ON COMPUTING DERIVATIVES OF TRANSFER OPERATORS AND LINEAR RESPONSES IN HIGHER DIMENSIONS

ANGXIU NI

Beijing International Center for Mathematical Research, Peking University, Beijing, China

ABSTRACT. We show that the derivative of the transfer operator with respect to perturbations of the map is a divergence. We show that, in high dimensions, approximating singular measures by isotropic finite-elements, and computing the derivative operator on such approximate measures, are both expensive. We show the equivalence between the operator and ensemble version of the linear response formula, and discuss how to combine both formula, as done by the fast linear response algorithm, to reduce cost.

Keywords. Transfer operator, SRB measures, Koopman operator, linear response, fast linear response algorithm.

1. Introduction

The transfer operator, $L$, also known as the Ruelle-Perron-Frobenius operator, is frequently used to study the behavior of dynamical systems. For a map, $f$, the transfer operator describes how the density of a measure is changed after evolving by $f$. For expanding maps, the transfer operator is very useful because it is regularizing in many norms. In contrast, the adjoint of the transfer operator, the Koopman operator, is regularizing for contracting maps. As a result, the Koopman operator is popular in contexts like machine learning, where most of the current systems are intentionally designed to be stable. In [18], Gouëzel andLiverani gave an optimal Banach space for considering the transfer operator of hyperbolic maps, which has both expanding and contracting directions. In the so-called anisotropic Banach space, the largest eigenvalue of the transfer operator is still 1; this enables many useful functional tools in hyperbolic systems. The unique eigenvector corresponding to eigenvalue 1 is the physical measure, or the SRB measure, which is typically singular with respect to the Lebesgue measure.

In numerical computations, a major difficulty is that the SRB measure, $h$, is typically singular. There are various methods to find an approximate measure, $\tilde{h}$, which is absolutely continuous to Lebesgue. Such finite-rank approximation of SRB measures were discussed in many papers [21, 14, 24, 11, 10, 31, 16, 17, 39, 9, 2, 38, 15]; it is very convenient for reusing algorithms intended for smooth densities. These algorithms are highly efficient for low-dimensional systems, but the cost can increase exponentially fast.

E-mail address: niangxiu@gmail.com
Date: September 1, 2021.
with respect to the dimension. For high-dimensional systems, if we are only interested in the integration of the SRB measure to a continuous observable function, then the most efficient approximation of SRB measure is to average over a sample orbit.

The derivative of the transfer operator, $\delta L$, with respect to $\delta f$, is useful in many settings. For SRB measures, $\delta L$ is singular, and a major numerical solution is to approximately compute it on a smooth approximate $\hat{h}$. Gutiérrez and Lucarini computed approximate $\delta L$ for a continuous-time 3-dimensional system [34], but that only requires a relatively degenerate formula of the discrete-time cases; Bahsoun, Galatolo, Nisoli, and Niu did computations on 1-dimensional expanding maps [3]. Theoretically, for high-dimensional hyperbolic systems, this approximated operator approach converges in the anisotropic Banach space, and it does not require computing hyperbolic structures of the system. However, computing $\delta L$ of SRB measures via this approximation scheme was not numerically realized for discrete-time systems with dimensions larger than 1, mainly because of two reasons:

- the lack of some convenient formulas for higher-dimensions;
- the cost is expected to be high, although we still lack a quantitative apriori estimation.

The first part of this paper addresses these issues. Section 2 first proves the divergence formula of $\delta L$ using a functional argument, then proves the same theorem using a pointwise argument, which also yields several formulas useful for computations. Section 3 uses the divergence formula to estimate the cost-error relation for isotropically approximating singular measures, and for computing derivative operators using approximate measures. Our estimations show that both costs increase exponentially fast with respect to the dimension of the attractors. In fact, even if we do not use isotropic approximations of SRB measures, the cost is still high for computing $\delta L$, because it has infinite sup norm.

The second part of this paper considers one of the most important applications of $\delta L$: the linear response, which is the derivative of the SRB measure with respect to $\delta f$ [4]. Since it is expensive to compute $\delta L$ on the entire SRB measure, the operator version of linear response formula is also expensive. However, section 4.2 shows that the derivative operator is still an important ingredient for efficiently computing linear responses. We give a new interpretation of some existing algorithms as using a blended formula which does not have large sup norms. The blended formula uses the operator formula for the unstable part of the linear response, and the ensemble formula for the stable part. Here the ensemble formula is another version of the linear response formula used by Ruelle and Dolgopyat [32, 12]; using the divergence formula of $\delta L$, section 4.1 shows that the ensemble formula is exactly the integrated-by-part operator formula. However, the unstable part involves an unstable divergence, which is very difficult to compute due to lack of regularities. As a result, previous blended algorithms still have high cost, such as the blended response algorithm and the S3 algorithm [1, 8].

The fast linear response algorithm resolves the regularity issues by a ‘fast’ formula of the unstable divergence [28]. Moreover, it requires data from only one sample orbit, which is the most efficient way to sample the SRB measure. Section 4.2 discusses its computational cost compared to the operator approach. Another ingredient of the fast
linear response is the non-intrusive shadowing algorithm, which efficiently computes the shadowing direction \(30, 29, 27, 37, 36, 20, 5, 35, 22, 6\); it was successfully applied to systems with over \(4 \times 10^6\) dimensions \[26\]. Non-intrusive shadowing can be a good approximation of the linear response when the unstable ratio is low \[27\].

2. Divergence formula of \(\delta L\)

2.1. A functional proof.

Let \(f\) be a smooth diffeomorphism on a smooth Riemannian manifold \(\mathcal{M}\), whose dimension is \(M\). For measures with a density function, say \(h \in C^r(\mathcal{M})\), the transfer operator, \(L : C^r \rightarrow C^r\), gives the new density function after pushing forward the measure by \(f\). More specifically, \(L\) of \(f\) is defined by the duality

\[
\int h \cdot \Phi \circ f =: \int Lh \cdot \Phi,
\]

where \(\Phi\) is any smooth observable function. In this paper, all integrals are taken with respect to the Lebesgue or Riemannian measure, except when another measure is explicitly mentioned.

We are interested in how a perturbation, \(\delta f\), would affect \(L\). We may assume that \(f\) is parameterized by some scalar \(\gamma\), and define

\[
\delta(\cdot) := \frac{\partial(\cdot)}{\partial \gamma}.
\]

**Theorem 1.** For measures absolutely continuous to Lebesgue,

\[
\delta L h = - \text{div}((Lh)X).
\]

Here \(X := \delta f \circ f^{-1}\), and \(X(\cdot)\) is to differentiate a function in the direction of \(X\).

**Remark.** (1) This theorem holds pointwisely. (2) For invariant measures, \(Lh = h\), and there is a simplification very useful in the following part of this paper,

\[
\delta Lh = - \text{div}(LhX) = - \text{div}(hX).
\]

**Proof.** Differentiate equation (11), for any \(\Phi\),

\[
\int h \cdot \delta(\Phi \circ f) = \int \delta Lh \cdot \Phi.
\]

Since \(\delta(\Phi \circ f) = \delta f(\Phi) = X(\Phi) \circ f\), the left-hand-side

\[
\int h \cdot \delta(\Phi \circ f) = \int h \cdot X(\Phi) \circ f = \int Lh \cdot X(\Phi),
\]

where we applied the definition of \(L\) in equation (11) again.

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

\[
\int \delta Lh \cdot \Phi = \int Lh \cdot X(\Phi) = - \int \text{div}(LhX) \cdot \Phi.
\]

Since this holds for any \(\Phi\), it must be \(\delta Lh = -\text{div}(LhX)\). When \(h\) is not compactly supported, just apply a smooth cutoff function to \(h\). \(\square\)
We define a notation
\[ \text{div}_Lh X := \frac{\text{div}((Lh)X)}{Lh} = \text{div}(X) + \frac{X(Lh)}{Lh}. \]

In typical geometry textbooks, the divergence is defined after choosing a Riemmanian metric. However, we do not need the full metric to define the divergence; the divergence is the same for any two metrics with the same volume measure. Here \( \text{div}_Lh \) is the divergence under the measure \( Lh \), and theorem 1 writes
\[ \delta Lh = -Lh \text{div}_Lh X. \]

2.2. A pointwise proof and more formulas.

This section derives \( \delta L \) using the pointwise definitions of \( L \), which also gives several formulas useful for computations, especially for non-invariant measures.

On a Riemannian manifold, \( L \) is equivalently defined by the pointwise expression,
\[ Lh = (hJ^{-1}) \circ f^{-1}. \]

Here \( J \) is the Jacobian determinant, which is how much the volume of a small cube grows via one pushforward of \( f \). More specifically,
\[ J = \frac{|f_*e|}{|e|} \quad \text{where} \quad e = e_1 \wedge \cdots \wedge e_M, \]
where \( e_i \)'s are smooth 1-vector fields; \( e \) is a smooth \( M \)-vector field, which is essentially an \( M \)-dimensional hyper-cube field, and \( | \cdot | \) is its volume. Here \( f_* \) is the pushforward of vectors. Notice that \( J \) 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 Riemmanian metric. For simple \( M \)-vectors,
\[ \langle e, r \rangle := \det \langle e_i, r_j \rangle, \quad \text{where} \quad e = e_1 \wedge \cdots \wedge e_u, \ r = r_1 \wedge \cdots \wedge r_v, \ e_i, r_j \in T_M. \]

When the operands are summations of simple \( M \)-vectors, the inner-product is the corresponding sum.

Applying \( \delta \) on both side of equation (2), notice that \( h \) is fixed, we have
\[ (\delta L)h = \delta(Lh) = -(h\delta(J^{-1})) \circ f^{-1} + \delta(f^{-1})(hJ^{-1}) \]
\[ = -(\frac{h}{J^2} \delta J) \circ f^{-1} + \left( \frac{1}{J} \circ f^{-1} \right)((\delta(f^{-1}))h) - \left( \frac{h}{J^2} \circ f^{-1} \right)((\delta(f^{-1}))J). \]

Here \( \delta(f^{-1})(x) \) is a vector at \( f^{-1}x \), so when it differentiates a function, say \( h \), we agree that the differentiation happens at \( f^{-1}x \). Then we give the detailed formula for each term in equation (3).

**Lemma 1.** \( \delta J = J \cdot (\text{div} X \circ f) \), where \( X := \delta f \circ f^{-1} \).
Remark. Notice that
\[ f(x) = \sum_{i=1}^{M} f_i(x) e_i, \]
where \( \{e_i\}_{i=1}^{M} \) is the basis of \( T_e \mathcal{M} \).

Lemma 2. \( \delta(f^{-1}) = -f^{-1}X. \)

Proof. Differentiate \( Id = f \circ f^{-1} \), we get
\[ 0 = \delta f \circ f^{-1} + f_i \delta(f^{-1}) = X + f_i \delta(f^{-1}). \]

Lemma 3. \( Y(J) = J(\text{div } f_*)Y. \)

Remark. Notice that \( J \), \( f_* \), and \( Y \) are at the same place. Hence, for \( Y = f_*^{-1}(X(x)) \in T_f \mathcal{M} \), we have \( Y(J) = J(f^{-1}(x)) \langle \text{div } f_*(f^{-1}(x)) \rangle f_*^{-1}(X(x)) \).

Proof. By definitions of \( J \),
\[ Y(J) = Y \left( \frac{\langle f_*e \rangle}{|e|} \right) = Y \left( \frac{f_*e}{|e|} \right) \frac{Y(|e|)}{|e|} = \frac{\langle Y f_* e, f_* e \rangle}{|f_* e| |e|} - \frac{|f_* e| |Y e, e|}{|e|^3}. \]
By the same argument as in equation (4), we have
\[ Y(J) = J(f,e)^i \nabla f,Y f,e_i - J e^i \nabla_Y e_i. \]

By definitions of \( \nabla f \) and \( \text{div} f \),
\[ Y(J) / J = (f,e)^i((\nabla_Y f,e_i + f,\nabla_Y e_i) - e^i \nabla_Y e_i) = \text{div}(f,e)Y + (f,e)^i f,\nabla_Y e_i - e^i \nabla_Y e_i. \]
The last two terms cancel because \((f,e)^i f,\cdot = e^i \cdot \).
\[ \square \]

**Lemma 4.** \( X(Lh) = \left( \frac{1}{J} \circ f^{-1} \right) f^{-1}_x X(h) - \left( \frac{h}{J} \circ f^{-1} \right) (\text{div} f)_x f^{-1}_x X. \)

**Proof.** Differentiate the expression of \( Lh \), we get
\[ (5) \quad X(Lh) = X \left( \frac{h}{J} \circ f^{-1} \right) = \frac{1}{J \circ f^{-1}} f^{-1}_x X(h) - \left( \frac{h}{J^2} \circ f^{-1} \right) f^{-1}_x X(J). \]
Then substitute lemma 3.
\[ \square \]

For a pointwise proof of theorem 1, substitute lemma 1, 2, and 3 into equation (3),
\[ (6) \quad \delta Lh = - \frac{h}{J} \circ f^{-1} \text{div} X - \left( \frac{1}{J} \circ f^{-1} \right) f^{-1}_x X(h) + \left( \frac{h}{J} \circ f^{-1} \right) (\text{div} f)_x f^{-1}_x X. \]
substitute lemma 4 into equation (6), then
\[ \delta Lh = - \frac{h}{J} \circ f^{-1} \text{div} X - X(Lh) = -(Lh \text{div} X + X(Lh)) = - \text{div}((Lh)X). \]
In fact, for proving the theorem, we do not need lemma 3 and lemma 4, we only need equation (5); but an explicit expression of \( X(Lh) \) is more useful for computations.

3. Cost-error estimation for computing \( \delta L \) of SRB measures

When the SRB measure is singular, both \( \text{div}(hX) \) and \( \text{div}_h X \) have infinite sup norm. Although both are well-defined mathematical objects in suitable spaces, computers cannot process infinite sup norm. Currently, the main practice in operator methods is to compute \( \delta L \) on an approximated measure, which is absolutely continuous to Lebesgue. More specifically, say a smooth function \( \tilde{h} \) is an approximation of \( Lh = h \), then, by theorem 1, we can approximate \( \delta Lh \) by \( \text{div} \tilde{h}X \). For \( \text{div} \tilde{h}X \) and \( \text{div}_h X \) to have finite sup norm, we need to use isotropic finite-elements, which are regular in all directions. This allows us to neglect the subtle structures of SRB measures; however, it is still affected by the fact that the true SRB measure is singular with hyperbolic structures, since approximating low-dimensional objects by isotropic elements is expensive/inaccurate.

3.1. Approximating SRB measures by isotropic elements.

We first estimate the cost-error relation for approximating a singular SRB measure by isotropic finite-elements. In [17], 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. This is a very precise bound, but it hides away the cost-error relation. Here we aim at giving an apriori estimation on a specific example, which captures only the error in the direction off the attractor: this could be the most significant error. The example does not capture the complete error for general cases,
but it is sufficient for showing our point: the cost of the approximation is cursed by dimensionality.

Consider the example where \( \mathcal{M} = \mathbb{T}^M = [-0.5, 0.5]^M \), the SRB measure is uniformly distributed on the \( a \)-dimensional attractor, \( \{0\}^{M-a} \times \mathbb{T}^a \). We use the zeroth order finite-elements in the \( M \)-dimensional cubes, \( \prod_{i=1}^M \varepsilon [n_i - 0.5, n_i + 0.5] \), where \( n_i \in \mathbb{Z} \), and \( 1/\varepsilon \in \mathbb{Z} \). The density of the SRB measure, \( \tilde{h} \), is a distribution. Let \( \hat{h} \) be the finite-element approximation of \( h \), so

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

For the smooth objective function, \( \Phi \), we assume that for any unit vector \( v \), \( \partial^2 \Phi / \partial v^2 \sim O(1) \), where \( \sim \) means to equal in absolute value, within some constant coefficients, with large probability.

Then we look at the approximation error, \( E_h \), caused by using \( \tilde{h} \) instead of \( h \).

\[
E_h := \int \Phi \tilde{h} - \int \Phi h \\
= \int_{T^a} \int_{\mathbb{T}^{M-a}} \Phi \tilde{h} d x^{1 \sim M-a} d x^{M-a+1 \sim M} - \int_{T^a} \Phi(0, x^{M-a+1}, \ldots, x^M) d x^{M-a+1 \sim M},
\]

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

\[
E_h \sim \int_{\mathbb{T}^{M-a}} \varphi \tilde{h} - \varphi(0) = \int_{\mathbb{T}^{M-a}} (\varphi(y) - \varphi(0)) \tilde{h} \sim \int_{\mathbb{T}^{M-a}} \frac{\partial \varphi}{\partial v}(0) y + \frac{\partial^2 \varphi}{\partial v^2}(0) \frac{y^2}{2} \tilde{h},
\]

where \( v = y/|y| \) is the direction of taking derivatives. The first term is zero due to symmetry, hence

\[
E_h \sim \int_{\mathbb{T}^{M-a}} y^2 \tilde{h} = \varepsilon^{-(M-a)} \int_{[-0.5\varepsilon, 0.5\varepsilon]^{M-a}} (y^1)^2 + \ldots + (y^{M-a})^2 d y^1 \ldots d y^{M-a} \\
\sim \varepsilon^{-(M-a)} (M-a) \varepsilon^3 \varepsilon^{M-a-1} = (M-a) \varepsilon^2.
\]

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

There are several different algorithms for finding a finite-rank approximation of the SRB measure and its distributional derivatives. The finite-element basis we chose is localized, hence we can find an approximation supported close to the low-dimensional attractor. With optimal implementation, we should be able restrict our computation to the attractor, and the cost

\[
S \sim O(\varepsilon^{-a}) \sim O \left( \frac{M-a}{E_h} \right)^{\frac{3}{2}}.
\]

On the other hand, if the finite-elements are all globally supported, such as the Fourier basis, or if the implementation is not optimal, the computation may need to consider the entire phase space, and the cost could be \( O(\varepsilon^{-M}) \). To conclude, approximation by isotropic elements is inefficient/inaccurate for SRB measures in higher dimensions; it is cursed by dimensionality.
3.2. Computing $\delta L$ on approximated singular measures.

Now we consider the cost-error relation for computing $\delta L$ on approximate SRB measures. Further assume that for any unit vector $v$, $\partial^2 \Phi/\partial x^1 \partial v^2 \sim O(1)$. Using the divergence formula for $\delta L$, we see that the approximation error, $E_\tilde{h}$, becomes

$$E_\tilde{h} := \delta L(h) - \delta L(\tilde{h}) = \int \Phi \operatorname{div}_{\tilde{h}} X h - \int \Phi \operatorname{div}_h X \tilde{h}$$

$$= \int \Phi X(h) - \int \Phi \tilde{h} X = \int X(\Phi)h - \int X(\Phi)\tilde{h}.$$

Replace $\Phi$ by $X(\Phi) = \partial \Phi/\partial x^1$ in the last subsection, the same estimation still applies, and we still have

$$E_\tilde{h} \sim (M-a)\varepsilon^2$$

and

$$S \sim O(\varepsilon^{-a}) \sim O\left(\frac{M-a}{E_\tilde{h}}\right)^{\frac{2}{3}}.$$

So the cost is still cursed by dimensionality.

Hypothetically, we can perhaps develop algorithms which compute $\operatorname{div}_{\tilde{h}} X$ using only data from a sample orbit of length $T$. We optimistically neglect other additional errors, which could be quite significant, and consider only the sampling error due to using a finite trajectory. Precisely speaking, $\operatorname{div}_{\tilde{h}} X$ is a distribution with singular support, but we can estimate its 'typical' sup norm by its average on the approximate SRB measure,

$$\int |\operatorname{div}_{\tilde{h}} X| \tilde{h} = \int |X(\tilde{h})| = \int_{T^a} \int_{T^{M-a-1}} \int_{T^{M-a}} |X(\tilde{h})| dx^1 dx^{2\sim M-a} dx^{M-a+1\sim M}.$$

The inner integration is the total variation of $\tilde{h}$ along the $x^1$ axis, that is,

$$\int_{T} |X(\tilde{h})| dx^1 = \int_{T} \left| \frac{\partial \tilde{h}}{\partial x^1} \right| dx^1 = \begin{cases} 2\varepsilon^{-(M-a)} & \text{if } |x^2|, \ldots, |x^{M-a}| \leq \varepsilon/2; \\ 0 & \text{otherwise}. \end{cases}$$

Hence,

$$\int |\operatorname{div}_{\tilde{h}} X| \tilde{h} = \int |X(\tilde{h})| = 2\varepsilon^{-(M-a)} \varepsilon^{M-a-1} = 2\varepsilon^{-1}.$$

Hence, $\operatorname{div}_{\tilde{h}} X \sim O(\varepsilon^{-1})$, and the sampling error $E_{\text{sam}} \sim O(\varepsilon^{-1} T^{-0.5})$. In practice we want $E_{\text{sam}} \sim E_\tilde{h}$, so $T \sim O(\varepsilon^{-6} (M-a)^{-2})$. Assuming that only one orbit is enough and we do not need any other data, then

$$S \sim O(T) \sim O((M-a)\varepsilon^{-3}).$$

To conclude, even if we could really get rid of the curse of dimensionality, our cost will still be affected by the large sup norm in the approximated derivative. To avoid large sup norm, we should differentiate $h$ only in the smooth directions, and this can not be done without knowing some details of the hyperbolic structures.

4. Reduce cost via the blended linear response formula

We now focus on one of the most important applications of $\delta L$: computing the linear response. Due to our previous analysis, it can be very expensive to compute the linear response by the operator formula for higher-dimensional attractors. It is also well known that another version of the linear response formula, the ensemble formula,
is also very expensive, due to exploding vectors. In this section, we first show the equivalence between the two formulas using the divergence formula for $\delta L$. Then we discuss how to combine the two formulas, as done by the fast linear response algorithm, and why this reduces the computational cost.

4.1. **Two versions of the linear response formula.**

The SRB measure, $h$, corresponding to a map $f$, hence its transfer operator $L$, is

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

where $\mu$ is any measure with a smooth density function. When changing $f$, we have a new SRB measure. By formal differentiation, we see that $\delta h$ has the expression

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

We call this the operator version of the linear response formula. 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 [18, 4].

The dual way to derive the linear response formula is to consider the pullback of observable functions, or the Koopman operators. For a smooth observable function $\Phi$,

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

Hence we can formally write the linear response,

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

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

We call this the ensemble version of the linear response formula, because it is formally an average of orbit-wise perturbations over an ensemble of trajectories. For contracting maps, the convergence is because the system lands onto a stable fixed point. For hyperbolic systems, above formula was proved in [32, 12]. This formula was numerically realized in [23, 13, 25, 19]; however, due to exponential growth of the sup norm of vectors, it is typically unaffordable for ensemble methods to actually convergence [28, 7].

By theorem 1, we can directly show that these two linear response formulas are equivalent. Formally integrate-by-parts the ensemble version, we have

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

Which we refer to as the integrated-by-parts version of linear response formula. For invariant measures, $h = Lh$, hence

$$\sum_{m=0}^{\infty} \int \Phi \circ f^m \text{div}_h X h = \sum_{m=0}^{\infty} \int \Phi L^m \delta L h = \Phi \sum_{m=0}^{\infty} \int L^m \delta L h.$$
Of course, all linear response formulas must be equivalent since they are expressions for the same derivative. With our divergence expression of $\delta L$, we further see that the operator version and integrated-by-parts version are exactly the same formula.

4.2. Blended formula and fast linear response.

This subsection gives a new interpretation of some existing linear response algorithms as combinations of the ensemble formula and the operator formula. Roughly speaking, we decompose $\delta f$ into stable and unstable components, then we use the ensemble formula for the stable part, and the operator formula for the unstable part. This gives a blended formula which avoids large sup norm, thus improving efficiency for algorithms based on this formula.

To achieve this, first decompose $X$ into stable and unstable part, $X^s$ and $X^u$. We use the ensemble formula for the linear response caused by the perturbation $X^s$,

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

The summation converges because the pushforward of stable vectors decay exponentially.

For the unstable part, notice that the SRB measure is smooth on the unstable manifolds, so we can consider the dynamical system as time-inhomogeneous, hopping from one unstable manifold to another. In this model, for a fixed $f$, 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.

As a result, the operator version of linear response formula still applies. Also notice that the measure on unstable manifold is now the conditional SRB measure, $\sigma$. Hence,

$$\delta^u \left( \int \Phi h \right) = \sum_{m=0}^{\infty} \int \Phi \text{div}^u_{\sigma} X^u h,$$

where $\text{div}^u_{\sigma}$ is the divergence on the unstable manifold under $\sigma$. The unstable divergence is a Holder continuous function on the entire attractor, in particular, it has a bounded sup norm. The above expression converges, because of the regularizing effect of transfer operators on expanding maps. We can now sum the two parts of the linear response,

$$\delta \left( \int \Phi h \right) = \sum_{m=0}^{\infty} \int (f^m_s X^s(\Phi) + \Phi \text{div}^u_{\sigma} X^u) h.$$

This blended formula is equivalent to performing integration-by-parts on the unstable manifolds for the ensemble formula [28, 33].

The next difficulty is to compute the unstable divergence. The caveat is that we should not compute by summing directional derivatives, which are infinite in sup norm. The blended response algorithm, by Abramov and Majda, first approximates the SRB measure by a Gaussian distribution, then computes the unstable divergence [1]. The S3 algorithm, by Q.Wang and Chandramoorthy, approximates the unstable divergence
by finite differences [8]. Because both try to compute the unstable divergence via summing directional derivatives, both suffer from high cost or large error.

The fast linear response algorithm resolves this regularity difficulty by computing an inductive relation on a sample orbit, which is the fast formula of the unstable divergence. Because the unstable divergence is a Holder function on the entire attractor, the sampling error for computing \( \int \Phi \text{div}^u X^u h \), the first term in the linear response, is only \( E \sim O(1/\sqrt{T}) \). Since the induction converges exponentially fast, the dominating error is the sampling error [28]. Fast linear response requires solving \( u \), the unstable dimension, many first and second-order tangent equations, hence the cost is

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

Fast linear response is not cursed by dimensionality; it is faster than current operator algorithms at least for cases where the attractor dimension \( a \geq 4 \). It is also faster than the hypothetical operator algorithm. Roughly speaking, this is because the fast formula completely gets rid of large sup norms.

Acknowledgements

The author is very grateful to Stefano Galatolo, Wael Bahsoun, Gary Froyland, and Caroline Wormell for very helpful discussions.

References

[1] R. V. Abramov and A. J. Majda. Blended response algorithms for linear fluctuation-dissipation for complex nonlinear dynamical systems. *Nonlinearity*, 20(12):2793–2821, 2007.
[2] F. Antown, G. Froyland, and S. Galatolo. Optimal linear response for Markov Hilbert-Schmidt integral operators and stochastic dynamical systems. *arXiv:2101.09411*, 2021.
[3] W. Bahsoun, S. Galatolo, I. Nisoli, and X. Niu. A rigorous computational approach to linear response. *Nonlinearity*, 31(3):1073–1109, 2018.
[4] V. Baladi. Linear response, or else. *ICM Seoul 2014 Proceedings*, 3:525–545, 2014.
[5] P. J. Blonigan. Adjoint sensitivity analysis of chaotic dynamical systems with non-intrusive least squares shadowing. *Journal of Computational Physics*, 348:803–826, 2017.
[6] P. J. Blonigan and Q. Wang. Multiple shooting shadowing for sensitivity analysis of chaotic dynamical systems. *Journal of Computational Physics*, 354:447–475, 2018.
[7] N. Chandramoorthy, P. Fernandez, C. Talnikar, and Q. Wang. An Analysis of the Ensemble Adjoint Approach to Sensitivity Analysis in Chaotic Systems. In *23rd AIAA Computational Fluid Dynamics Conference, AIAA AVIATION Forum (AIAA 2017-3799)*, AIAA AVIATION Forum, pages 1–11. American Institute of Aeronautics and Astronautics, 2017.
[8] N. Chandramoorthy and Q. Wang. A computable realization of Ruelle’s formula for linear response of statistics in chaotic systems. *arXiv:2002.04117*, 2020.
[9] H. Crimmins and G. Froyland. Fourier approximation of the statistical properties of Anosov maps on tori. *Nonlinearity*, 33(11):6244–6296, 2020.
[10] J. Ding, Q. Du, and T. Y. Li. High order approximation of the Frobenius-Perron operator. *Applied Mathematics and Computation*, 53(2-3):151–171, 1993.
[11] J. Ding and A. Zhou. The projection method for computing multidimensional absolutely continuous invariant measures. *Journal of Statistical Physics*, 77(3-4):899–908, 1994.
[12] D. Dolgopyat. On differentiability of SRB states for partially hyperbolic systems. *Inventiones Mathematicae*, 155(2):389–449, 2004.
[13] G. L. Eyink, T. W. N. Haine, and D. J. Lea. Ruelle’s linear response formula, ensemble adjoint schemes and Lévy flights. *Nonlinearity*, 17(5):1867–1889, 2004.
[14] G. Froyland. On ulam approximation of the isolated spectrum and eigenfunctions of hyperbolic maps. *Discrete and Continuous Dynamical Systems*, 17(3):671–689, 2007.

[15] G. Froyland, O. Junge, and P. Koltai. Estimating long-term behavior of flows without trajectory integration: The infinitesimal generator approach. *SIAM Journal on Numerical Analysis*, 51(1):223–247, 2013.

[16] S. Galatolo and I. Nisoli. An elementary approach to rigorous approximation of invariant measures. *SIAM Journal on Applied Dynamical Systems*, 13(2):958–985, 2014.

[17] S. Galatolo and I. Nisoli. Rigorous computation of invariant measures and fractal dimension for maps with contracting fibers: 2D Lorenz-like maps. *Ergodic Theory and Dynamical Systems*, 36(6):1865–1891, 2016.

[18] S. Gouëzel and C. Liverani. Banach spaces adapted to Anosov systems. *Ergodic Theory and Dynamical Systems*, 26(1):189–217, 2006.

[19] A. Gritsun and V. Lucarini. Fluctuations, response, and resonances in a simple atmospheric model. *Physica D: Nonlinear Phenomena*, 349:62–76, 2017.

[20] S. Günther, N. R. Gauger, and Q. Wang. A framework for simultaneous aerodynamic design optimization in the presence of chaos. *Journal of Computational Physics*, 328:387–398, 2017.

[21] M. Keane, R. Murray, and L. S. Young. Computing invariant measures for expanding circle maps. *Nonlinearity*, 11(1):27–46, 1998.

[22] D. Lasagna, A. Sharma, and J. Meyers. Periodic shadowing sensitivity analysis of chaotic systems. *Journal of Computational Physics*, 391:119–141, 2019.

[23] D. J. Lea, M. R. Allen, and T. W. N. Haine. Sensitivity analysis of the climate of a chaotic system. *Tellus Series a-Dynamic Meteorology and Oceanography*, 52(5):523–532, 2000.

[24] C. Liverani. Rigorous numerical investigation of the statistical properties of piecewise expanding maps. A feasibility study. *Nonlinearity*, 14(3):463–490, 2001.

[25] V. Lucarini, F. Ragone, and F. Lunkeit. Predicting Climate Change Using Response Theory: Global Averages and Spatial Patterns. *Journal of Statistical Physics*, 166(3-4):1036–1064, 2017.

[26] A. Ni. Hyperbolicity, shadowing directions and sensitivity analysis of a turbulent three-dimensional flow. *Journal of Fluid Mechanics*, 863:644–669, 2019.

[27] A. Ni. Approximating linear response by non-intrusive shadowing algorithms. https://arxiv.org/abs/2003.09801, to appear in *SIAM Journal on Numerical Analysis*, pages 1–12, 2020.

[28] A. Ni. Fast linear response algorithm for differentiating chaos. *arXiv:2009.00595*, pages 1–28, 2020.

[29] A. Ni and C. Talnikar. Adjoint sensitivity analysis on chaotic dynamical systems by Non-Intrusive Least Squares Adjoint Shadowing (NILSAS). *Journal of Computational Physics*, 395:690–709, 2019.

[30] A. Ni and Q. Wang. Sensitivity analysis on chaotic dynamical systems by Non-Intrusive Least Squares Shadowing (NILSS). *Journal of Computational Physics*, 347:56–77, 2017.

[31] M. Pollicott and O. Jenkinson. Computing invariant densities and metric entropy. *Communications in Mathematical Physics*, 211(3):687–703, 2000.

[32] D. Ruelle. Differentiation of SRB States. *Commun. Math. Phys.*, 187:227–241, 1997.

[33] D. Ruelle. Differentiation of SRB States: Correction and Complements. *Communications in Mathematical Physics*, pages 185–190, 2003.

[34] M. Santos Gutiérrez and V. Lucarini. Response and Sensitivity Using Markov Chains. *Journal of Statistical Physics*, 179(5-6):1572–1593, 2020.

[35] K. Shawki and G. Papadakis. A preconditioned multiple shooting shadowing algorithm for the sensitivity analysis of chaotic systems. *Journal of Computational Physics*, 398:108861, 2019.

[36] Y. S. Shimizu and K. J. Fidkowski. Output-based error estimation for chaotic flows using reduced-order modeling. *AIAA Aerospace Sciences Meeting*, 2018, (210059), 2018.

[37] Q. Wang. Convergence of the Least Squares Shadowing Method for Computing Derivative of Ergodic Averages. *SIAM Journal on Numerical Analysis*, 52(1):156–170, 2014.
[38] C. Wormell. Spectral Galerkin methods for transfer operators in uniformly expanding dynamics. Numerische Mathematik, 142(2):421–463, 2019.

[39] C. L. Wormell and G. A. Gottwald. Linear response for macroscopic observables in high-dimensional systems. Chaos, 29(11), 2019.

URL: https://math.berkeley.edu/~niangxiu/