gamma} \nabla_{e} \tilde{f} = \nabla_{\delta y} \nabla_{e} \tilde{f} + \nabla_{e} \frac{\partial}{\partial \gamma} \tilde{f} = \nabla_{e} X.
\]

Here \( \nabla_{\delta y} \nabla_{e} \tilde{f} = 0 \) because \( \tilde{f}(y, 0) = y \), so \( \tilde{f} \)^{'s second order partial derivative in the location variable is zero.

Because the stable part decays via pushforwards, for any \( r = \sum_i e_1 \wedge \cdots \wedge e_r \wedge \cdots \wedge e_u \),

\[
\lim_{k \to \infty} \frac{\langle f_s^k r, f_s^k e \rangle}{|f_s^k e|^2} = \varepsilon r.
\]

A more careful proof of this intuitive statement is in appendix C. Since \( f_s^n e_{-k} = e_{n-k} f_s^n e_{-k} \),

\[
\lim_{k \to \infty} \frac{\langle f_s^{2k-n-1} (\nabla_{-f_s^{n-k} X_u} f_s) f_s^n e_{-k}, f_s^{2k} e_{-k} \rangle}{|f_s^{2k} e_{-k}|^2}
\]

\[
= \lim_{k \to \infty} \frac{\langle f_s^{2k-n-1} (\nabla_{-f_s^{n-k} X_u} f_s) e_{n-k}, f_s^{2k-n-1} e_{n-k+1} \rangle}{|f_s^{2k-n-1} e_{n-k+1}|^2 |f_s e_{n-k}|}
\]

\[
= \frac{\varepsilon_{n-k+1} (\nabla_{-f_s^{n-k} X_u} f_s) e_{n-k}}{|f_s e_{n-k}|} = \left( \frac{\varepsilon_{1} \nabla_{e} f_s}{|f_s e|} \right)_{n-k} f_s^{n-k} X u.
\]

Hence,

\[
- \frac{\delta \tilde{L} u |\sigma(x)|}{\sigma} = \varepsilon \nabla_{e} X + \lim_{k \to \infty} \sum_{n=0}^{k-1} - (\text{div}^u f_s)_{n-k} f_s^{n-k} X u + (\text{div}^u f_s)_{n} f_s^{n} X u.
\]

\[
\square
\]

### 3.3. Recursive formula.

We define the adjoint shadowing operator \( S : T^* M \to T^* M \),

\[
S(\text{div}^u f_s) := \sum_{n=0}^{\infty} f_s^n \mathcal{P}^u (\text{div}^u f_s)_{n} - \sum_{m=1}^{\infty} f_s^{m} \mathcal{P}^u (\text{div}^u f_s)_{-m}.
\]

Here \( \mathcal{P}^u \), \( \mathcal{P}^u \), and \( f_s \) are transposed matrices, or adjoint operators, of \( P^u \), \( P^u \), and \( f_s \). Hence, we have proved theorem 2. In fact, this theorem may as well be proved...\]
via the fast formula in [37], which is shown in appendix B, but that proof is longer and less intuitive.

The significance of this formula is that it can be sampled by an orbit, just as how the physical measure is defined. More specifically, this means two things

- The formula is pointwisely defined.
- The formula can be computed by recursively applying a map on a few vectors and covectors.

The formula is pointwisely defined: all differentiations hit only $C^\infty$ functions $X$ and $f_*$, and all intermediate quantities have bounded sup norm. There are previous works achieving pointwise formula for the unstable part of linear responses [45, 27]. However, it was not clear back then that those formulas were related to unstable transfer operators, and the formulas are not recursive.

More importantly, our formula can be sampled on an orbit via only $2u + 1$ many recursive relations. It is not obvious that previous pointwise formulas, even with extra work, can be realized by this many recursive relations. First, $e$ can be efficiently computed via $u$-many forward recursion. Since unstable vectors grow while stable vectors decay, we can pushforward almost any set of $u$ vectors, and their span will converge to $V^u$, while their normalized wedge product converges to $e$. This classical result is used in the ‘dynamical’ algorithms for Lyapunov vectors by Ginelli and Benettin [24, 23, 7], although here we only need the unstable subspace instead of individual unstable Lyapunov vectors. Similarly, $\varepsilon$ can be efficiently computed via pulling-back $u$-many covectors, since it is the unstable subspace of the adjoint system.

The adjoint shadowing form $\nu := S(\text{div}^v f_*)$ can also be efficiently computed with one more backward recursion and an orthogonal condition at the first step. The adjoint shadowing lemma states that $\nu$ is the only bounded solution of the inhomogeneous adjoint equation,

$$\nu_n = f^* \nu_{n+1} + (\text{div}^v f_*)_n.$$

Hence $\nu$ can be well approximated by

$$\nu = \nu' + \sum_{i=1}^u \varepsilon^i a_i, \quad \text{s.t.} \quad \langle \nu_0, \varepsilon^i_0 \rangle = 0 \quad \text{for all} \quad 1 \leq i \leq u.$$

Here $\nu'$ is a particular inhomogeneous adjoint solution. Intuitively, the unstable modes are removed by the orthogonal projection at the first step, where the unstable adjoint modes are the most significant. This is known as the nonintrusive (adjoint) shadowing algorithm [40] (also see [8, 41, 38, 47]).

Hence, we can compute the $v$-divergence formula on a sample orbit, with sampling error $E \sim O(1/\sqrt{T})$, and the cost is

$$S \sim O(uT) \sim O(uE^{-2}).$$

In particular, this is not cursed by dimensionality. Compared with the zeroth-order finite-elements method for the whole $\delta L$, whose cost is estimated in appendix A, the efficiency advantage is significant when the dimension is larger than 4. The numerical implementations of our formula takes seconds to run on an $M = 21$ system, which is almost out of reach for finite-element methods [39].
4. Sampling linear responses by an orbit

This section uses our equivariant divergence formula to sample linear responses recursively on an orbit, which is the derivative of the physical measure with respect to the parameter of the system. We do not seek to reprove linear responses, rather, the focus is to sample it by recursively applying a map to evolve vectors. We first review the two linear response formula of physical measures. Then we explain how to blend the two linear response formulas for physical measures. In particular, the unstable part is given by the unstable perturbation of the unstable transfer operator, which can be sampled by an orbit.

4.1. Two formulas for linear response.

The application that we are interested in is the linear response of physical measures. In fact, most cases where we favor derivative operators are when the perturbation is evolved for a long-time, as in the case of linear responses. Otherwise, we may as well use the Koopman formula, the left side of equation (2), which can be evaluated much more easily than derivative of transfer operators for a few steps. This subsection reviews the linear response and its two more well-known formulas, the ensemble formula and the operator formula.

We denote our diffeomorphism by \( \tilde{f} \circ f \), that is, adding a perturbation \( \tilde{f} \) to a fixed map \( f \). The corresponding physical measure \( \tilde{h} \) is

\[
\tilde{h} := \lim_{n \to \infty} (LL)^n \mu, \quad h := \lim_{n \to \infty} L^n \mu,
\]

where \( \mu \) is any smooth density function of a measure. The physical measure encodes the long-time-average statistics, and it has regularities in the unstable directions for axiom A systems. A perturbation \( \tilde{f} \) gives a new physical measure, and their linear relation was discussed by the pioneering works [21, 13, 31, 9], then justified rigorously for uniform hyperbolic systems. There are other attempts to compute the linear response which do not need ergodic theory, such as the gradient clipping and the reservoir computing method from machine learning [42, 30].

One way to derive the linear response formula is to integrate the perturbation of individual orbits. For a smooth observable function \( \Phi \),

\[
\int \Phi \tilde{h} = \lim_{n \to \infty} \int \Phi \circ (\tilde{f} f)^n \mu.
\]

We can formally write the linear response by recursively applying the chain rule,

\[
\delta \left( \int \Phi \tilde{h} \right) = \lim_{n \to \infty} \int \delta(\Phi \circ (\tilde{f} f)^n) \mu = \lim_{n \to \infty} \sum_{m=0}^{n-1} \int \delta(\tilde{f}(\Phi \circ f^m) \circ f^{n-m}) \mu
\]

\[
= \lim_{n \to \infty} \sum_{m=0}^{n-1} \int X(\Phi \circ f^m) \circ f^{n-m} \mu = \sum_{m=0}^{\infty} \int X(\Phi \circ f^m) h = \sum_{m=0}^{\infty} \int f^m X(\Phi) h.
\]

We call this the ensemble formula for the linear response, because it is formally an average of orbit-wise perturbations over an ensemble of trajectories.

For contracting maps, the ensemble formula convergences, and we we only need one orbit to sample each attractor and its perturbation. For hyperbolic systems, above formula was proved in [44, 15]. This formula was numerically realized in [34, 16, 36, 28]. However, due to exponential growth of the integrand, it is typically
unaffordable for ensemble methods to actually converge [37, 10]. This issue is sometimes known as the ‘gradient explosion’.

The dual way to derive the linear response formula is to differentiate transfer operators, which shows that $\delta \tilde{h}$ and hence $\int \Phi \delta \tilde{h}$ have the expression

$$
\delta \tilde{h} = \lim_{n \to \infty} \sum_{m=0}^{n-1} L^m \delta \tilde{L} L^{n-m} \mu = \sum_{m=0}^{\infty} L^m \delta \tilde{L} h,
$$

$$
\int \Phi \delta \tilde{h} = \int \Phi \delta \tilde{L} h = \sum_{m=0}^{\infty} \int \Phi L^m \delta \tilde{L} h = \sum_{m=0}^{\infty} \int \Phi \circ f^m \delta \tilde{L} h.
$$

We call this the operator formula for the linear response. The convergence is due to decay of correlations, but the convergence speed can be faster than normal, due to that $\delta \tilde{L} h$ has mean zero [25, 33]. For expanding maps, $L$ has smoothing effects on densities, and the sum convergences in $C^r$. For hyperbolic systems with both stable and unstable directions, the sum still converges in the anisotropic Banach space [26, 4].

For expanding maps, $\delta \tilde{L} h$ is a function, and we can sample it on an orbit recursively; to do this, just linearly remove the stable part from our equivariant divergence formula. However, for maps with contracting directions, the physical measure is typically singular, and $\delta \tilde{L} h$ is not even pointwise defined. Hence, we have to resolve the full phase space to approximate $\delta \tilde{L} h$. As shown in appendix A, the cost is exponential to the large dimension of the phase space, which is too high for typical physical systems. This issue is known as ‘curse by dimensionality’.

The operator formula and the ensemble formula are formally equivalent under integration-by parts. From the ensemble formula,

$$
\sum_{m=0}^{\infty} \int f^m \Phi(X) h = \sum_{m=0}^{\infty} \int X(\Phi \circ f^m) h = -\sum_{m=0}^{\infty} \int \Phi \circ f^m (\text{div}_h X) h.
$$

By theorem 1, we have

$$
\sum_{m=0}^{\infty} \int \Phi \circ f^m (\text{div}_h X) h = -\sum_{m=0}^{\infty} \int \Phi L^m \delta \tilde{L} h = -\int \Phi \delta \tilde{h}.
$$

To summarize, both the ensemble formula and the operator formula give the true derivative for hyperbolic systems, which have both expanding and contracting directions. However, in high dimensions, we want to sample by orbits, and the ensemble formula is still suitable mainly for contracting systems, whereas the operator formula is suitable mainly for expanding systems.

4.2. Blending two linear response formulas.

It is a natural idea to combine the two linear response formulas. That is, to use the ensemble formula for the stable part of the linear response, and the operator formula for the unstable part. This subsection formally explains this decomposition, which is a variant of Gallavotti’s framework for proving the linear response [22, 9]. Our presentation takes a transfer-operator perspective on the unstable part, which makes it more apparent that our $\nu$-divergence formula can sample the unstable part by an orbit. We do not prove the linear response, rather, we shall assume that linear response exists, so we can obtain the full linear response by adding the perturbation caused $X^s$ and $X^u$. Our focus is to sample by an orbit.
Define the ‘stable contribution’ of the linear response as the part caused by the perturbation $X^s$,

$$\delta^s \left( \int \Phi \tilde{h} \right) := \sum_{m=0}^{\infty} \int f_m^s X^s(\Phi)h.$$  

The summation converges because stable vectors decay exponentially via pushforward. This formula can be naturally sampled by an orbit.

The unstable perturbation by $X^u = \delta(\xi \tilde{f})$ will re-distribute the densities within each unstable manifold, but will not move densities across different unstable manifolds. Intuitively, since the stable direction contracts the measures, the measures eventually lands onto unstable manifolds, and the physical measure is carried by the unstable manifolds. Hence, we can think of the dynamical system as time-inhomogeneous, hopping from one unstable manifold to another: this model is purely expanding. In this model, the phase spaces are a family of unstable manifolds, which is preserved under the unstable perturbation.

Hence, the operator version of linear response formula still applies. Let $\sigma'$ be the quotient measure in the stable direction, so $\int \sigma' \int \sigma \Phi = \int h \Phi$ for any smooth function $\Phi$. Let $L^u$ and $\tilde{L}^u$ be the transfer operator of $f$ and $\xi \tilde{f}$ on unstable manifolds. Let $\tilde{\sigma}$ be the conditional measure of the SRB measure of $\xi \tilde{f}f$, and $\sigma = L^u \sigma_{-1} = \cdots = (L^u)^m \sigma_{-m}$ be the sequence of conditional measures on unstable manifolds crossing $x, x_{-1}, \cdots x_{-m} = f^{-m}x$, where $x$ is the dummy variable in the integration below. The ‘unstable contribution’ of the linear response is

$$\delta^u \left( \int \Phi \tilde{h} \right) := \int \sigma' \int \Phi \tilde{\sigma} = \sum_{m \geq 0} \int \sigma' \int \Phi (L^u)^m \tilde{L}^u \sigma_{-m}$$  

Here $\tilde{L}^u \sigma_{-m}$ is a density on $V(x_{-m})$, which is pushed forward by $(L^u)^m$ to the current unstable manifold $V(x)$, where the inner integration is performed. By the pointwise definition of transfer operators, for any measure $\sigma'_{-m}$ on $V^u(x_{-m})$,

$$\frac{(L^u)^m \sigma'_{-m}}{\sigma'_{-m}} = \frac{(L^u)^m \sigma_{-m}}{\sigma_{-m}} = \frac{\sigma}{\sigma_{-m}}.$$  

Let $\sigma'_{-m}$ be $\tilde{L}^u \sigma_{-m}$, and apply the invariance of $h$, we have

$$\delta^u \left( \int \Phi \tilde{h} \right) = \sum_{m \geq 0} \int \sigma' \int \sigma \frac{\delta \tilde{L}^u \sigma_{-m}}{\sigma_{-m}} = \sum_{m \geq 0} \int h \Phi \circ f^m . \delta \tilde{L}^u \sigma.$$  

We may also prove this expression via integrating-by-parts the ensemble formula on unstable manifolds, but that is less intuitive [44, 37].

Adding up the two contributions, we get the so-called blended formula, in name of the blended response algorithm by Majda and Abramov [1]. But they computed the unstable divergence by summing directional derivatives, which is not pointwisely defined. With our formula for the unstable perturbations of transfer operators, we can sample the unstable divergence and hence the entire linear response by an orbit.

The $\nu$-divergence formula is part of the so-called fast (adjoint) response algorithm. It is numerically demonstrated on a 21 dimensional example with 20 unstable dimensions. There we use a slightly different decomposition of the linear response, a decomposition into shadowing and unstable contributions, because the shadowing contribution codes easier and runs faster than the stable contribution, and we use shadowing anyway for the unstable contribution [39, 37].
5. Conclusions

The phase space is typically high dimensional, so efficient computations demand sampling by an orbit rather than resolving the phase space. In this paper we solve this problem for the more difficult part, the unstable perturbation operator of a physical measure. It was well known that the physical measure can be sampled on an orbit; now, with our results, we know that its derivative operator and hence the linear response can also be sampled on an orbit by $2u + 1$ recursive relations. This cost is perhaps optimal, since we need at least $u$ many modes to capture all the unstable perturbative behaviors of a chaotic system.

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Data Availability Statements

This manuscript has no associated data.

Appendix A. A very rough cost estimation of finite-element method for approximating high-dimensional measures

When the measure is singular, $\delta Lh$ has infinite sup norm. Although this is a well-defined mathematical object in suitable Banach spaces, computers can not process infinite sup norm. Currently, the main numerical practice for computing derivative operators is to first approximate the measure by isotropic finite-elements [32, 17, 35, 14, 43, 19, 20, 49, 12, 2, 48, 18], then compute the derivative operator. This allows us to ignore the singularities and subtle structures of measures; however, the cost can still be affected.

Computing the entire derivative operator was not numerically realized for discrete-time systems with dimensions larger than 1. In particular, Gutiérrez and Lucarini numerically computed the derivative operator for a continuous-time 3-dimensional system [29], Bahsoun, Galatolo, Nisoli, and Niu did computations on 1-dimensional expanding maps [3]. There are two difficulties, the easier one is the lack of convenient formulas, which we solved via theorem 1. The more essential difficulty is that the finite-elements method is cursed by the dimension of the dynamical system.

Galatolo and Nisoli gave a rigorous posterior error bound for the finite-elements method, where some quantities in the bound are designated to be computed by numerical simulations [20]. That bound, though precise, does not give the cost-error relation and how it depends on dimensions.

This section gives an apriori cost-error estimation on a simple singular measure approximated by zero-order isotropic finite elements. A more general and precise estimation is more difficult, but should not change the qualitative conclusion. That is, the cost is ‘cursed by dimensionality’, or it increases exponentially fast with respect to the dimension of the attractor. For physical or engineering systems, this cost is too high.
Consider the example where the singular measure is uniformly distributed on the $a$-dimensional attractor, \( \{0\}^{M-a} \times T^a \), where \( T := [-0.5, 0.5] \). We use the zeroth order finite-elements in the $M$-dimensional cubes of length $b$ on each side. The density $h$ is a distribution; and we still formally denote the SRB measure as the integration of $h$ with respect to the Lebesgue measure. Let $h'$ be the finite-element approximation of $h$, so

\[
h'(x) = \begin{cases} 
    b^{-(M-a)} & \text{for } |x^1|, \ldots, |x^{M-a}| \leq b/2; \ |x^{M-a+1}|, \ldots, |x^M| \leq 0.5; 
    0 & \text{otherwise.}
\end{cases}
\]

For the smooth objective function, $\Phi$, we assume that for any unit vector $Y$, the second order derivative $Y^2(\Phi)(x) := Y(Y(\Phi))(x) \sim 1$. Where $\sim$ means the two terms are on the same order as $x$ or $b$ goes to zero.

The approximation error $E$ caused by using $h'$ instead of $h$ is

\[
E := \int \Phi h' - \int \Phi h
\]

\[
= \int_{T^a} \int_{T^{M-a}} \Phi' dx^{1\sim M-a} dx^{M-a+1\sim M} - \int_{T^a} \Phi(0, x^{M-a+1}, \ldots, x^M) dx^{M-a+1\sim M},
\]

where $dx^{1\sim M-a} = dx^1 \ldots dx^{M-1}$. We only need an estimation of $E$, so we can just sample the outside integration at any point; denote $\varphi(y) := \Phi(y, x^{M-a+1}, \ldots, x^M)$, then

\[
E \sim \int_{T^{M-a}} \varphi h' - \varphi(0) = \int_{T^{M-a}} (\varphi(y) - \varphi(0))h' \sim \int_{T^{M-a}} (Y(\varphi)(0)y + Y^2(\varphi)(0)\frac{|y|^2}{2})h',
\]

where $Y = y/|y|$ is the direction of taking derivatives. The first term is zero due to symmetry, hence

\[
E \sim \int_{T^{M-a}} y^2 h' = b^{-(M-a)} \int_{-0.5b,0.5b} (y^1)^2 + \ldots + (y^{M-a})^2 dy^1 \ldots dy^{M-a}
\]

\[
\sim b^{-(M-a)}(M-a)b^3b^{M-a-1} = (M-a)b^2.
\]

For more general cases, there should be another error due to approximation within the attractor, but here we neglect it.

It is nontrivial to achieve optimal mesh adaptation in higher dimensions. For now we assume optimal mesh, then we can restrict our computation to the attractor, and the cost

\[
S \sim b^{-a} \sim \left( \frac{M-a}{E} \right)^{\frac{a}{2}}.
\]

On the other hand, if the finite-elements are all globally supported, such as the Fourier basis, or if the optimal implementation is not achieved, the cost can be $O(b^{-M})$.

In higher dimensions, it is expensive to resolve the entire attractor by finite-elements. Hence, it is also expensive to compute $\delta \tilde{L}h$ via finite-elements.

**APPENDIX B. ANOTHER PROOF OF THE EQUIVARIANT DIVERGENT FORMULA**

This section uses the fast formula from \cite{37} to give another proof of theorem 2. This proof is less intuitive and slightly weaker, since it can only prove the formula for $\rho$-almost everywhere. The main purpose of this proof is to verify the previous fast formula, which runs only forwardly on an orbit, hence is faster for one parameter.
In fact, if we revert this proof, we can prove the fast formula from the equivariant divergence formula.

This proof is based on ‘adjoining’ the fast formula of the unstable contribution. More specifically, we shall expand the unstable divergence, move major computations away from $X$ and $\psi$, and obtain an expansion formula for an adjoint operator. Then we seek a neat characterization of the expansion formula, and we prove theorem 2 by further using the adjoint shadowing lemma.

B.1. Fast formula for the unstable contribution.

The unstable contribution is defined as

$$ U.C. = \rho (\psi \text{div}_u X) $$

where $\psi := \sum \Phi f^m - \rho(\Phi)$. (7)

Here $\text{div}_u$ is the submanifold divergence on the unstable manifold under the conditional SRB measure. The norm of this integrand is $O(\sqrt{W})$, much smaller than the ensemble formula. Note that the directional derivatives of $X$ are distributions.

We gave a fast formula for the unstable divergence. It involves only $u$ many second-order tangent equations on one sample orbit, which runs forwardly in time.

**Theorem 3** (fast formula for unstable contribution [37]). For any $r_0 \in D^u$, $U.C. = \lim_{N \to \infty} \frac{1}{N} \sum_{n=0}^{N-1} \langle \tilde{\beta}_r, e_n+1 \rangle$, where $r_{n+1} = P^\perp \tilde{\beta}_r$.

Here $e = e_1 \wedge \cdots \wedge e_u$ is the unit $u$-dimensional cube spanned by unstable vectors, $\langle \cdot, \cdot \rangle$ is the inner product between $u$-vectors;

$$ D^u := \{ r = \sum_i e_1 \wedge \cdots \wedge r_i \wedge \cdots \wedge e_u : r_i \in T_x M, e_i \in V^u \} $$

is the space of derivatives of unstable cubes; for any $r \in D^u$,

$$ P^\perp r := \sum_i e_1 \wedge \cdots \wedge P^\perp r_i \wedge \cdots \wedge e_u, $$

where the second $P^\perp$ orthogonally projects a vector to the subspace perpendicular to $V^u$. Here $\tilde{\beta}$ is the renormalized second-order tangent equation governing the propagation of derivatives of cubes,

$$ r_{n+1} = P^\perp \tilde{\beta}_r = \frac{P^\perp f_s}{J} r_n + \frac{P^\perp (\nabla \tilde{e} f_s)}{J} e_n + P^\perp (\psi \nabla e X)_{n+1}, $$

where the Jacobian determinant $J$ is regarded as an operator, when applied to quantities at $x_n$, $J := |f_s e_n|$. $\tilde{\nu}$ is the shadowing vector of $\psi X$, which is the only bounded solution to

$$ \tilde{\nu}_{n+1} = f_s \tilde{\nu}_n + (\psi X)_n. $$

The fast response algorithm based on the fast formula was demonstrated on a 21-dimensional system with a 20-dimensional unstable subspace. For the same accuracy, fast response is orders of magnitude faster than ensemble and operator algorithms; it is even faster than finite difference [37]. Some later algorithms also use orthogonally projected second order tangent equations to compute some other divergences, such as the second version of S3 algorithm, whose complexity is now $O(M u^3)$ per step, more than $O(u)$ times higher than the fast response [11, 46]. The
first version of S3 was earlier than the fast response, but it assumes and heavily depends on the differentiability of the Lyapunov vectors, or the convergence of the recursive formula for the derivative of Lyapunov vectors, which are typically not true.

Comparing to the adjoint formulas in this paper, the fast formula runs only forwardly, so the corresponding algorithm is faster, though the number of flops (float point operations) are the same for one parameter. However, the forward algorithm’s marginal cost for a new parameter is much larger than the adjoint algorithm.

B.2. Expansion formulas of unstable contribution.

**Lemma 4.** U.C.\(_W\) = \(\rho(e^bTq)\) = \(\rho((\mathcal{T}e^b)q)\), where
\[
e^b(\cdot) := \langle e, \cdot \rangle, \quad q := \frac{\nabla_e f_s}{J} \tilde{v}_{-1} + \psi \nabla_e X, \]
\[
T(\cdot) := \sum_{k \geq 0} \left( \frac{f_s P_{\perp}}{J} \right)^k (\cdot)_{-k}, \quad T e^b(\cdot) := \sum_{k \geq 0} \left( \frac{f_s P_{\perp}}{J} \right)^k (\cdot, e_k). \]

**Remark.** (1) Here \(q\) is in the space of derivative-like \(u\)-vectors \(D^u\), \(e^b\) is in the dual space \(D^{u^*}\); \(T\) is a linear operator on \(L^2(\rho, D^u)\), its adjoint operator is \(\mathcal{T}\), which is an operator on \(L^2(\rho, D^{u^*})\). (2) This is not the full expansion, since \(\tilde{v}\) can be further expanded. But there is no need to expand \(\tilde{v}\), since the adjoint shadowing lemma has told us very well how to deal with it. Also note that the expansion formula of \(p\) in [37] is also not the full expansion, and is different from our current one.

**Proof.** Due to the stability of the induction on \(r\), its solution of any initial condition converges to the equivariant solution, \(p_k\), which satisfies \(p_k(x) = p(f^k x)\). Its expression can be written out using Duhamel’s principle,
\[
p = \sum_{n \geq 0} \left( \frac{P_{\perp} f_s}{J} \right)^n \left( \frac{P_{\perp} (\nabla_e f_s)}{J} \tilde{v}_{n-1} + P_{\perp} (\psi \nabla_e X)_{-n} \right)
= \sum_{n \geq 0} P_{\perp} \left( \frac{f_s P_{\perp}}{J} \right)^n \left( \frac{\nabla_e f_s}{J} \tilde{v}_{n-1} + (\psi \nabla_e X)_{-n} \right).
\]

We further write down the expansion formula for \(\tilde{\beta} p_{-1}\):
\[
\tilde{\beta} p_{-1} = \frac{f_s}{J} \sum_{n \geq 0} P_{\perp} \left( \frac{f_s P_{\perp}}{J} \right)^n \left( \frac{\nabla_e f_s}{J} \tilde{v}_{n-2} + (\psi \nabla_e X)_{-n-1} \right) + \frac{\nabla_e f_s}{J} \tilde{v}_{-1} + \psi \nabla_e X
= \sum_{n \geq -1} \left( \frac{f_s P_{\perp}}{J} \right)^{n+1} \left( \frac{\nabla_e f_s}{J} \tilde{v}_{n-2} + (\psi \nabla_e X)_{n-1} \right)
= \sum_{k \geq 0} \left( \frac{f_s P_{\perp}}{J} \right)^k \left( \frac{\nabla_e f_s}{J} \tilde{v}_{-k-1} + (\psi \nabla_e X)_{-k} \right).
\]

Substituting this into the unstable contribution in theorem 3, we proved
\[
U.C.\_W = \lim_{N \to \infty} \frac{1}{N} \sum_{n=0}^{N-1} \langle \tilde{\beta} p_n, e_{n+1} \rangle = \rho(\tilde{\beta} p_{-1}, e) = \rho(e^b \tilde{\beta} p_{-1}) = \rho(e^b T q).
\]

The formula for \(\mathcal{T}\) is proved by the invariance of SRB measures. \(\square\)
B.3. Characterizing $\mathcal{T}e^b$ by unstable co-cube.

**Lemma 5.** $\mathcal{T}e^b(r) = \varepsilon(r), \forall r \in \mathcal{D}^u$.

**Proof.** Since $P_\perp f_* P_\perp = P_\perp f_*, P_\parallel$ projects to the span of $e$, for any $r \in \mathcal{D}^u$,

\[
\left\langle \left( \frac{f_* P_\perp}{J} \right)^k r, e_k \right\rangle = \left\langle \frac{f_* P_\perp}{J} f_*^{k-1} r, e_k \right\rangle = \left\langle \frac{f_*}{J} f_*^{k-1} r, e_k \right\rangle - \left\langle \frac{f_*}{J} f_*^{k-1} r, e_k \right\rangle = \left\langle \frac{f_*}{J} f_*^{k-1} r, e_k \right\rangle.
\]

The last equality is because $\left\langle P_\parallel, e \right\rangle = \left\langle \cdot, e \right\rangle$. Hence,

\[
\mathcal{T}e^b(r) = \langle f, e_0 \rangle + \lim_{N \to \infty} \sum_{k \geq 1} \left( \left\langle \frac{f_*}{J} f_*^{k-1} r, e_k \right\rangle - \left\langle \frac{f_*}{J} f_*^{k-1} r, e_k \right\rangle \right) = \lim_{N \to \infty} \left( \left\langle \frac{f_*}{J} f_*^{N} r, e_N \right\rangle \right).
\]

The lemma is proved once we show that this equals $\varepsilon(r)$. Intuitively, this is because the stable parts decay while the unstable parts grow. A more careful proof of this statement is in appendix C. $\square$ 

**Proof.** (theorem 2 for $\rho$-almost everywhere) Substituting lemma 5 into lemma 4, we get

\[
U.C.\ W = \rho \left( \varepsilon \nabla e f_* \tilde{v}_{-1} + \varepsilon \psi \nabla e X \right) = \rho \left( (\text{div}^u f_*) \tilde{v} + \psi \text{div}^u X \right).
\]

Recall that $\tilde{v}$ is the shadowing vector for $\psi X$; hence, by definition of the shadowing covector,

\[
U.C.\ W = \rho \left( \psi (\mathcal{S}(\text{div}^u f_*) X + \text{div}^u X) \right).
\]

Compare with the definition of the unstable contribution in equation (7), since the equality holds for any smooth $\psi$, we have proved the theorem $\rho$-almost everywhere.

Note that the proof in the main body of the paper holds on the entire attractor with a continuous splitting of stable and unstable subspace. $\square$

**Appendix C. Relative decay of pushing forward $\mathcal{D}^u$**

We prove a lemma used in both proofs of the $v$-divergence formula.

**Lemma 6** (relative decay of pushing forward $\mathcal{D}^u$). $\forall r \in \mathcal{D}^u$,

\[
\lim_{N \to \infty} \left\langle \frac{f_*^N r}{|f_*^N e|}, e_N \right\rangle = \varepsilon(r).
\]

**Proof.** We claim that

\[
\mathcal{T}e^b(r) = \lim_{N \to \infty} \left\langle \frac{f_*^N r}{|f_*^N e|}, e_N \right\rangle = \begin{cases} 1, & \text{if } r = e, \\ 0, & \text{if } r = \sum_i e_1 \wedge \cdots \wedge r_i \wedge \cdots \wedge e_u, r_i \in V^s. \end{cases}
\]

If the claim is true, $\mathcal{T}e^b = \varepsilon$ for all basis of $\mathcal{D}^u$, hence, the equality also holds for all $r \in \mathcal{D}^u$, finishing the proof of the lemma. The first case is straightforward, and we only need to prove the second case.
Intuitively, the claim that $T e^b(r) = 0$ in the second case is because that $r_i \in V^s$ decays exponentially fast; but we should be more careful when proving it for $u$-vectors. Assume for convenience that $\{e_i\}_{i=1}^n$ is any orthogonal basis for $V^u$ such that $e = e_1 \wedge \cdots \wedge e_u$. In the rest of this proof, fix $C$ as the constant used in the definition of hyperbolicity. We claim that

$$C\lambda^n |f^n e| \geq |f^n(e_2 \wedge \cdots \wedge e_u)||e_1||, \quad \forall n \geq 0. \quad (9)$$

To prove this claim, assume that it is false, that is, for some $n$,

$$C\lambda^n |f^n e| < |f^n(e_2 \wedge \cdots \wedge e_u)||e_1||.$$

We can find $e'_1 \in V^u$, such that $f^n e'_1 \perp \text{span}\{f^n e_2, \ldots, f^n e_u\}$, and $e'_1 \wedge e_2 \wedge \cdots \wedge e_u = e$. As a result, $|e'_1| \geq |e_1|$. Hence, by our assumption,

$$C\lambda^n |f^n e'_1| = C\lambda^n |f^n e| < |f^n(e_2 \wedge \cdots \wedge e_u)||e_1|| \Rightarrow C\lambda^n |f^n e'_1| < |e_1| \leq |e'_1|.$$

Denote $w := f^n e'_1$, then $C\lambda^n |w| < |f^{-n} w|$, contradicting our hyperbolicity assumption.

We can rewrite $r$ on the orthogonal basis $\{e_i\}_{i=1}^n$, still as $r = \sum_{i} e_i \wedge \cdots \wedge r_i \wedge \cdots \wedge e_u$, with $r_i \in V^s$ (see [37] for the detailed formula). With equation (9),

$$\frac{|f^N (r_1 \wedge e_2 \wedge \cdots \wedge e_u)|}{|f^N e|} \leq C\lambda^N \frac{|f^N r_1||f^N (e_2 \wedge \cdots \wedge e_u)|}{|e_1||f^N (e_2 \wedge \cdots \wedge e_u)|} = C\lambda^N \frac{|f^N r_1|}{|e_1|} \leq C^2 \lambda^{2N} \frac{|r_1|}{|e_1|} \rightarrow 0,$$

as $N \rightarrow \infty$. Similarly, we can prove this for any $r_i$. Hence $|f^N r / J^N| \rightarrow 0$, and $T e^b(r) = 0$. ☐

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