FAST ADJOINT DIFFERENTIATION OF CHAOS

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ABSTRACT. We devise a fast algorithm for the gradient of the long-time-average statistics of chaotic systems, with cost almost independent of the number of parameters. It runs on one sample orbit; its cost is linear to the unstable dimension. The algorithm is based on two theoretical results in this paper: the adjoint shadowing lemma for the shadowing contribution and the fast adjoint formula for the unstable divergence in the linear response.

Keywords. Adjoint method, backpropagation, chaos, gradient explosion, nonintrusive shadowing, fast linear response.

1. Introduction

1.1. Literature review.

The long-time-average behavior of chaotic systems is typically deterministic, and can be predicted using parameters of the system. We are interested in the derivative of the long-time-average of an objective function with respect to the parameters of the system. This derivative is also called the linear response or sensitivity, and it is one of the most basic numerical tools for many purposes. The long-time-average statistic of a chaotic system is given by the physical measure, or the SRB measure, which is a model for fractal limiting invariant measures of chaos [40, 33, 10].

There are several different formulas for the linear response; the most well-known are the ensemble formula and the operator formula, and they are formally equivalent under integration-by-parts [16, 34, 35, 36, 13, 17, 5]. Direct implementation of the ensemble formula is also known as stochastic methods, where the perturbations of individual orbits are averaged over SRB measures. However, it is very expensive to average out the orbit-wise perturbation, which grows exponentially fast [19, 14, 20, 11]. The current operator methods typically requires approximating singular SRB measures by isotropic finite-elements, which is inefficient in higher dimensions [4, 15, 3, 38, 25].

A promising direction is to ‘blend’ two different formulas, one for the stable/shadowing contribution, the other for the unstable contribution of the linear response. This was first attempted in computation by the blended response algorithm, which used the ensemble formula and the operator formula for the two
parts [1, 2]. In this paper, we decompose into the shadowing contribution and the unstable contribution: the formulas we use are explained below.

The shadowing contribution is given by the shadowing direction, which is the difference between two orbits close to each other but with perturbed parameters [9, 31]. When the ratio of unstable direction is low, with some additional statistical assumptions, shadowing can be good approximations of the entire linear response [24]. The shadowing direction is efficiently computed by the nonintrusive shadowing algorithm [26, 28, 29, 22].

For the unstable contribution, we start from the operator formula, which is in the form of an unstable divergence [25]. Previous algorithms could not compute the unstable divergence accurately due to lack of regularities. Recently, following the theoretical works on the linear response, we derived the computable expansion formula for the unstable divergence. Moreover, we find a fast formula for the expansion in the form of renormalized second-order tangent equations, whose second derivative is taken in a modified shadowing direction. This leads to the fast linear response algorithm, which is precise and highly efficient [23].

Many real-life applications desire an adjoint algorithm for sensitivity, whose cost is almost independent of the number of parameters. Such adjoint algorithms are also called backpropagation algorithms, because major terms are typically solved backwards in time. Currently, only the ensemble and operator algorithms have adjoint versions, but both are expensive for typical real-life chaotic systems. Pioneering attempts, such as the gradient clipping method, lack theoretical support [30]. An efficient and precise adjoint algorithm for chaos is an important open problem, and this paper gives an answer for an important basic scenario, the discrete-time autonomous systems with some hyperbolicity.

Readers may also find a previous preprint for the adjoint shadowing theory useful, which works only in Euclidean spaces [21]. Our overall logic here for the adjoint shadowing theory is better than the preprint, which now looks more like a reverse of the (tangent) shadowing theory. The nonintrusive adjoint shadowing algorithm has already been developed; it uses only the backward-running adjoint solutions, and has been applied to computational fluid problems with over $3 \times 10^6$ dimensions [27]. There are several other adjoint shadowing algorithms [7, 26]; in this paper, we mostly refer to the nonintrusive adjoint shadowing algorithm.

1.2. Main results.

For discrete-time chaotic systems, we devise adjoint theories and algorithms for the two parts of the linear response, the shadowing and the unstable contribution. This subsection summarizes our main results. Note that we will mostly use $m, n, k$ to label steps, and $i, j, l$ to label directions.

For most orbits on the attractor, \( \{ x_n = f(x_{n-1}) \}_{n \in \mathbb{Z}} \), the long-time-average statistic coincides with the SRB measure \( \rho \) on the phase space. The linear response is the linear relation between \( \delta \rho \) and \( \delta f \); it can be decomposed into

\[
\delta \rho(\Phi) = S.C. - U.C.
\]

Here \( \Phi \) is a fixed function representing the instantaneous objective; \( \delta(\cdot) := \partial(\cdot)/\partial \gamma \), where \( \gamma \) is some parameter of the system; \( S.C. \) and \( U.C. \) are the shadowing contribution and the unstable contribution of the linear response.
We first devise the adjoint shadowing theory. Denote the space of covectors, or forms, or linear functions on vectors at \( x \), by \( T^*_x \). We define the adjoint shadowing form, \( \{ \nu_n \in T^*_x \}_{n \in \mathbb{Z}} \), as such that

\[
S.C. = \rho(\nu X) = \lim_{N \to \infty} \frac{1}{N} \sum_{n=1}^{N} \nu_n X_n ,
\]

where \( X := \delta f \circ f^{-1} \). We show that \( \nu \) is the unique bounded solution of the inhomogeneous adjoint equation,

\[
\nu_{n-1} = f^* \nu_n + d\Phi_{n-1} ,
\]

where the differential of \( \Phi \), \( d\Phi_k := d\Phi(x_k) \); \( f^* \) is the pullback of covectors. We say that \( \nu = L(\rho) \) is the adjoint shadowing form corresponding to the 1-form \( d\Phi \). This characterization can be efficiently computed by the nonintrusive adjoint shadowing algorithm.

Then we give the fast adjoint formula of the unstable contribution,

\[
U.C. := \lim_{W \to \infty} \rho(\psi \, \text{div}^u \, X^u) , \quad \text{where} \quad \psi := \sum_{m=-W}^{W} (\Phi \circ f^m - \rho(\Phi)) ,
\]

via the fast adjoint formula of the unstable divergence:

\[
\text{div}^u \, X^u = L(\omega) X + \tilde{\varepsilon} \nabla_{\tilde{e}} X .
\]

Here \( \tilde{e} = e_1 \wedge \cdots \wedge e_u \in \land^u T^* \mathcal{M} \) is the unit hypercube in the \( u \)-dimensional unstable subspace, \( \tilde{\varepsilon} \in \land^u T^* \mathcal{M} \) is its co-hypercube with \( \tilde{\varepsilon}(\tilde{e}) = 1 \); \( \nabla_{\tilde{e}} X \in \land^u T^* \) is the Riemannian derivative of \( X \) in the direction of \( \tilde{e} \),

\[
\nabla_{\tilde{e}} X := \sum_{i=1}^{u} e_1 \wedge \cdots \wedge \nabla_{e_i} X \wedge \cdots \wedge e_u .
\]

Moreover, \( L \) is the adjoint shadowing operator, and \( \omega \) is the covector

\[
\omega := \frac{1}{J} \tilde{\varepsilon}_1 \nabla_{\tilde{e}} f^* , \quad \text{where} \quad \tilde{\varepsilon}_1 := \tilde{\varepsilon} \circ f .
\]

Here \( J \) is the growth rate of the unstable hypercube, and the 3-tensor \( \nabla_{\tilde{e}} f^* \) is the derivative of the Jacobian matrix in the direction of \( \tilde{e} \).

Our adjoint formulas separate major computations away from \( X \): this makes the cost of a new \( X \) negligible. Hence, our third result is the fast adjoint response algorithm for chaotic systems, which is highly efficient and its cost is almost independent of the number of parameters; in fact, the cost for the unstable contribution is further independent of the number of objectives. Our algorithm only needs to perform computations on one sample orbit; since all terms in our expressions are continuous functions on the attractor, the main error is the sampling error of the orbit. The computational cost is mainly in computing \( u \)-many tangent and adjoint solutions and contracting them with \( \nabla_{\tilde{e}} f^* \). On our numerical example, the cost of fast adjoint response is similar to finite-differences, but is almost unaffected by the number of parameters: this is orders of magnitude more efficient than previous precise adjoint algorithms.

This paper is organized as follows. First, we review the linear response theory, the nonintrusive shadowing algorithm for computing the shadowing contribution,
and the fast linear response algorithm for the unstable contribution. Section 3 develops the adjoint shadowing lemma. Section 4 gives the fast adjoint formula for the unstable divergence. Section 5 addresses some practical issues in implementing the algorithms. Finally, we illustrate the fast adjoint response algorithm on a numerical example.

2. Preliminaries

2.1. Hyperbolicity and linear response.

The main difficulty in this paper is finding a nice formula for the linear response; once the formula is found, its equivalence to other formulas can be proved more easily than the existence of the linear response, which requires more technical assumptions. For simplicity of discussions, we assume uniform hyperbolicity; the more detailed statements can be found in [34, 23].

Let $f$ be a smooth diffeomorphism on a smooth Riemannian manifold $M$, whose dimension is $M$. Assume that $K$ is a hyperbolic compact invariant set, that is, $T_K M$ (the tangent bundle restricted to $K$) has a continuous $f_*$-invariant splitting into stable and unstable subspaces, $T_K M = V^s \oplus V^u$, such that there are constants $C > 0$, $0 < \lambda < 1$, and

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

Here $f_*$ is the pushforward operator on vectors, when $M = \mathbb{R}^M$, $f_*$ is represented by multiplying with matrix $\partial f/\partial x$ on the left. Define the oblique projection operators $P^u$ and $P^s$, such that

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

We further assume that $K$ is an attractor, that is, there is an open neighborhood $U$, called the basin of the attractor, such that $\bigcap_{n \geq 0} f^n U = K$.

With some more assumptions, the attractor admits SRB measures, denoted by $\rho$. In this paper, we define SRB measures as physical measures, that is,

$$\rho := \lim_{n \to \infty} f_*^n \rho',$$

where $\rho'$ is absolutely continuous to Lebesgue; $f_*$ is the pushforward of measures, in $\mathbb{R}^M$, it is represented by multiplying the density function with $\det(\partial f/\partial x)^{-1}$.

Here the limit is in the weak sense, that is, for every continuous observable $\Phi : M \to \mathbb{R}$ and almost all $x \in U$

$$\lim_{N \to \infty} \frac{1}{N} \sum_{k=0}^{N-1} \Phi(f^k x) = \rho(\Phi).$$

In other words, SRB measures give the long-time-average statistic of the chaotic system. The SRB measure has several other characterizations [40], which were very important for the linear response theory and the fast linear response algorithm [34, 23], but our paper does not directly use those characterizations.

Assume that the system is parameterized by some parameter, $\gamma$; the linear response formula is an expression of $\delta\rho$ by $\delta f$, where

$$\delta(\cdot) := \partial(\cdot)/\partial \gamma.$$
may as well be regarded as small perturbations. Linear response formulas are proved to give the correct derivative for various hyperbolic systems [34, 13], yet it fails for some cases [5, 39]. The earliest proof is:

**Theorem 1** (Ruelle [34]). Assume that $f$ is parameterized by some scalar $\gamma$, and define $\delta(\cdot) := \frac{\partial (\cdot)}{\partial \gamma}$. Then, the derivative of the SRB measure is given by:

$$\delta \rho(\Phi) = \lim_{W \to \infty} \rho \left( \sum_{n=0}^{W} X(\Phi_n) \right),$$

where $X := \delta f \circ f^{-1}$, $X(\cdot)$ is to differentiate in the direction of $X$, and $\Phi \in C^2$ is a fixed observable function. Here $\Phi_n = \Phi \circ f^n$.

There are several different linear response formulas expressing the same derivative in different ways: they are good for different purposes. We shall refer to theorem 1 as the ensemble formula. Note that the integrand in this formula grows exponentially fast to $W$, and directly evaluating this integrand via ensemble or stochastic approaches is extremely expensive. For faster computation, we decompose the linear response formula into two parts,

$$\delta \rho(\Phi) = S.C. - U.C.,$$

which we call the shadowing and the unstable contribution. Like a Leibniz rule, the shadowing contribution accounts for the change of the location of the attractor, while the unstable contribution accounts for the change of the measure if the attractor is fixed.

### 2.2. Shadowing contribution.

We review tangent theories and nonintrusive shadowing algorithms for the shadowing contribution. In this paper, ‘tangent’ means that the main solver in the algorithm is running forward in time, whereas ‘adjoint’ means computing the gradient of one objective with respect to many parameters at once. Conventionally, the definitions are symmetric, since the cost of tangent solvers is typically independent of the number of objective functions, and the adjoint solvers runs backward. However, such convention is true only for shadowing methods, but not for the unstable contribution. Hence, our definitions for tangent and adjoint are not symmetric in this paper.

We first review the tangent shadowing theory. We define the shadowing direction by its characterizing properties. That is, on an orbit $\{x_n = f(x_{n-1})\}_{n \in \mathbb{Z}}$ on the attractor, the shadowing direction $\{v_n \in T_{x_n}M\}_{n \in \mathbb{Z}}$ is the only bounded solution of the inhomogeneous tangent equation,

$$v_{n+1} = f_* v_n + X_{n+1}, \quad \text{where} \quad X := \delta f \circ f^{-1}.$$
initial condition, \( v' \). The Duhamel’s principle says that it can be done by first propagate previous perturbations to step \( k \), then sum up. This procedure is shown in figure 1, and the formula for \( v' \) is

\[
v'_k = \sum_{n=1}^{k} D_n^k X_n, \quad v'_0 = 0.
\]

The expression of the tangent shadowing direction can be obtained similarly, but we need to first decompose \( X \), then propagate stable components to the future, unstable components to the past. This procedure is also in figure 1, and the expansion formula for \( v \) is

\[
v = \sum_{n \geq 0} f^n_s P_s X_{-n} - \sum_{n \leq -1} f^n_u P_u X_{-n} =: L(X),
\]

where the linear operator \( L : L^2(\rho) \rightarrow L^2(\rho) \) is the shadowing operator. By the exponential decay of stable and unstable vectors, we can see that \( v \) is bounded for all \( k \). The variant Duhamel’s principle guarantees that \( v \) is still an inhomogeneous tangent solution: the proof is similar to that of theorem 3.

\[\text{Figure 1. Inhomogeneous tangent solution with zero initial condition (left), and the tangent shadowing direction (right).}\]

For us, the utility of conventional tangent solutions is to compute the sensitivity of stable dynamical systems. Similarly, the shadowing direction can be used to compute the shadowing contribution of the linear response for chaotic systems. Comparing the expression of \( v \) with the expression of the shadowing contribution, we can find that [24]

\[ S.C. = \rho(d\Phi v). \]

The best way to compute the shadowing direction is to recover its characterizing properties. Currently, the most efficient algorithm is the nonintrusive shadowing algorithm [28, 29], which has been applied to a \( 4 \times 10^6 \) dimensional system in computational fluids. Nonintrusive means to solve only \( O(u) \) many solutions of the most basic inductive relations. In the case of the tangent shadowing algorithm, nonintrusive means to use only \( u \) many tangent solutions. The nonintrusive shadowing algorithm solves the constrained minimization,

\[
\min_{a \in \mathbb{R}^u} \frac{1}{2N} \sum_{n=0}^{N-1} |v_n|^2, \quad \text{s.t.} \quad v_n = v'_n + \xi_n a,
\]

where \( v' \) is the conventional inhomogeneous tangent solution, \( \xi \) is a matrix with \( u \) columns of homogeneous tangent solutions. Intuitively, the boundedness property is approximated by a minimization, while the \( M \)-dimensional feasible space of all inhomogeneous tangent solutions is reduced to an affine subspace of only \( u \) dimensions.
2.3. **Unstable contribution.**

We review the tangent theory and the fast linear response algorithm for the unstable contribution, defined as

\[
U.C. := \lim_{W \to \infty} U.C. W, \quad U.C. W := -\rho \left( \sum_{n=-W}^{W} X^u(\Phi_n) \right). 
\]

The integrand in the unstable contribution grows exponentially fast. To treat this, integrate-by-parts on the unstable manifold, we get

\[
U.C. W = \rho (\psi \text{div}^u X^u), \quad \text{where} \quad \psi := \sum_{m=-W}^{W} (\Phi \circ f^m - \rho(\Phi)).
\]

Here \( \text{div}^u \) is the divergence on the unstable manifold under the conditional SRB measure. The unstable divergence turns out to be the derivative of the transfer operator on unstable manifolds [25]; its norm is \( O(\sqrt{W}) \), much smaller than the ensemble formula. However, the directional derivatives are distributions, so using directional derivatives as an intermediate quantities incur high cost or large error.

A precise and computable formula for the unstable divergence was given in [23]. It is obtained by expanding the unstable divergence into a series of functions whose sup norm decay exponentially: this idea was previously used in proving the regularity of the unstable divergence [34]. Directly computing the expansion formula already gives a precise algorithm, which is typically much faster than ensemble or operator methods.

We further derived the fast formula of the unstable divergence, which allows the unstable contribution be computed even more efficiently and robustly than directly using the expansion formula. Using the idea for fast algorithms, we combine many small terms into a big term, then apply a uniform rule of propagation only once on the big term. Here the propagation rule is given by second-order tangent equations, whose second derivative is taken in a modified shadowing direction. Computing the fast formula requires solving only \( u \) many second-order tangent equations on one sample orbit, and the main error is the sampling error of the orbit.

**Theorem 2** (fast formula for unstable divergence). For any \( r_0 \in D^u \),

\[
U.C. W = \lim_{N \to \infty} \frac{1}{N} \sum_{n=0}^{N-1} \left\langle \bar{\beta}_r n, \bar{\epsilon}_{n+1} \right\rangle, \quad \text{where} \quad r_{n+1} = P^\perp \bar{\beta}_r n.
\]

Here \( \bar{\epsilon} = e_1 \wedge \cdots \wedge e_u \) is the unit \( u \)-dimensional cube spanned by unstable vectors, \( \left\langle \cdot, \cdot \right\rangle \) 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 \( V^u \). Roughly speaking, \( \bar{\beta} \) is the renormalized second-order tangent equation governing the propagation of derivatives of cubes (see section 4.1).
The fast formula leads to a precise, efficient, robust, and easy-to-implement algorithm for the linear response of SRB measures, the fast linear response algorithm. The algorithm was demonstrated on a 21-dimensional system with a 20-dimensional unstable subspace. For the same accuracy, fast linear response is orders of magnitude faster than ensemble and operator algorithms; it is even slightly faster than finite difference [23]. After the fast linear response, some other algorithms also start to use orthogonally projected second order tangent equations to compute some other divergences, such as the second S3 algorithm, whose complexity is about $O(u)$ times higher than the fast linear response [12, 37].

3. ADJOINT SHADOWING CONTRIBUTION

This section finds a characterization of the adjoint shadowing operator convenient for numerical computations. As a preparation, we first show that the pullback of covectors is also hyperbolic. Then we develop the adjoint shadowing theory in the reversed order of its tangent counterpart. First, we shall define the adjoint shadowing form by its utility of adjointly computing the shadowing contribution; then we find its expansion formula; finally, we characterize it as the bounded inhomogeneous adjoint solution.

3.1. Adjoint hyperbolicity.

The pullback operator $f^*$ is the adjoint of $f_*$, that is, for any $x \in \mathcal{M}$, $w \in T_x \mathcal{M}$, and $\eta \in T_{f_x} \mathcal{M}$, $f^*$ is the operator such that

$$\eta(f_*w) = f^* \eta(w).$$

When $\mathcal{M} = \mathbb{R}^M$, $\eta$ is represented by multiplying with a column vector and $f^*$ is represented by multiplying with the transposed Jacobian matrix on the left. Moreover, define the norm on covectors

$$|\eta| = \sup_w \eta(w)/|w|.$$

Define the adjoint projection operator, $\mathcal{P}^u$ and $\mathcal{P}^s$, such that for any $w \in T_x \mathcal{M}$, $\eta \in T_{f_*} \mathcal{M}$,

$$\eta(P^u w) = P^u \eta(w), \quad \eta(P^s w) = P^s \eta(w).$$

Define the image space of $\mathcal{P}^u$ and $\mathcal{P}^s$ as $V^{u*}$ and $V^{s*}$. For any $v^u \in V^u$, $v^s \in V^s$, $\nu^u \in V^{u*}$, and $\nu^s \in V^{s*}$,

$$\nu^u v^s = \nu^s v^u = 0.$$

The next lemma shows that $V^{u*}$ and $V^{s*}$ are in fact unstable and stable subspaces for the adjoint system. Hence, the adjoint system is dual to the tangent system and is also hyperbolic.

**Lemma 1** (adjoint hyperbolicity). There are $C > 0$, $0 < \lambda < 1$, such that for any $x \in K$, $\eta \in T_{f_*} \mathcal{M}$, $n \geq 0$, we have

$$|f^{*n} P^u \eta| \leq C \lambda^n |P^u \eta|, \quad |f^{*n} P^s \eta| \leq C \lambda^n |P^s \eta|.$$
Remark. (1) Notice that $f^\ast$ moves covectors backwards in time. (2) By this lemma, if we pullback $u$-many covectors for many steps, they automatically occupy the unstable subspace, since their unstable parts grow while stable parts decay.

Proof. Since $K$ is compact, there is constant $C > 0$, such that for any $w \in T_xM$, $|P^s w| \leq C |w|$. Hence

$$|f^n P^s \eta| = \sup_w \frac{f^n P^s \eta(w)}{|w|} = \sup_w \frac{P^s \eta(f^n P^s w)}{|w|} \leq C\lambda^n |P^s \eta| \sup_w \frac{|P^s w|}{|w|} \leq C\lambda^n |P^s \eta|.$$  

Here $C$ does not depend on the quantities appearing on both side of the inequality, but its exact value may change from line to line. The statement on $P^u$ can be proved similarly. \hfill \Box

3.2. Definition and expansion of the adjoint shadowing form.

First, we define the adjoint shadowing form by its utility in adjointly computing the shadowing contribution.

Definition (adjoint shadowing form). The adjoint shadowing form $\nu$ of $d\Phi$ is the unique $\nu$ such that the following formula holds for all $X \in L^2(\rho)$:

$$S.C. = \rho(d\Phi v) = \rho(\nu X),$$

where $v$ is the shadowing direction corresponding to $X$. In other words,

$$\nu := L(d\Phi).$$

where $L$ is the adjoint of the shadowing operator $L$.

Lemma 2 (expansion of the adjoint shadowing form).

$$\nu = \sum_{n \geq 0} f^n \Phi P^s d\Phi_n - \sum_{n \leq -1} f^n \Phi P^u d\Phi_n.$$

Proof. Substitute the expansion formula of $v$ in equation (1) into the shadowing contribution in equation (2), then move all operations to $d\Phi$, and apply the invariance of SRB measures, we get

$$\rho(d\Phi v) = \rho \left( \sum_{n \geq 0} f^n \Phi P^s X_{-n} - \sum_{n \leq -1} f^n \Phi P^u X_{-n} \right)$$

$$= \rho \left( \sum_{n \geq 0} (f^n \Phi P^s d\Phi_n)X_{-n} - \sum_{n \leq -1} (f^n \Phi P^u d\Phi_n)X_{-n} \right)$$

$$= \rho \left( \sum_{n \geq 0} (f^n \Phi P^s d\Phi_n)X - \sum_{n \leq -1} (f^n \Phi P^u d\Phi_n)X \right)$$

$$= \rho \left( \sum_{n \geq 0} f^n \Phi P^s d\Phi_n - \sum_{n \leq -1} f^n \Phi P^u d\Phi_n \right).$$

\hfill \Box
The expression of the adjoint shadowing direction is similar to the tangent one. That is, first decompose $d\Phi$ according to the adjoint hyperbolicity, propagate stable components to the past, unstable components to the future; then $\nu$ is the summation of the 1-forms propagated to the step of interest. This procedure, illustrated in figure 2, is a variant of the Duhamel’s principle for writing out conventional adjoint solutions. The conventional adjoint solution, $\nu'$, is just the sum of $d\Phi$’s from the future, and its inner-product with $X$ gives sensitivity for stable dynamical systems. Similarly, the inner-product of $\nu$ with $X$ gives the shadowing contribution.

![Figure 2. Illustrations for inhomogeneous adjoint solution with zero initial condition (left), and the adjoint shadowing form (right).](image)

3.3. Adjoint shadowing lemma and the nonintrusive algorithm.

An idea frequently used in nonintrusive shadowing and fast linear response algorithms is to avoid directly computing expansion formulas. Rather, we seek neat characterizations of these formulas, and recovering these characterizing properties can be numerically much more efficient. For the adjoint shadowing form, it can be characterized similarly to its tangent counterpart.

In view of figure 2, by the exponential decay of stable and unstable covectors, $\nu$ is bounded; the variant Duhamel’s principle makes $\nu$ an inhomogeneous adjoint solution. It turns out these two properties uniquely characterizes the adjoint shadowing form.

**Theorem 3** (adjoint shadowing lemma). The adjoint shadowing form of $d\Phi$ is the unique bounded solution of the inhomogeneous adjoint equation,

$$\nu = f^*\nu_1 + d\Phi,$$

where $\nu_1 := \nu \circ f$.

**Proof.** $\nu$ is bounded on the entire attractor $K$ and on every orbit, due to the exponential decay of adjoint hyperbolicity. For the governing equation,

$$\nu - f^*\nu_1 = \sum_{n \geq 0} f^{sn}P^s d\Phi_n - \sum_{n \leq -1} f^{sn}P^u d\Phi_n - \sum_{n \geq 0} f^{sn+1}P^s d\Phi_{n+1} + \sum_{n \leq -1} f^{sn+1}P^u d\Phi_{n+1}$$

$$= \sum_{n \geq 0} f^{sn}P^s d\Phi_n - \sum_{n \leq -1} f^{sn}P^u d\Phi_n - \sum_{k \geq 1} f^{sk}P^s d\Phi_k + \sum_{k \leq 0} f^{sk}P^u d\Phi_k$$

$$= P^s d\Phi + P^u d\Phi = d\Phi.$$

For uniqueness, pick any orbit and any other inhomogeneous adjoint solution, $\nu'$, then $\nu' - \nu$ is a homogeneous adjoint solution. If this difference is not zero, then it grows exponentially fast either in the positive or negative time direction; hence, $\nu'$ can not be bounded. $\square$
The characterizing properties of the adjoint shadowing form can be efficiently and conveniently recovered by nonintrusive shadowing algorithms. More specifically, we solve the nonintrusive adjoint shadowing problem,

$$\min_{a \in \mathbb{R}^u} \frac{1}{2N} \sum_{n=0}^{N-1} |\nu_n|^2, \quad \text{s.t.} \quad \nu_n = \nu'_n + \xi_n a,$$

where $\nu'$ is the inhomogeneous adjoint solution with $\nu'_{N-1} = 0$. $\xi$ is a matrix with $u$ columns of homogeneous adjoint solutions. Then the solution is a good approximation of the true adjoint shadowing form, since its characterizing properties are recovered [24].

When $u \ll M$, if the system has fast decay of correlation, and $X, d\Phi$ are not particularly aligned with unstable directions, the shadowing contribution can be a good approximation of the entire linear response [24]. The nonintrusive adjoint shadowing algorithm was used on fluid problems with $u = 8$, and $M \approx 3 \times 10^6$; the cost was on the same order of simulating the flow, and the approximate derivative was useful [27]. However, when the unstable contribution is large, or when better accuracy is desired, for example near design optimal, we need to further compute the unstable contribution [32, 18, 6]. Since adjoint shadowing is also an important part for the unstable contribution, no work will be wasted.

4. Adjoint unstable contribution

This section derives a fast adjoint formula for the unstable divergence. We shall expand the unstable divergence, move major computations away from $X$ and $\psi$, obtain an expansion formula for an adjoint operator. Then we seek a neat characterization of the expansion formula. Further using the adjoint shadowing lemma, we obtain the fast adjoint formula of the unstable divergence.

4.1. Expansion formulas.

The second-order tangent equation governing $r$ in theorem 2 is

$$r_{n+1} = P^\perp \tilde{r}_n = \frac{P^\perp f_s}{J} r_n + \frac{P^\perp (\nabla_{\tilde{v}} f_s)}{J} \tilde{e}_n + P^\perp (\psi \nabla_{\tilde{v}} X)_{n+1},$$

where $\tilde{v}$ is the shadowing direction of $\psi X$, $\psi$ defined in equation (3). The Jacobian determinant $J$ is regarded as an operator, when applied to quantities at $x_n$, $J := |f_s \tilde{e}_n|$. Here $\nabla f_s$ is the symmetric Hessian tensor, and

$$(\nabla_{\tilde{v}} f_s) \tilde{e} := \nabla_{\tilde{v}} f_s(f_s \tilde{e}) - f_s \nabla \tilde{v} \tilde{e} = \sum_{i=1}^u f_s e_1 \wedge \cdots \wedge (\nabla_{\tilde{v}} f_s) e_i \wedge \cdots \wedge f_s e_u$$

$$= \sum_{i=1}^u f_s e_1 \wedge \cdots \wedge (\nabla_{e_i} f_s) \tilde{v} \wedge \cdots \wedge f_s e_u =: (\nabla_{\tilde{v}} f_s) \tilde{v}.$$

Due to the stability of this induction, 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,

\[ p = \sum_{n \geq 0} \left( \frac{P^\perp f_s}{J} \right)^n \left( \frac{P^\perp(\partial_\varepsilon f_s)}{J} \tilde{v}_{n-1} + P^\perp(\psi \nabla_\varepsilon X)_{-n} \right) \]

\[ = \sum_{n \geq 0} P^\perp \left( \frac{f_s P^\perp}{J} \right)^n \left( \frac{\nabla_\varepsilon f_s}{J} \tilde{v}_{n-1} + (\psi \nabla_\varepsilon X)_{-n} \right). \]

Remark. This is not the full expansion of \( p \), since \( \tilde{v} \) can be further expanded using lemma 2. 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 \( \beta \) in [23] is also not the full expansion, and is different from our current one.

We further write down the expansion formula for \( \tilde{\beta}_{p-1} \):

\[ \tilde{\beta}_{p-1} = \frac{f_s}{J} \sum_{n \geq 0} P^\perp \left( \frac{f_s P^\perp}{J} \right)^n \left( \frac{\nabla_\varepsilon f_s}{J} \tilde{v}_{n-2} + (\psi \nabla_\varepsilon X)_{-n-1} \right) + \frac{\nabla_\varepsilon f_s}{J} \tilde{v}_{n-1} + \psi \nabla_\varepsilon X \]

\[ = \sum_{n \geq 1} \left( \frac{f_s P^\perp}{J} \right)^{n+1} \left( \frac{\nabla_\varepsilon f_s}{J} \tilde{v}_{n-2} + (\psi \nabla_\varepsilon X)_{-n-1} \right) \]

\[ = \sum_{k \geq 0} \left( \frac{f_s P^\perp}{J} \right)^k \left( \frac{\nabla_\varepsilon f_s}{J} \tilde{v}_{k-1} + (\psi \nabla_\varepsilon X)_{-k} \right). \]

Substituting this into the unstable contribution in theorem 2, we have

\[ U.C.W = \lim_{N \to \infty} \frac{1}{N} \sum_{n=0}^{N-1} \langle \tilde{\beta}_{p_n}, \tilde{e}_{n+1} \rangle = \rho \langle \tilde{\beta}_{p-1}, \tilde{e} \rangle = \rho \langle \tilde{e}^b \tilde{\beta}_{p-1} \rangle = \rho \left( \tilde{e}^b T q \right), \]

where \( \tilde{e}^b (\cdot) := \langle \tilde{e}, \cdot \rangle \) \( T (\cdot) := \sum_{k \geq 0} \left( \frac{f_s P^\perp}{J} \right)^k (\cdot)_{-k} \), \( q := \nabla_\varepsilon f_s \tilde{v}_{-1} + \psi \nabla_\varepsilon X \).

Here \( q \) is in the space of derivative-like \( u \)-vectors \( D^u, \tilde{e}^b \) is in the dual space \( D^{u^*} \), and \( T \) is a linear operator on \( L^2(\rho, D^{u^*}) \).

Denote the adjoint operator of \( T \) by \( T^* \), then \( T^* \) is operator on \( L^2(\rho, D^{u^*}) \), and

(4) \[ U.C.W = \rho \left( (T\tilde{e}^b)q \right). \]

By the invariance of SRB measures, we see that \( T \) has the expansion formula

\[ T\tilde{e}^b (\cdot) = \sum_{k \geq 0} \left( \frac{f_s P^\perp}{J} \right)^k (\cdot)_{-k}, \]

4.2. Characterizing \( T\tilde{e}^b \) by unstable co-cube.

Once again, we are going to find a simple characterization for \( T\tilde{e}^b \). Define the unit unstable \( u \)-covectors \( \varepsilon \), one such that \( \varepsilon(\varepsilon) = 1 \), by

\[ \varepsilon := \varepsilon^1 \land \cdots \land \varepsilon^u, \quad \varepsilon := \varepsilon/\varepsilon(\varepsilon), \quad \text{where} \quad \varepsilon^i \in V^{u^*}. \]

Lemma 3. \( T\tilde{e}^b (r) = \varepsilon(r), \forall r \in D^u. \)
Proof. Since \( P^\perp f_s P^\perp = P^\perp f_s \), \( P^\parallel \) projects to the span of \( \tilde{e} \), for any \( r \in D^n \),

\[
\begin{align*}
\langle \left( \frac{f_s P^\perp}{J} \right)^k r, \tilde{e}_k \rangle & = \langle f_s P^\perp f_s^{k-1} r, \tilde{e}_k \rangle = \langle \frac{f_s}{J} f_s^{k-1} r, \tilde{e}_k \rangle - \langle f_s P^\parallel f_s^{k-1} r, \tilde{e}_k \rangle \\
& = \langle \frac{f_s}{J} f_s^{k-1} r, \tilde{e}_k \rangle - \langle \frac{f_s}{J} f_s^{k-1} r, \tilde{e}_{k-1} \rangle = \langle \frac{f_s f_s^{k-1}}{J} r, \tilde{e}_k \rangle = \langle \frac{f_s f_s^{k-1}}{J} r, \tilde{e}_{k-1} \rangle.
\end{align*}
\]

The last equality is because \( \langle P^\parallel, e \rangle = \langle \cdot, e \rangle \). Hence,

\[
\mathcal{T}e^b(r) = \langle f_s, \tilde{e}_0 \rangle + \lim_{N \to \infty} \sum_{k \geq 1} \langle \frac{f_s}{J} f_s^k r, \tilde{e}_k \rangle - \langle \frac{f_s}{J} f_s^k r, \tilde{e}_{k-1} \rangle = \lim_{N \to \infty} \langle \frac{f_s^N}{J} r, \tilde{e}_N \rangle.
\]

We claim that

\[
\mathcal{T}e^b(r) = \begin{cases} 
1, & \text{if } r = \tilde{e}, \\
0, & \text{if } r = \sum_i e_1 \wedge \cdots \wedge r_i \wedge \cdots \wedge e_u, r_i \in V^s.
\end{cases}
\]

If the claim is true, \( \mathcal{T}e^b = \mathcal{T} \) for all basis of \( D^n \), hence, the equality also holds for all \( r \in D^n \), finishing the proof of the lemma. The first case is straightforward, and we only need to prove the second case.

Intuitively, the claim that \( \mathcal{T}e^b(r) = 0 \) 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 \( \{e_i\}_{i=1}^u \) is any orthogonal basis for \( V^u \) such that \( \tilde{e} = e_1 \wedge \cdots \wedge e_u \). In the rest of this proof, fix \( C \) as the constant used in the definition of hyperbolicity. We claim that

\[
(5) \quad C \lambda^n |f_s^u \tilde{e}| \geq |f_s^u (e_2 \wedge \cdots \wedge e_u)| |e_1|, \quad \forall n \geq 0.
\]

To prove this claim, assume that it is false, that is, for some \( n \),

\[
C \lambda^n |f_s^u \tilde{e}| < |f_s^u (e_2 \wedge \cdots \wedge e_u)| |e_1|.
\]

We can find \( e'_1 \in V^u \), such that \( f_s^u e'_1 \downarrow \) span\{\( f_s^u e_2, \dots, f_s^u e_u \)\}, and \( e'_1 \wedge e_2 \wedge \cdots \wedge e_u = \tilde{e} \). As a result, \(|e'_1| \geq |e_1|\). Hence, by our assumption,

\[
C \lambda^n |f_s^u (e_2 \wedge \cdots \wedge e_u)| |f_s^u e'_1| = C \lambda^n |f_s^u \tilde{e}| < |f_s^u (e_2 \wedge \cdots \wedge e_u)| |e_1| \Rightarrow C \lambda^n |f_s^u e'_1| < |e_1| \leq |e'_1|.
\]

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

We can rewrite \( r \) on the orthogonal basis \( \{e_i\}_{i=1}^u \), still as \( r = \sum_i e_1 \wedge \cdots \wedge r_i \wedge \cdots \wedge e_u \), with \( r_i \in V^s \) (see [23] for the detailed formula). With equation (5),

\[
\begin{align*}
\left| \frac{f_s^N (r_1 \wedge e_2 \wedge \cdots \wedge e_u)}{|e_1| |f_s^N \tilde{e}|} \right| & = \left| \frac{f_s^N (r_1 \wedge e_2 \wedge \cdots \wedge e_u)}{|e_1| |f_s^N \tilde{e}|} \right| \\
& \leq C \lambda^N |f_s^N r_1| |f_s^N (e_2 \wedge \cdots \wedge e_u)| |e_1| |f_s^N \tilde{e}| \\
& \leq C \lambda^N |f_s^N r_1| |e_1| \to 0,
\end{align*}
\]

as \( N \to \infty \). Similarly, we can prove this for any \( r_i \). Hence \( |f_s^N r/J^N| \to 0 \), and \( \mathcal{T}e^b(r) = 0 \). \( \square \)
4.3. Fast adjoint formula for the unstable divergence.

**Theorem 4** (fast adjoint formula). For any smooth $X$, almost $\rho$-surely

$$\text{div}^u_a X^u = \mathcal{L}(\omega)X + \tilde{\epsilon}\nabla\tilde{e}X,$$

where $\omega(\cdot) := \tilde{\epsilon}_1 \frac{\nabla \tilde{e}}{|\nabla \tilde{e}|} f_s(\cdot)$.

Here $\tilde{e}$ is the unit $u$-vector, $\tilde{\epsilon}$ is dual of $\tilde{e}$, $\omega$ is a 1-form, and $\mathcal{L}$ is the adjoint shadowing operator.

**Remark.** (1) This is not a local statement, since both $\mathcal{L}$ and the conditional SRB measure $\sigma$ encode information from the whole dynamical system. (2) This formula is also ‘adjoint’ in the utility sense, that is, to compute $\text{div}^u_a X^u$ for a new $X$, we only need to apply $\mathcal{L}\omega$ on $X$ and contract the 2-tensor $\nabla_X$, whose cost are negligible compared to computing quantities not affected by $X$, such as $\tilde{e}, \tilde{\epsilon}, \mathcal{L}\omega$.

**Proof.** Substituting lemma 3 into equation (4), we get

$$U.C. W = \rho \left( \tilde{\epsilon} \frac{\nabla \tilde{e} f_s}{|\nabla \tilde{e}|} \tilde{v}_1 + \tilde{\epsilon}_1 \psi \nabla \tilde{e}X \right) = \rho \left( \tilde{\epsilon}_1 \frac{\nabla \tilde{e}}{|\nabla \tilde{e}|} f_s \tilde{v} + \tilde{\epsilon}_1 \psi \nabla \tilde{e}X \right) = \rho \left( \omega \tilde{v} + \tilde{\epsilon}_1 \psi \nabla \tilde{e}X \right).$$

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

$$U.C. W = \rho \left( \mathcal{L}(\omega) \psi X + \tilde{\epsilon}_1 \psi \nabla \tilde{e}X \right).$$

Compare with the definition of the unstable contribution in equation (3), since the equality holds for any smooth $\psi$, we have proved the theorem.

**Lemma 4** (formulas using non-normalized $e$ and $\epsilon$). For any unstable $e$ and $\epsilon$,

$$\tilde{\epsilon} \nabla \tilde{e}X = \frac{1}{\epsilon e} \nabla eX; \quad \omega = \frac{1}{\epsilon_1 f_s e} \epsilon_1 \nabla \epsilon f_s.$$

**Proof.** Recall that $\tilde{\epsilon} = \epsilon / \epsilon(\tilde{e})$, $\tilde{e} = e / |e|$, so

$$\tilde{\epsilon} \nabla \tilde{e}X = \frac{\epsilon}{\epsilon \tilde{e}} \nabla |e| X = \frac{\epsilon}{\epsilon(|e|)} \nabla \epsilon X = \frac{1}{\epsilon e} \nabla eX.$$

$$\omega := \tilde{\epsilon}_1 \frac{\nabla \tilde{e} f_s}{J} = \frac{\epsilon_1}{\epsilon_1 \tilde{e}_1} \frac{\nabla e / |e| f_s}{J} = \frac{\epsilon_1}{\epsilon_1 \tilde{e}_1} \frac{|e| f_s}{J} = \frac{1}{\epsilon_1 f_s e} \epsilon_1 \nabla e f_s,$$

where we used that $|e| J = |f_s e|, |f_s e| \tilde{e}_1 = f_s e$.

5. Fast adjoint response algorithm

Now we switch to the numerical aspect of our work. In this section, we first show how to compute the adjoint response on a long orbit divided into small segments. This multi-segment treatment will help reduce numerical error and reduce the frequency of some expensive operations. Then we give a detailed procedure list of the algorithm. Finally, we give some potentially helpful remarks on the implementation of the algorithm.
5.1. Multi-segment treatment.

In the algorithm, we evolve tangent and adjoint solutions to approximate unstable subspaces. Due to the exponential growth, we should renormalize them to avoid overflow in float numbers. A good renormalization will also keep the duality between tangent and adjoint solutions: this will save the cost for computing contractions. However, also for cost reasons, we want to perform renormalizations only occasionally. The solution is to divide a long orbit into multiple segments and renormalize at interfaces.

Our convention for subscripts on multi-segments is shown in figure 3, which is the same as the nonintrusive shadowing and the fast linear response. We divide an orbit into small segments of \( N \) steps. The \( \alpha \)-th segment consists of step \( \alpha N \) to \( \alpha N + N \), where \( \alpha \) runs from \( 0 \) to \( A - 1 \); notice that the last step of segment \( \alpha \) is also the first step of segment \( \alpha + 1 \). We use double subscripts, such as \( x_{\alpha,n} \), to indicate the \( n \)-th step in the \( \alpha \)-th segment, which is the \( (\alpha N + n) \)-th step in total. Note that for some quantities defined on each step, for example, \( e_{\alpha,N} \neq e_{\alpha+1,0} \), since renormalization is performed at the interface across segments. Continuity across interfaces is true only for some quantities, such as adjoint shadowing forms \( \nu, \tilde{\nu} \), and unit unstable cubes \( \tilde{e}, \tilde{\epsilon} \). Later, we will define some quantities on the \( \alpha \)-th segment, such as \( C_{\alpha}, d_{\alpha} \): their subscripts are the same as the segment they are defined on. For quantities to be defined at interfaces, such as \( Q_\alpha, R_\alpha, b_\alpha \), their subscripts are the same as the total step number of the interface divided by \( N \).

![Figure 3. Subscript convention on multiple segments.](image)

We introduce some matrix notations. Let \( I \) be the \( u \times u \) identity matrix. Moreover, denote \( \xi := [e_1, \cdots, e_u], \xi := [\epsilon^1, \cdots, \epsilon^u], \)

\[
\xi^T \xi := [\epsilon^i e_j]_{ij}, \quad \text{so} \quad \epsilon e = \det(\xi^T \xi).
\]

Here \( [\cdot]_{ij} \) is the matrix with \( (i, j) \)-th entry given inside the bracket. Similarly,

\[
\xi^T \xi := \langle \xi^i, \xi^j \rangle_{ij}, \quad \xi^T \xi := \langle e_i, e_j \rangle_{ij}.
\]

Here \( \langle \cdot, \cdot \rangle \) is the inner product. For any vector \( w \),

\[
\epsilon_1(\nabla e f_s)w = \sum_{i=1}^u \det \begin{bmatrix}
\epsilon^1 e_1 f_s e_1 & \cdots & \epsilon^1 e_1 (\nabla e_i f_s)w & \cdots & \epsilon^1 e_1 f_s e_u \\
\vdots & \ddots & \vdots & \ddots & \vdots \\
\epsilon^u e_1 f_s e_1 & \cdots & \epsilon^u e_1 (\nabla e_i f_s)w & \cdots & \epsilon^u e_1 f_s e_u
\end{bmatrix}.
\]
The expression for $\nabla_\epsilon X$ is similar. When $\epsilon$ and $e$ have duality, the above expression admits a significant reduction, relieving us from computing the determinant.

**Lemma 5** (duality condition). *Within any segment $\alpha$, let*

$$e_{\alpha,n} := f^*_\epsilon e_{\alpha,n-1}, \quad \epsilon_{\alpha,n} := f^*\epsilon_{\alpha,n+1}.$$  

*For any invertible matrix $R_\alpha$, when moving across segments, if*

$$(\xi^T_\epsilon)_{\alpha,0} = I, \quad \xi_{\alpha-1,N} = \xi_{\alpha,0} R_\alpha, \quad \xi_{\alpha-1,N} = \xi_{\alpha,0} R_\alpha^{-T};$$

*Then for all suitable $n$ in segment $\alpha - 1$, we have $(\xi^T_\epsilon)_n = (\xi^T_\epsilon f_\epsilon)_n = I,$ and*

$$(\xi \nabla_\epsilon X)_n = \sum_{i=1}^n (\epsilon_i^n \nabla e_i X)_n, \quad \omega_n = \sum_{i=1}^n \epsilon_{n+1}^i (\nabla e_{n,i} f_\epsilon).$$

**Remark.** (1) Typically we perform QR factorization to $\xi_{\alpha-1,N}$, so $\xi_{\alpha,0}$ is orthogonal, and $R_\alpha$ is upper triangular. (2) If not for round-off errors, $\xi^T_{\alpha,0} \xi_{\alpha-1,N} = \xi^T_{\alpha,0} \xi_{\alpha,0} R_\alpha = R_\alpha$. To guarantee the duality, we compute via the more expensive expression, $\xi_{\alpha-1,N} = \xi_{\alpha,0} (\xi^T_{\alpha,0} \xi_{\alpha-1,N})^{-T}$.

**Proof.** Since $\xi^T_\epsilon f_\epsilon \xi = \xi^T_\epsilon \xi = \xi^T_\epsilon \xi$ is constant on segment $\alpha - 1$, we only need to show $(\xi^T_\epsilon)_\alpha - 1,N = I,$ and this is because

$$(\xi^T_\epsilon)_{\alpha-1,N} = (\xi_{\alpha,0} R_\alpha^{-T})^T \xi_{\alpha,0} R_\alpha = R^{-1}_\alpha \xi_{\alpha,0} R_\alpha = R^{-1}_\alpha R_\alpha = I.$$  

Then use lemma 4. □

In the nonintrusive adjoint shadowing algorithm, we need to compute a particular inhomogeneous adjoint solution $\nu'$. To avoid it from growing too large, we need to throw out its unstable part after every segment; meanwhile, we should keep a continuous affine space, $\nu' + \text{span } \xi$, so that later we can recover a continuous adjoint shadowing form $\nu$. This was a standard part of nonintrusive shadowing algorithms, but since we changed the renormalizing scheme on $\xi$, we shall re-derive the renormalizing scheme for $\nu'$ and continuity conditions.

**Lemma 6** (inhomogeneous continuity). *Let*

$$\nu'_{\alpha-1,N} = \nu'_{\alpha,0} - \xi_{\alpha,0} b_\alpha, \quad \text{where} \quad b_\alpha = (\xi^T_{\alpha,0} \xi_{\alpha,0})^{-1} \xi^T_{\alpha,0} \nu'_{\alpha,0};$$

*then $\nu'_{\alpha-1,N} \perp V^*_{\alpha-1,N}$, and the affine space $\nu'_{\alpha-1,N} + \text{span } \xi_{\alpha-1,N} = \nu'_{\alpha,0} + \text{span } \xi_{\alpha,0}$. If the adjoint shadowing form is represented nonintrusively as*

$$\nu_{\alpha,n} = \nu'_{\alpha,n} + \xi_{\alpha,n} a_\alpha,$$

*then the continuity of $\nu$ across segments, $\nu_{\alpha,N} = \nu_{\alpha+1,0}$, is equivalent to*

$$a_{\alpha-1} = R^T_\alpha (a_\alpha + b_\alpha).$$

**Proof.** To see the orthogonality, notice that $V^*_{\alpha-1,N} = \text{span } \xi_{\alpha-1,N} = \text{span } \xi_{\alpha,0}$, so

$$\xi^T_{\alpha,0} \nu'_{\alpha-1,N} = \xi^T_{\alpha,0} \nu'_{\alpha,0} - \xi^T_{\alpha,0} \xi_{\alpha,0} b_\alpha = 0.$$
The continuity of the affine space follows from definitions. For \( \nu \),

\[
\nu_{\alpha-1,N} = \nu_{\alpha,0} \iff \nu_{\alpha-1,N} + \xi_{\alpha-1,N}a_{\alpha-1} = \nu_{\alpha,0} + \xi_{\alpha,0}a_{\alpha} \\
\iff -\xi_{\alpha,0}b_{\alpha} + \xi_{\alpha-1,N}a_{\alpha-1} = \xi_{\alpha,0}a_{\alpha} \\
\iff \xi_{\alpha,0}(R_{\alpha}^{-T}a_{\alpha-1} - a_{\alpha} - b_{\alpha}) = 0 \iff a_{\alpha-1} = R_{\alpha}^{T}(a_{\alpha} + b_{\alpha}).
\]

Here the last equivalence is because \( \xi \) is a basis. \( \square \)

5.2. Procedure list.

This subsection gives a detailed procedure list of the fast adjoint response algorithm. When \( \mathcal{M} = \mathbb{R}^{M} \), corresponding simplifications are explained. The subscript explanation is in figure 3.

i. Evolve the dynamical system for a sufficient number of steps before \( n = 0 \), so that \( x_{0,0} \) is on the attractor at the beginning of our algorithm. Then, evolve the system from segment \( \alpha = 0 \) to \( \alpha = A - 1 \), each containing \( N \) steps, to obtain the orbit,

\[
x_{\alpha,n+1} = f(x_{\alpha,n}), \quad x_{\alpha+1,0} = x_{\alpha,N}.
\]

ii. Compute tangent solutions. Set random initial conditions for each column in \( e := [e_{1}, \cdots, e_{u}] \). For \( \alpha \) from \( 0 \) to \( A - 1 \) do the following:

(a) From initial conditions, solve tangent equations, \( \alpha \) neglected,

\[
\xi_{\alpha+1} = f_{*}\xi_{\alpha}.
\]

Here \( f_{*} \) is the pushforward operator. In \( \mathbb{R}^{M} \), the vectors are column vectors, and \( f_{*} \) is the Jacobian matrix,

\[
f_{*} = [\partial f^{i}/\partial z^{j}]_{ij},
\]

multiplied on the left of column vectors. Here \( [\cdot]_{ij} \) is the matrix with \( (i, j) \)-th entry given inside the bracket, \( f^{i} \) is the \( i \)-th component of \( f \), \( z^{j} \) is the \( j \)-th coordinate of \( \mathbb{R}^{M} \).

(b) At step \( N \) of segment \( \alpha \), orthonormalize \( \xi \) with a QR factorization

\[
\xi_{\alpha,N} = Q_{\alpha+1}R_{\alpha+1}.
\]

(c) Set initial conditions of the next segment,

\[
\xi_{\alpha+1,0} = Q_{\alpha+1}.
\]

iii. Compute adjoint solutions. Set terminal condition \( \nu'_{A-1,N} = \nu'_{A-1,N} = 0 \), and \( \xi_{A-1,N} \) such that \( (\xi^{T}\xi)_{A-1,N} = I \); here \( \xi = [\xi^{1}, \cdots, \xi^{u}] \). In \( \mathbb{R}^{M} \) we can set \( \xi_{A-1,N} = Q_{A}R_{A}^{-T} \). For \( \alpha \) from \( A - 1 \) to \( 0 \) do the following:

(a) From terminal conditions, solve homogeneous adjoint equations,

\[
\xi_{\alpha-1} = f^{*}\xi_{\alpha}.
\]

In \( \mathbb{R}^{M} \), covectors are represented by inner-product with column vectors, and the pullback operator \( f^{*} \) at \( x_{n} \) is the transposed Jacobian matrix evaluated at \( x_{n-1} \), multiplied on the left of column vectors.
(b) Compute the inhomogeneous term \( \omega \) for the modified adjoint shadowing equation, note that we do not compute \( \omega_n \) at \( n = N \):

\[
\omega_{n-1} = \sum_{i=1}^{u} \varepsilon_i (\nabla c_{n-1,i} f_*).
\]

Here \( \nabla (\cdot) f_* \) is the Riemannian derivative of \( f_* \) [23]. In \( \mathbb{R}^M \),

\[
\omega_{n-1} = \sum_{i=1}^{u} \sum_{l=1}^{M} \sum_{k=1}^{M} \left[ \varepsilon_{n,l} \frac{\partial^2 f_i}{\partial x^k \partial x^j} c_{n-1,l}^k \right] j \in \mathbb{R}^M,
\]

where \( \varepsilon_i, c^k \) are components in \( \mathbb{R}^M \).

(c) Solve inhomogeneous adjoint equations,

\[
\nu'_{n-1} = f^* \nu'_n + d\Phi_{n-1}, \quad \tilde{\nu}'_{n-1} = f^* \tilde{\nu}'_n + \omega_{n-1}.
\]

Note that the terminal values come from terminal conditions.

(d) Compute and store the covariance matrix and the inner product,

\[
C_\alpha := \sum_{n=1}^{N} \xi^T_{a,n} \xi_{a,n}, \quad d_\alpha := \sum_{n=1}^{N} \xi^T_{a,n} \nu'_{a,n}, \quad \tilde{d}_\alpha := \sum_{n=1}^{N} \xi^T_{a,n} \tilde{\nu}'_{a,0} dt.
\]

Here \( \xi^T \xi := [\langle \varepsilon_i, \varepsilon_j \rangle]_{ij} \), and \( \langle \cdot, \cdot \rangle \) in \( \mathbb{R}^M \) is the inner product between column vectors.

(e) At step 0 of segment \( \alpha \), compute and store

\[
b_\alpha = \left( \xi^T_{a,0} \xi_{a,0} \right)^{-1} \xi^T_{a,0} \nu'_{a,0}, \quad \tilde{b}_\alpha = \left( \xi^T_{a,0} \xi_{a,0} \right)^{-1} \xi^T_{a,0} \tilde{\nu}'_{a,0}.
\]

(f) Set initial conditions of the next segment,

\[
\xi_{a-1,N} = \xi_{a,0} (\xi^T_{a,0} \xi_{a-1,N})^{-T}, \quad \nu'_{a-1,N} = \nu'_{a,0} - \xi_{a,0} b_\alpha, \quad \tilde{\nu}'_{a-1,N} = \tilde{\nu}'_{a,0} - \xi_{a,0} \tilde{b}_\alpha.
\]

iv. Solve the nonintrusive adjoint shadowing problem,

\[
\min_{\{a_\alpha \}} \sum_{\alpha=0}^{A-1} \frac{1}{2} a_\alpha^T C_\alpha a_\alpha + d_\alpha^T a_\alpha
\]

s.t. \( a_{\alpha-1} = R_\alpha^T (a_\alpha + b_\alpha). \quad \alpha = 1, \ldots, A - 1. \)

Appendix A shows how to solve this with \( O(A) \) cost. Solve the same problem again, with \( b \) and \( d \) replaced by \( \tilde{b} \) and \( \tilde{d} \), for \( \tilde{a} \). Compute adjoint shadowing forms

\[
\nu_\alpha := \mathcal{L}(d\Phi) = \nu'_{a} + \xi_{\alpha} a_\alpha, \quad \tilde{\nu}_{\alpha} := \mathcal{L}(\omega) = \tilde{\nu}'_{a} + \xi_{\alpha} \tilde{a}_\alpha.
\]

v. Compute the shadowing contribution,

\[
S.C. = \lim_{A \to \infty} \frac{1}{AN} \sum_{\alpha=0}^{A-1} \sum_{n=1}^{N} \nu_{\alpha,n} X_{\alpha,n}.
\]

Here \( X_n := (\partial f / \partial \gamma)_{n-1} \), where \( \gamma \) is the parameter of the system. Note that we do not compute \( X_n \) at \( n = 0 \). Also note that \( X \) is used only after major computations have been done; no previous procedure depends on \( X \).
vi. (a) Compute the unstable divergence.

\[ \text{div}_u X^u_n = (\tilde{\nu} X)_n + (\varepsilon \nabla \sigma X)_n. \]

In \( \mathbb{R}^M \),

\[ (\varepsilon \nabla \sigma X)_n = \sum_{i=1}^u \sum_{j=1}^M \sum_{l=1}^M \varepsilon_{n,l}^i \frac{\partial^2 f_{n-1}^l}{\partial \gamma \partial x_j} \epsilon_{n-1,i}^j. \]

(b) Compute the unstable contribution

\[ U.C. W = \lim_{A \to \infty} \frac{1}{AN} \sum_{\alpha=0}^{A-1} \sum_{n=1}^N \psi_{\alpha,n} \text{div}_u X^u_{\alpha,n}, \]

where \( \psi := \sum_{m=-W}^W (\Phi \circ f^m - \rho(\Phi)) \) for a large \( W \).

vii. The linear response is

\[ \delta \rho(\Phi) = \lim_{W \to \infty} S.C. - U.C. W. \]

5.3. Remarks on implementation.

The main cost of the algorithm is computing \( \omega \) in step iii.b of the procedure. For a dense 3-tensor \( \nabla f_\alpha \), this can be very expensive, since for each \( j \), \( \omega^j \) requires summing \( uM^2 \) terms: this is a total of \( O(uM^3) \) float operations to get \( \omega \). However, for many engineering applications, such as fluid mechanics and convolutional neural networks, \( \nabla f_\alpha \) is sparse. This means that for each \( j \), \( \frac{\partial^2 f^j}{\partial x^k \partial x^l} \) is nonzero only for a few \( l \) and \( k \). Hence, for these situations, computing \( \omega \) costs only \( O(uM) \), and the overall complexity is the same order as the nonintrusive shadowing and the tangent fast response algorithm.

Although the number of float number operation for computing adjoint solutions are similar to tangent ones, adjoint solvers can take longer time. This is because adjoint solvers runs backward in time, which requires storing and reading data of the orbit. It seems that the most time-saving solution is to save checkpoints of the orbit and then rerun a segment of the orbit when solving the adjoint equations. This makes the adjoint solver a few times slower than tangent solvers.

Note that the cost for computing the unstable contribution is not only almost independent of the number of parameters; it is also almost independent of the number of objectives. This is different from conventional adjoint methods, whose cost depends almost linearly on the number of objectives. On the other hand, we require both tangent and adjoint solvers, whereas conventional adjoint and adjoint shadowing algorithms require only adjoint solvers.

Many practical comments for the fast linear response algorithm still apply in the adjoint version. For example, why our work may hold beyond the strong hyperbolicity assumptions we used in the proof; how to choose the number of steps in each segment; how to efficiently contract a higher tensor with several lower tensors; the cost-error estimation and its comparison with ensemble or stochastic methods.
6. A numerical example

This section illustrates the fast adjoint response algorithm on a 21-dimensional solenoid map with 20 unstable dimensions. Here $\mathcal{M} = \mathbb{R} \times \mathbb{T}^{20}$, and the governing equation is

$$
\begin{align*}
    x_{n+1}^1 &= 0.05x_n^1 + \gamma_1 + 0.1 \sum_{i=2}^{21} \cos(5x_n^i) \\
    x_{n+1}^i &= 2x_n^i + \gamma_2 (1 + x_n^1) \sin(2x_n^i) \mod 2\pi, \quad \text{for } 2 \leq i \leq 21
\end{align*}
$$

where the superscript labels the coordinates, and the instantaneous objective function is

$$
\Phi(x) := (x^1)^3 + 0.005 \sum_{i=2}^{21} (x^i - \pi)^2.
$$

This is almost the same example as in the paper for fast linear response [23], except for that now we have two parameters, $\gamma_1$ and $\gamma_2$.

The default setting, $N = 20$ steps in each segment, $A = 200$ segments, and $W = 10$, is used unless otherwise noted. The code is at https://github.com/niangxiu/far.

We first let $\gamma = \gamma_1 = \gamma_2$ and consider derivatives computed with respect to one parameter. We choose the default value $\gamma = 0.1$. Figure 4 shows that the variance of the computed derivative is proportional to $A^{-0.5}$, that is, the error decreases like the sampling error of an orbit. Figure 5 shows that the bias in the averaged derivative decreases as $W$ increases, but the variance increases roughly like $W^{0.5}$. Figure 6 shows that the derivative computed by the fast adjoint response correctly reflects the trend of the objective as $\gamma$ changes. The plots we obtained via the fast adjoint response is almost identical to that of the fast linear response [23]; this is expected, since they are two algorithms for the same quantity.

![Figure 4](image-url)  

**Figure 4.** Effects of $A$. Left: derivatives from 30 independent computations for each $A$. Right: the sample standard deviation of the computed derivatives, where the dashed line is $A^{-0.5}$.

On a single-core 3.0GHz CPU, for $10^4$ segments, which is a total of $2 \times 10^5$ steps, the time for computing the orbit is 5.5 seconds; the fast adjoint response on the same orbit takes another 186 seconds. So the time cost of fast adjoint response is about 34 times of simulating the orbit, or 6 times of the fast linear
Figure 5. Effects of $W$. Left: derivatives computed by different $W$’s. Right: standard deviation of derivatives, where the dashed line is $0.005W^{0.5}$.

Figure 6. Averaged objectives for different parameter $\gamma$. The grey lines are the derivatives computed by fast adjoint response.

response. Also, our algorithm can run even faster if we use the sparsity of the system, either via sparse matrices or graph tracing.

By the same analysis we have done in the tangent paper, on our example, fast adjoint response is about $10^6$ times faster than ensemble or stochastic adjoint algorithms; the isotropic operator method would take about $10^{20}$ GB storage. Other algorithms do not yet have adjoint versions. When there is only one parameter and one objective, fast linear response has cost similar to finite differences, which require data from several orbits to cancel the noise.

Finally, we demonstrate the fast adjoint response on two parameters $\gamma_1 \neq \gamma_2$. Fast adjoint response computes sensitivities with respect to multiple parameters with almost no additional cost; in fact, the cost of the unstable contribution is also independent of the number of objectives. Figure 7 illustrates the contour of $\rho(\Phi)$ and the gradients computed. Since we use the same length unit for both parameters, gradients should be perpendicular to the level sets of the objective: our algorithm indeed gives the correct gradient.
Figure 7. Gradients computed by fast adjoint response and the contour of \( \rho(\Phi) \). Here \( \rho(\Phi) \) is averaged over 30 orbits with 1000 segments, while the gradient is averaged over 30 orbits of 200 segments. The arrow’s length is 1/15 of the gradient.

Appendix A. Solving the Adjoint Shadowing Problem

The adjoint shadowing problem in this paper is slightly different from [27] since the renormalizing scheme is different. Also, we give the detailed formulas for the tridiagonal matrix algorithm, which can be convenient for readers.

The Lagrange function of the nonintrusive adjoint shadowing problem in step iv. of section 5.2 is:

\[
\sum_{\alpha=0}^{A-1} \frac{1}{2} a_\alpha^T C_\alpha a_\alpha + d_\alpha^T a_\alpha + \sum_{\alpha=1}^{A-1} \lambda_\alpha^T \left( a_{\alpha-1} - R_\alpha^T (a_\alpha + b_\alpha) \right),
\]

where \( \lambda_\alpha \) is the Lagrange multiplier for the continuity condition at step \( \alpha N \). The minimizer is given by

\[
\begin{bmatrix}
C & B \\
B^T & 0
\end{bmatrix}
\begin{bmatrix}
a \\
\lambda
\end{bmatrix} =
\begin{bmatrix}
-d \\
b'
\end{bmatrix},
\]

where

\[
C =
\begin{bmatrix}
C_0 & & \\
& C_1 & \\
& & \ddots
\end{bmatrix},
\quad
B =
\begin{bmatrix}
I & & \\
& -R_1 & I \\
& \dot{\cdots} & \ddots & \ddots
\end{bmatrix},
\quad
a =
\begin{bmatrix}
a_0 \\
\vdots \\
a_{A-1}
\end{bmatrix},
\quad
d =
\begin{bmatrix}
d_0 \\
\vdots \\
d_{A-1}
\end{bmatrix},
\quad
\lambda =
\begin{bmatrix}
\lambda_1 \\
\vdots \\
\lambda_{A-1}
\end{bmatrix},
\quad
b' =
\begin{bmatrix}
R_1^T b_1 \\
\vdots \\
R_{A-1}^T b_{A-1}
\end{bmatrix}.
\]

Here \( \{C_\alpha\}_{\alpha=0}^{A-1} \), \( \{R_\alpha\}_{\alpha=1}^{A-1} \) \( \in \mathbb{R}^{u \times u} \); \( \{a_\alpha\}_{\alpha=0}^{A-1} \), \( \{d_\alpha\}_{\alpha=0}^{A-1} \), \( \{\lambda_\alpha\}_{\alpha=1}^{A-1} \), \( \{b_\alpha\}_{\alpha=1}^{A-1} \) \( \in \mathbb{R}^u \). Note that \( C_\alpha \) and \( C \) are symmetric matrices.

We first solve the Schur complement for \( \lambda \) [8],

\[
B^T C^{-1} B \lambda = -(B^T C^{-1} d + b').
\]
We can write the left side in block form,
\[
C^{-1}B = \begin{bmatrix}
C_0^{-1} & & \\
-D_1 & \ddots & \\
& \ddots & C_{A-2}^{-1} \\
-D_{A-2} & \cdots & -D_{A-1}
\end{bmatrix},
\]
where
\[
D_\alpha := C_\alpha^{-1}R_\alpha, \quad E_\alpha := C_{\alpha-1}^{-1} + R_\alpha^T D_\alpha, \quad \alpha = 1, \cdots, A-1.
\]

For the right side, denote
\[
\begin{bmatrix}
y_1 \\
\vdots \\
y_{A-1}
\end{bmatrix} := -(B^T C^{-1}d + b'),
\]
where
\[
y_\alpha = D_\alpha^T d_\alpha - C_{\alpha-1}^{-1}d_{\alpha-1} - R_\alpha^T b_\alpha, \quad \alpha = 1, \cdots, A-1.
\]

The linear equation system \( \Lambda \lambda = y \) is a block-tridiagonal matrix; to solve it efficiently, we use the tridiagonal matrix algorithm, whose cost is only \( O(A) \).

First, we run a ‘forward chasing’ to eliminate below-diagonal blocks in \( \Lambda \),
\[
W := D_{A-1} E_{A-1}^{-1}, \quad E_\alpha \leftarrow E_\alpha - W D_{\alpha-1}^T, \quad y_\alpha \leftarrow y_\alpha + W y_{\alpha-1},
\]
sequentially for \( \alpha = 2, 3, \cdots, A-1 \).

Here ‘\( \leftarrow \)’ means to replace with new values. Then we run a ‘backward chasing’ to compute \( \lambda_\alpha \).
\[
\lambda_{A-1} = E_{A-1}^{-1} y_{A-1};
\]
\[
\lambda_\alpha = E_\alpha^{-1}(D_\alpha^T \lambda_{\alpha+1} + y_\alpha), \quad \text{sequentially for } \alpha = A-2, \cdots, 1.
\]

Then we solve for \( a \) via
\[
a = -C^{-1}(B \lambda + d).
\]

More specifically,
\[
a_0 = C_0^{-1}(-d_0 - \lambda_1);
\]
\[
a_\alpha = C_\alpha^{-1}(-d_\alpha - \lambda_{\alpha+1} + R_\alpha \lambda_\alpha), \quad \alpha = 2, \cdots, A-2;
\]
\[
a_{A-1} = C_{A-1}^{-1}(-d_{A-1} + R_{A-1} \lambda_{A-1}).
\]

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