DIVERGENCE FORMULAS FOR SAMPLING DERIVATIVES OF TRANSFER OPERATORS ON AN ORBIT

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Abstract. For discrete time systems, we show that the derivative of the (measure) transfer operator with respect to the system parameters is a divergence. For singular physical measures, which are limits of an orbit, we show that we typically only need the transfer operator to handle the unstable derivatives. Then we derive a divergence formula for the unstable derivative of transfer operators, which has no exploding intermediate quantities. This formula and hence the derivative of physical measures can be sampled by a few recursive relations on an orbit.

Keywords. transfer operator, unstable divergence, SRB measures, linear response, fast response algorithm, Markov chain Monte Carlo.

1. Introduction

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 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 [19, 20, 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 [35, 12, 4, 18]. The operator formula is particularly attractive in numerical computations because it is not affected by the exponential growth of unstable vectors.

Currently, the main numerical practice for computing derivative operators is to first approximate the measure by isotropic finite-elements [24, 14, 26, 11, 34, 16, 17, 40, 10, 2, 39, 15], then compute the derivative operator. In particular, Gutiérrez and Lucarini numerically computed the derivative operator for a continuous-time 3-dimensional system [22], Bahsoun, Galatolo, Nisoli, and Niu did computations on 1-dimensional expanding maps [3].
However, computing the entire derivative operator was not numerically realized for
discrete-time systems with dimensions larger than 1. There are two difficulties, the easier
one is the lack of convenient formulas. In this paper, we derive a divergence formula for
the derivative operator. The more essential difficulty is that the finite-elements method
is cursed by the dimension of the dynamical system. In this paper, on a toy problem, we
give an apriori cost-error estimation, which shows that the cost increase exponentially
fast with respect to the dimension of the attractor. For physical or engineering systems,
this cost is too high.

When the underlying measure is a higher-dimensional physical measure, 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
could not be achieved for the entire derivative operator, which is typically singular,
and its value at a point is not defined. However, we typically only need the transfer
operator to handle the unstable perturbations. In this paper, we further derive a new
divergence formula for the unstable derivative of unstable transfer operators on physical
measures; it involves only a few recursive relations on an orbit.

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 inspired by our recent numerical algorithm, the fast response algorithm,
for computing the linear response on a sample orbit [28]. The second version of the S3
algorithm later achieved similar goals with less efficiency [9, 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 may be viewed as
the generalization of the well-known backpropagation method to unstable and chaotic
neural networks [30].

The main results of our paper are the two divergence formulas in theorem 1 and
theorem 2. This paper is organized as follows. Section 2 proves the divergence formula
of entire derivative operator. Section 3 motivates why we mostly care about the unstable
part of the derivative operator, and why it has the potential to be sampled on an orbit.
Section 4 derives the divergence formula for the unstable derivative of the unstable
transfer operator. This paper is intended to be intuitive and simple, so we restrict our
discussions to uniform hyperbolic systems in \( \mathbb{R}^M \). Generalizations are possible.

2. DIVERGENCE FORMULA OF DERIVATIVE OPERATOR

We first assume that the measure on which we apply the transfer operator is smooth
(means \( C^{\infty} \)) 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 as MCMC, samples by an orbit; but an orbit is not necessary here.

2.1. A functional proof.

Let \( \tilde{f} = \eta \circ f \) be a smooth diffeomorphism on \( \mathbb{R}^M \). For measures with a smooth density function, 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

\[
\int h_{-1} \cdot \Phi \circ \tilde{f} =: \int \tilde{L}h_{-1} \cdot \Phi,
\]

where \( \Phi \) is any smooth observable function, and

\[
h := \tilde{L}h_{-1}
\]

are smooth densities not affected by \( \gamma \); here \( L \) is the operator of \( f \). We use subscript to label steps. Note that \( L \) operates on the entire density function, and \( Lh(x) := (Lh)(x) \). In this paper, all integrals are taken with respect to the Lebesgue or Riemannian measure, except when another measure is explicitly mentioned.

Throughout this paper, we assume that \( f \) is fixed, whereas \( \eta \) and hence \( \tilde{f} \) are controlled by a parameter \( \gamma \), whose default value is \( \gamma = 0 \), and \( \eta|_{\gamma=0} = I_d \) is the identity map. We are interested in how perturbations in \( \gamma \) would affect \( \tilde{L} \). Define

\[
\delta(\cdot) := \left. \frac{\partial(\cdot)}{\partial \gamma} \right|_{\gamma=0}.
\]

We emphasize that when a function, such as \( \eta \), has more than one variables, \( \delta \) is the partial derivative with respect to \( \gamma \). Define the perturbation vector field \( X \) as

\[
X := \delta \eta = \delta \tilde{f} \circ f^{-1}.
\]

**Remark.** For this paper, we only consider the derivatives at \( \gamma = 0 \). Hence, we can freely assume the value of \( \partial \eta / \partial \gamma \) 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

\[
\frac{\partial \eta}{\partial \gamma} = X, \quad \text{for any small } \gamma.
\]

In other words, we may assume that \( \eta \) is the flow of \( X \).

**Theorem 1.** For a measure with fixed density \( h_{-1} \), and any \( \eta \) such that \( \delta \eta = X \), denote \( h := \tilde{L}h_{-1} \), then

\[
\delta \tilde{L}(h_{-1}) := \delta (\tilde{L}h_{-1}) = -\text{div}(hX).
\]

**Remark.** If \( \tilde{f} : \mathcal{M}_{-1} \to \mathcal{M} \) is a map between two manifolds, then \( X \) is a vector field on \( \mathcal{M} \).

**Proof.** Differentiate equation (1), notice that \( \delta (\Phi \circ \tilde{f}) = \delta \tilde{f}(\Phi) = X(\Phi) \circ f \), where \( X(\cdot) \) is to differentiate a function in the direction of \( X \), we have

\[
\int h_{-1} \cdot \delta(\Phi \circ \tilde{f}) = \int \delta \tilde{L}h_{-1} \cdot \Phi.
\]
We call the left hand side the Koopman formula, and the right side the operator formula for the perturbation. Hence,

\[ \int h_{-1} \cdot \delta(\Phi \circ \tilde{f}) = \int L h_{-1} \cdot X(\Phi) = \int h \cdot X(\Phi), \]

where we applied the definition of \( L \) in equation (1) again.

First assume that \( h_{-1} \) is compactly supported, then there is no boundary term for integration-by-parts, and we have

\[ \int \delta \tilde{L} h_{-1} \cdot \Phi = \int h \cdot X(\Phi) = -\int \text{div}(h X) \cdot \Phi. \]

Since this holds for any \( \Phi \), it must be \( \delta \tilde{L} h_{-1} = -\text{div}(h X) \). When \( h_{-1} \) is not compactly supported, just apply a smooth cutoff function. \( \square \)

We define \( \text{div}_h \) as the divergence under the measure \( h \),

\[ \text{div}_h X := \frac{\text{div}(h X)}{h} = \text{div}(X) + \frac{X(h)}{h}. \]

For two measures \( h' \) and \( h'' \), if \( h' \propto h'' \), that is, \( h' = C h'' \) for a constant \( C > 0 \), then \( \text{div}_{h'} = \text{div}_{h''} \). Now theorem 1 writes

\[ \delta \tilde{L} h_{-1} = -h \text{div}_h X. \]

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,

\[ \tilde{L} h_{-1}(x) := \frac{h_{-1}}{|f_*|}(f^{-1}(x)) = \frac{h_{-1}}{|f_*|} \circ f^{-1} \circ \eta^{-1} \cdot \frac{1}{|\eta_*|} \circ \eta^{-1}(x) \]

\[ = \frac{L h_{-1}}{|\eta_*|} \circ \eta^{-1}(x) = \frac{h(y)}{|\eta_*|(y)}, \quad \text{where} \quad y := \eta^{-1} x. \]

Here the point \( x \) is fixed, and \( y \) varies according to \( \gamma \). \( |f_*| \) and \( |\eta_*| \) are Jacobian determinants, or the norms as operators on \( M \)-vectors,

\[ |f_*| := \frac{|f_* e|}{|e|}, \quad |\eta_*| := \frac{|\eta_* e|}{|e|} \quad \text{where} \quad e = e_1 \wedge \cdots \wedge e_M. \]

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 \( f_* \) is the Jacobian matrix. Note that \( f_* \) changes our point of interest, that is, \( f_* (X(x)) \) is a vector at \( fx \). Also note that \( |f_*| \) and \( |\eta_*| \) are 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,

\[ \langle e, r \rangle := \det \langle e_i, r_j \rangle, \quad \text{where} \quad e = e_1 \wedge \cdots \wedge e_u, \quad r = r_1 \wedge \cdots \wedge r_u, \quad e_i, r_j \in TM. \]
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 $L$ and $h$ are fixed functions, also that $|\eta_*| = 1$ when $\gamma = 0$, we have

$$\delta \tilde{L}h_{-1} = \delta y(h) - h \frac{d}{d\gamma}(|\eta_*|(y)).$$

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: $\eta$ has two direct parameters $y$ and $\gamma$, $y$ implicitly depends on $\gamma$.

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

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

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

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

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

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

where $\epsilon^i$ 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 $\eta_* e_i = \nabla_{e_i} \eta$. We can change the order of the derivative in the location and the derivative in the parameter, hence

$$\delta \eta_* e_i = \frac{\partial}{\partial \gamma} \nabla_{e_i} \eta = \nabla_{e_i} \frac{\partial}{\partial \gamma} \eta = \nabla_{e_i} X.$$

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

Substituting this lemma into equation (4), we get a pointwise proof of theorem 1. We restate it with new notations used in this proof, such as the perturbation map $\eta$ and the co-basis $\epsilon$.

**Proposition 1.** For a measure with fixed density $h$, and any $\eta$ such that $\delta \eta = X$,

$$\frac{1}{h} \delta \tilde{L}h_{-1} = \frac{1}{h} \delta \left( \frac{Lh_{-1}}{|\eta_*| \circ \eta^{-1}} \right) = \frac{-X(h)}{h} - \text{div } X = -\text{div}_h X.$$ 

3. **Motivating unstable derivative of unstable transfer operators**

Many important measures are singular, such as the physical measures of chaotic systems. But there is not much hope in numerically computing the entire $\delta \tilde{L}$ efficiently in higher dimensions. However, we only need the derivative operator to handle the
unstable perturbations; the stable perturbations are typically computed by the Koopman formula on the left of equation \(2\).

This section uses the application in the linear response to motivate our study of the unstable derivative of unstable transfer operators. First, we show that the finite-elements approach can be expensive in higher dimensions. Then we review the two linear response formula of physical measures. Finally, we explain how to blending the two formulas yields the unstable derivative of the unstable transfer operator, which has the potential to be sampled on an orbit; the next section shows how to realize this potential.

3.1. 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 objects in suitable Banach spaces, computers can not process infinite sup norm. Currently, the main practice in operator methods is to compute \(\delta L\) on a measure approximated by finite-elements, which is absolutely continuous to Lebesgue. This allows us to ignore the singularities and subtle structures of measures; however, the cost can still be affected. Galatolo and Nisoli gave a rigorous posterior bound for such error, where some quantities in the bound are designated to be computed by numerical simulations \[17\]. That bound, though precise, does not give the cost-error relation and how it depends on dimensions.

We give 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 increase at a faster rate than the accuracy when the dimension is high.

Consider the example where the singular measure is uniformly distributed on the \(a\)-dimensional attractor, \(\{0\}^{M-a} \times \mathbb{T}^a\), where \(\mathbb{T} := [-0.5, 0.5]\). 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

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

(6)
where $dx^{1\cdots M-a} = dx^1 \cdots dx^{M-1}$. 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

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

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

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

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

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 $\delta \tilde{L}$ via finite-elements.

### 3.2. Two formulas for linear response.

For a physical measure $h$, though singular, we can sample the measure efficiently by an orbit. So it is natural to ask if we could also sample $\delta \tilde{L} h$ by an orbit. No, since $\delta \tilde{L} h$ is a distribution, and it is not defined at a single point on an orbit. But for many applications, we only need a part of $\delta \tilde{L} h$, which is well-defined at a point, and has the potential to be sampled by an orbit.

The application that we are interested in is the linear response of physical measures, or SRB measures. In fact, the only case we might favor derivative operators is 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 formulas, the ensemble formula and the operator formula.

The physical measure $\tilde{h}$ corresponding to $\tilde{f}$ and its transfer operator $\tilde{L}$ is

$$\tilde{h} := \lim_{n \to \infty} \tilde{L}^n \mu, \quad h := \lim_{n \to \infty} L^n \mu,$$

where $\mu$ is any measure with a smooth density function. The physical measure encodes the long-time-average statistics, and it has regularities in the unstable directions.
A perturbation in \( \tilde{f} \) gives a new physical measure. By formal differentiation, we see that \( \delta \tilde{h} \) has the expression

\[
\delta \tilde{h} = \lim_{n \to \infty} \sum_{m=0}^{n-1} L^m \delta \tilde{L} L^{n-m-1} \mu = \sum_{m=0}^{\infty} L^m \delta \tilde{L} h.
\]

We call this the operator formula for the linear response. For expanding maps, \( L \) has smoothing effects on densities, and the sum converges in \( C^r \). For hyperbolic systems with both stable and unstable directions, the sum still converges in the anisotropic Banach space \([19, 4]\).

In computations, we have seen that finite elements do not work well in high dimensions. For expanding maps, \( \delta \tilde{L} h \) is a function, and theoretically speaking we can sample it on an orbit, preferably by iterating some simple recursive formulas. Note that we do not have such formulas yet, but it is theoretically possible. Such formula will be a degenerate case of the formulas we derive in the next section. However, for maps with contracting directions, the physical measure is typically singular, and there is theoretically no hope to sample \( \delta \tilde{L} h \) on an orbit.

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

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

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

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

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 converges, and we only need one orbit to sample each attractor and its perturbation. For hyperbolic systems, above formula was proved in \([35, 12]\). This formula was numerically realized in \([25, 13, 27, 21]\). However, due to exponential growth of the integrand, it is typically unaffordable for ensemble methods to actually convergence \([28, 8]\). This issue is sometimes known as the ‘gradient explosion’.

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

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

For invariant measures, \( h_{-1} = h \); by theorem \([1]\), we have

\[
\sum_{m=0}^{\infty} \int \Phi \circ f^m (\text{div}_h X) h = - \sum_{m=0}^{\infty} \int \Phi L^m \delta \tilde{L} h_{-1} = - \int \Phi \sum_{m=0}^{\infty} L^m \delta \tilde{L} h = - \int \Phi \delta \tilde{h}.
\]
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, the cost can be high if we directly implement them for numerical computations. In particular, we want to sample by orbits when the dimension is high, and the ensemble formula is still suitable mainly for contracting systems, whereas the operator formula is suitable mainly for expanding systems.

3.3. Blending two linear response formulas.

It is natural to ask if we can combine the two linear response formulas. That is, to use the ensemble formula for the contracting part of the linear response, and the operator formula for the expanding part. This subsection shows that such decomposition is possible. In particular, the main term in the expanding part of the linear response is the unstable derivative of the transfer operator on unstable manifolds. This shows the necessity and sufficiency of sampling the unstable derivative operator for the purpose of linear responses.

We assume that the underlying dynamical system has a mixing Axiom A attractor; hence, the physical measure can be sampled by an orbit. Moreover, 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

$$\max_{x \in K} |f_*^{-n}|V^u(x)|, |f_*^n|V^s(x)| \leq C \lambda^n$$

for $n \geq 0$, where $f_*$ is the Jacobian matrix. Define oblique projection operators $P^u$ and $P^s$, such that

$$X = P^u X + P^s X, \quad \text{where} \quad X^u := P^u X \in V^u, \quad X^s := P^s X \in V^s.$$ 

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.

We start with the ensemble formula. Define the ‘stable contribution’ of the linear response as the part caused by the perturbation $X^s$,

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

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

We define the unstable contribution similarly. Since the physical measure is smooth on the unstable manifolds, we can integrate-by-parts on the unstable manifolds under the conditional SRB measure $\sigma$ at $\gamma = 0$, which is smooth on each unstable manifold, hence,

(7) $$\delta^u \left( \int \Phi \hat{h} \right) := \sum_{m=0}^{\infty} \int f_*^m X^u(\Phi) h = \sum_{m=0}^{\infty} \int X^u(\Phi \circ f^m) h = - \sum_{m=0}^{\infty} \int \Phi \circ f^m h \text{div}_u X^u.$$ 

To be rigorous, we should first apply a Markov partition and then integrate-by-parts within each rectangle; the boundary terms cancel. This formula converges due to decay of correlations.
Adding up the two contributions, we get the so-called blended formula, partly in name of the blended response algorithm by Majda and Abramov \cite{1}. The blended formula suggests computing the unstable divergence by summing directional derivatives; this is again a trap, since directional derivatives of $X^u$ are still infinite. However, Ruelle showed that $\text{div}_\sigma^u X^u$ is Holder continuous \cite{36}. This opens up the possibility of sampling $\text{div}_\sigma^u X^u$ on an orbit, but we need another formula for it.

By the divergence formula in section 2, we know that the unstable divergence is the derivative of the transfer operator on the unstable manifold for the conditional physical measure $\sigma$. More specifically,

$$-\text{div}_\sigma^u X^u = \delta^u \tilde{L}^u \sigma_{-1},$$

where $\sigma_{-1}$ is the conditional physical measure on $V^u(f^{-1}x)$.

Finally, we give an alternative derivation of the unstable contribution formula in equation (7); this derivation is formal, but is operator-oriented and intuitive. 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. A perturbation by $X^u$ will re-distribute the densities within each unstable manifold, but will not move densities across different unstable manifolds.

Hence, the family of phase spaces of this time-inhomogeneous system is preserved, and the operator version of linear response formula still formally applies. Let $\sigma'$ be the quotient measure in the stable direction, so $\int \sigma' \int \sigma \Phi = \int h \Phi$ for any smooth function $\Phi$. Also let $\tilde{\sigma}$ be the conditional measure of $\tilde{f}$, and $\sigma = L^u \sigma_{-1} = \cdots = (L^u)^m \sigma_m$ be the sequence of conditional measures on unstable manifolds crossing $x, x_{-1}, \cdots x_{-m}$. Hence, formally,

$$\delta^u \left( \int \Phi \tilde{h} \right) = \int \sigma' \int \Phi \delta^u \tilde{\sigma} = \sum_{m \geq 0} \int \sigma' \int \Phi L^m \delta^u \tilde{L}^u \sigma_{-m-1}$$

$$= \sum_{m \geq 0} \int \sigma' \int \frac{\delta^u \tilde{L}^u \sigma_{-m-1}}{\sigma_{-m}} \circ f^{-m} \cdot \Phi \sigma$$

$$= \sum_{m \geq 0} \int \sigma' \int \text{div}_\sigma^u X^u \circ f^{-m} \cdot \Phi \sigma = \sum_{m \geq 0} \int \text{div}_\sigma^u X^u \circ f^{-m} \cdot \Phi \tilde{h}$$

This formula is the same as equation (7).

We also mention that there are many other attempts to compute the linear response which do not fall into our main logic of this paper, such as the gradient clipping, and the reservoir computing method from the machine learning community \cite{33, 23}. These methods do not need ergodic theory.

4. **Equivariant divergence formula for the unstable derivative operator**
We derive the recursive formula of the unstable derivative operator on the unstable manifold. 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.

4.1. Notations.

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 $|e| = 1$, 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 $\varepsilon(e) = 1$, where $\varepsilon := \varepsilon^1 \wedge \cdots \wedge \varepsilon^u$.

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 $Y$. $\nabla_{(\cdot)} f_s$, the derivative of the Jacobian, is the Hessian matrix, such that

$$\nabla_{f_s} Y (f_s X) = (\nabla_X f_s) X + f_s \nabla_Y X.$$

This is essentially the Leibniz rule. Note that $(\nabla_Y f_s) X = (\nabla_X f_s) Y$. Denote

$$\nabla e X := \sum_{i=1}^u e_i \wedge \cdots \wedge \nabla e_i X \wedge \cdots \wedge e_u, \quad \nabla X e := \sum_{i=1}^u e_1 \wedge \cdots \wedge \nabla X e_i \wedge \cdots \wedge e_u.$$

One of the slots of $\nabla_{(\cdot)} f_s (\cdot)$ can take a $u$-vector, in which case

$$(\nabla_X f_s) e := (\nabla e f_s) X := \sum_{i=1}^u f_s e_1 \wedge \cdots \wedge (\nabla e_i f_s) X \wedge \cdots \wedge f_s e_u,$$

$$\nabla_{f_s} e f_s X = (\nabla e f_s) X + f_s \nabla e X, \quad \nabla_{f_s} X f_s e = (\nabla X f_s) e + f_s \nabla X e.$$

There are two different divergences on an unstable manifold, which coincide only if $u = M$. The first divergence is taken within the unstable submanifold,

$$\text{div}^u X^u := \langle \nabla e X, e \rangle.$$

We call this the submanifold unstable divergence, or $u$-divergence. We may further specify a measure for this submanifold divergence, such as in $\text{div}^u X^u$. This is the unstable divergence we have been using.
The second kind of unstable divergence might be more essential for hyperbolic systems. Define the equivariant unstable divergence, or \( v \)-divergence, as
\[
\text{div}^v X^u := \varepsilon \nabla e X^u.
\]
We define the \( v \)-divergence of the Jacobian matrix \( f_* \),
\[
\text{div}^v f_* := \frac{\varepsilon_1 \nabla e f_*}{|f_* e|}, \quad (\text{div}^v f_*) X := \frac{\varepsilon_1 (\nabla e f_*) X}{|f_* e|}, \quad \text{where } \varepsilon_1(x) := \varepsilon(f x).
\]
Note that \( \text{div}^v f_* \) is a Holder continuous covector field on the attractor.

4.2. One volume ratio for the entire unstable derivative operator.

As illustrated in figure 1, for any \( z \in V^u(x) \), define \( \eta(z) : V^u \rightarrow M \) as the unique curve such that \( \delta \gamma := \partial \eta / \partial \gamma = X \) and \( \eta(z)|_{\gamma=0} = z \). For fixed \( \gamma \), \( V^u\gamma := \{ \eta(z) : z \in V^u \} \) is a \( u \)-dimensional manifold. For any \( z \in V^u\gamma \), denote the stable manifold that goes through it by \( V^s(z) \). Define \( \xi(z) \) as the unique intersection point of \( V^s(z) \) and \( V^u(x) \).

Since \( \xi \) is the projection along stable directions, \( \delta(\xi \eta) = X^u \). Hence, we can use \( \xi \eta \) to compute \( \delta^u \tilde{L}^u \), although it is not the same as the flow of \( X^u \) for large \( \gamma \).

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, \( \delta^u \tilde{L}^u \sigma_{-1}(x) = l_2 / l_1 = l'_2 / l'_1 \), where \( l_1, l_2 \) are lengths of dotted lines.

Denote the conditional measure at \( \gamma = 0 \) by \( \sigma \), fix a point \( x \), we want to compute \( \delta^u \tilde{L}^u \sigma_{-1}(x) \), where \( \sigma_{-1} \) is the conditional SRB measure on \( V^u(f_{-1} x) \). Let \( y = (\xi \eta)^{-1} x \), according to equation (3),
\[
\tilde{L}^u \sigma_{-1} = \frac{\sigma}{|\eta_*|} \circ \eta^{-1} = \frac{\sigma(y)}{\sigma(x) |\eta_*(y)| |\xi_*(\eta y)|}.
\]
To find \( \sigma \), we consider how the Lebesgue measure on \( V^u(x_{-k}) \) is evolved. Let \( e_{-k} \) be the unit \( u \)-vector field on \( V^u(x_{-k}) \). The mass contained in the cube \( e_{-k} \) is preserved via pushforwards, but the volume increased to \( f^k e_{-k} \). Hence the density
\[
\sigma \propto \lim_{k \to \infty} \frac{1}{|f^k e_{-k}|}.
\]
We use the proportional sign to indicate that the conditional measure is determined up to a constant coefficient. Let \( x^{-k} := f^{-k}x \),

\[
\frac{\dot{L}^u\sigma^{-1}}{\sigma}(x) = \lim_{k \to \infty} \frac{|f^k e^{-k}(x^{-k})|}{|f^k e^{-k}(y^{-k})|} = \lim_{k \to \infty} \frac{|f^k e^{-k}(x^{-k})|}{|\xi_n(y)| \cdot |\xi_n(\eta y)|}.
\]

Both \( f^k e^{-k}(x^{-k}) \) and \( \xi_n f^k e^{-k}(y^{-k}) \) are in \(^nV^u(x)\), which is a one-dimensional subspace. Hence, their ratio does not change via pushforwards, and

\[
\frac{\dot{L}^u\sigma^{-1}}{\sigma}(x) = \lim_{k \to \infty} \frac{|f^k e^{-k}(x^{-k})|}{|f^k \xi_n f^k e^{-k}(y^{-k})|}.
\]

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

\[
\lim_{k \to \infty} f^k \xi_n = \lim_{k \to \infty} f^k.
\]

This intuitive statement is proved as a corollary of the absolute continuity of the holonomy map \([6, \text{theorem 4.4.1}]\). Hence

\[
\frac{\dot{L}^u\sigma^{-1}}{\sigma}(x) = \lim_{k \to \infty} \frac{|f^k e^{-k}(x^{-k})|}{|f^k \xi_n f^k e^{-k}(y^{-k})|}.
\]

Formally differentiate above expressions,

\[
-\frac{\delta \dot{L}^u\sigma^{-1}}{\sigma}(x) = \lim_{k \to \infty} \frac{d}{d\gamma} \frac{f^k \xi_n f^k e^{-k}(y^{-k})}{f^k e^{-k}(x^{-k})} = \lim_{k \to \infty} \frac{\left\langle \frac{d}{d\gamma} f^k \xi_n f^k e^{-k}(y^{-k}), f^k e^{-k} \right\rangle}{|f^k e^{-k}|^2},
\]

where

\[
\frac{d}{d\gamma} f^k \xi_n f^k e^{-k} = \sum_{i=1}^u f^k \xi_n f^k e^{-k,1} \wedge \cdots \wedge \frac{d}{d\gamma} f^k \xi_n f^k e^{-k,i} \wedge \cdots \wedge f^k \xi_n f^k e^{-k,u}.
\]

Here \( e^{-k,i} = e_i(y^{-k}) \). We emphasize that \( \frac{d}{d\gamma} \) is the total derivative: \( \eta \) has two direct parameters \( y \) and \( \gamma \); \( f \) has only one variable \( y \), and \( y \) depends on \( \gamma \). Recursively apply the Leibniz rule, note that \( \eta_n = d\eta \) when \( \gamma = 0 \), we get

\[
-\frac{\delta \dot{L}^u\sigma^{-1}}{\sigma}(x) = \lim_{k \to \infty} \frac{\left\langle \frac{d}{d\gamma} f^k \xi_n f^k e^{-k}(y^{-k}), f^k e^{-k} \right\rangle}{|f^k e^{-k}|^2} + \frac{\left\langle \frac{d}{d\gamma} \nabla_{-f^k X_n} e^{-k}, f^k e^{-k} \right\rangle}{|f^k e^{-k}|^2} + \frac{\left\langle \frac{d}{d\gamma} \nabla_{-f^k X_n} e^{-k}, f^k e^{-k} \right\rangle}{|f^k e^{-k}|^2} + \frac{\left\langle \frac{d}{d\gamma} \nabla_{-f^k X_n} e^{-k}, f^k e^{-k} \right\rangle}{|f^k e^{-k}|^2}.
\]

The uniform convergence of this expansion justifies the formal differentiation.

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

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

Then we resolve \( d\eta_n / d\gamma \) in the first term. For fixed \( e \),

\[
\left( \frac{d}{d\gamma} \eta_n \right) e = \frac{d}{d\gamma} \nabla_e \eta(y, \gamma) = \nabla_{\delta y} \nabla_e \eta + \frac{\partial}{\partial \gamma} \nabla_e \eta = \nabla_{\delta y} \nabla_e \eta + \nabla_e \frac{\partial}{\partial \gamma} \eta = \nabla_e X.
\]

Here \( \nabla_{\delta y} \nabla_e \eta \) is zero because \( \eta(y, 0) = y \), so \( \eta \)'s second order partial derivative in the location variable is zero.
Because the stable part decays via pushforwards,
\[ \lim_{k \to \infty} \frac{\langle f^k r, f^k e \rangle}{|f^k e|^2} = \varepsilon r. \]
Since \( f^ne_{-k} = e_{n-k} |f^ne_{-k}| \),
\[ \lim_{k \to \infty} \frac{\langle f^{2k-n-1}(\nabla_{-\sigma^k X} f_s) f^ne_{-k}, f^{2k-1}e_{-k} \rangle}{|f^{2k-1}e_{-k}|^2} = \lim_{k \to \infty} \frac{\langle f^{2k-n-1}(\nabla_{-\sigma^k X} f_s) e_{n-k}, f^{2k-n}e_{n-k+1} \rangle}{|f^{2k-n}e_{n-k+1}|^2} = \frac{\varepsilon_{n-k+1}(\nabla_{-\sigma^k X} f_s) e_{n-k}}{|f^ne_{n-k}|} = -\left( \frac{\varepsilon_{n-k+1}(\nabla_{-\sigma^k X} f_s) X^u}{|f^ne_{n-k}|} \right). \]
Hence,
\[ -\frac{\delta \tilde{L}^u \sigma^{-1}}{\sigma}(x) = \varepsilon \nabla e X + \lim_{k \to \infty} \sum_{n=0}^{k-1} -(\text{div}^u f_s)_{n-k} f^u_{n-k} X^u + (\text{div}^u f_s)_{n} f^u_{n} X^u \]
\[ = \text{div}^u X - \sum_{m=1}^{\infty} (\text{div}^u f_s)_{-m} f^u_{-m} X^u + \sum_{n=0}^{\infty} (\text{div}^u f_s)_{n} f^u_{n} X^u. \]

4.3. Recursive formula.

We define the shadowing form \( \nu \) and the adjoint shadowing operator \( \mathcal{L} \).
\[ \mathcal{L}(\text{div}^u f_s) := \sum_{n=0}^{\infty} f^{u*n} \mathcal{P}^u(\text{div}^u f_s)_n - \sum_{m=1}^{\infty} f^{s-m} \mathcal{P}^u(\text{div}^u f_s)_{-m}. \]
Here \( \mathcal{P}^s, \mathcal{P}^u \), and \( f^* \) are transposed matrices, or adjoint operators, of \( P^s, P^u \), and \( f_s \). Hence, we have proved the following theorem.

**Theorem 2.** The \( \nu \)-divergence formula for unstable derivative of the transfer operator on unstable manifolds is
\[ \text{div}^u X^u = -\frac{\delta \tilde{L}^u \sigma^{-1}}{\sigma} \nu X = \text{div}^u X + (\mathcal{L}(\text{div}^u f_s)) X. \]

There are two significances of this formula. The first is that now all differentiation hits only \( C^\infty \) functions \( X \) and \( f_s \). We got rid of all intermediate quantities with infinite sup norm. The second significance is that, as we shall explain, the formula can be sampled on an orbit via \( 2u + 1 \) 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 \( e \). Similarly, \( \varepsilon \) can be efficiently computed via \( u \)-many backward recursion, since it is the unstable subspace of the adjoint system.

The adjoint shadowing form \( \nu := \mathcal{L}(\text{div}^u f_s) \) can also be efficient computed with one more backward recursion and an orthogonal condition. The adjoint shadowing lemma
states that $\nu$ is the only bounded solution of the adjoint equation,

$$\nu = f^*\nu_1 + \text{div}^\nu f_*.$$ 

Hence $\nu$ can be well approximated by

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

Here $\nu'$ is a particular inhomogeneous adjoint solution. This is known as the nonintrusive (adjoint) shadowing algorithm [31] (also see [7, 32, 29, 38]).

Hence, we can compute the $\nu$-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 $\delta L$, the efficiency advantage is significant when the attractor dimension is larger than 4.

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 [30, 28].

5. Conclusions

In perturbation theories for measures, we typically deal with the stable and unstable part separately, then assemble the two parts into a uniform transfer operator formula or ensemble/Koopman formula: this is very important for many analytical applications. However, in numerics, for sampling on an orbit via a few recursive relations, we might still want to use different formulas for the two parts. In this paper we solve this problem for the more difficult part, the unstable derivative operator of a physical measure. It was well known that the physical measure can be sampled on a orbit; now, with our results, we know that its derivative operator and hence the linear response can also be sampled on a orbit by $2u + 1$ recursive relations. This cost is perhaps optimal, since we need at least $u$ many modes to capture all the unstable behaviors of a chaotic system.

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This manuscript has not associated data.
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