Least Squares Shadowing for sensitivity analysis of chaotic dynamical systems

by

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Submitted to the Department of Aeronautics and Astronautics in partial fulfillment of the requirements for the degree of

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Abstract

In numerous scientific and engineering fields, sensitivity analysis tools are essential for design optimization as well as uncertainty quantification. For instance, adjoint algorithms are common place in aerospace engineering when it comes to optimize the shape of an airfoil, the configuration of a rocket or to quantify the impact of a manufacturing imperfection on the performance of a product. The quantities of interest are long-time averaged outputs such as the average drag on a plane wing. However, these conventional methods fail to compute the right sensitivity when the physical model exhibits chaos. This is the case of many turbulent fluid flows and atmospheric modelisations.

A recently developed method, Least Squares Shadowing or simply LSS, tackles this problem and proposes an alternative approach to compute the desired sensitivities. The results are very promising and this thesis is intended to lay the mathematical foundations of this new algorithm. A latter part is dedicated to some improvements of LSS which make it faster and more reliable.

Thesis Supervisor: Qiqi Wang
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Chapter 1

Introduction

In many scientific and engineering applications, quantities of interest are time averages of some specific instantaneous output and this output may be affected by parameters of the physical system/model. For example, when evaluating the performance of a wing, the time averaged drag produced by the wing is of great importance for aerodynamicists. Any shape characteristic of the wing (width, length, curvature, ...) clearly has an impact on the produced drag and could be consequently considered a parameter. Computing the derivative of the quantity of interest (time-averaged output) with respect to the system’s parameters is crucial in:

- **Numerical design optimization**: the derivative feeds a gradient-based algorithm that is then used to optimize the system’s parameters [1],[2],[3]

- **Uncertainty quantification**: the derivative itself gives a useful assessment of the sensitivity and/or uncertainty of the system with respect to its parameters [4],[5]

Conventional tangent and adjoint methods are very efficient at computing these sensitivities for many physical problems [6]. However, whenever the physics involves chaotic nonlinear dynamics, the so-called *butterfly effect* makes the conventional tangent/adjoint algorithms fail when computing the derivative of the quantity of interest. Indeed, the computed values are, in general, orders of magnitude bigger than the real values [7]. Unfortunately, many crucial applications involve simulations of nonlinear
dynamical systems that exhibit chaotic behavior. For example, chaos can be encountered in the following fields: fluid dynamics, climate and weather prediction [8],[9], turbulent combustion simulation [10], nuclear reactor physics [11], plasma dynamics in fusion [12], and multi-body problems [13].

1.1 Brief overview of dynamical systems

We will briefly present the essential concepts and notations that will be used in this thesis. For a more in-depth introduction to dynamical systems, the reader can consult [14]. Dynamical systems can be separated into two classes: continuous (including differential equations) and discrete (dynamical maps). In this thesis, continuous dynamical systems will be of the form of a differential equation parameterized by a parameter $s \in \mathbb{R}$ and governing $u(t) \in \mathbb{R}^m$ where $\mathbb{R}^m$ is called phase space:

$$\begin{cases} \frac{du}{dt} = f(u, s), \\ u(0) = u_0 \quad u_0 \in \mathbb{R}^m. \end{cases} \quad (1.1)$$

Discrete dynamical systems will presented as:

$$\begin{cases} u_{i+1} = f(u_i, s), \quad i \in \mathbb{N}, \\ u_0 \in \mathbb{R}^m. \end{cases} \quad (1.2)$$

The trajectory of $u$ in phase space is $\{u(t), t \in \mathbb{R}\}$ for the continuous case and $\{u_i, i \in \mathbb{N}\}$ for the discrete case. Depending on the characteristics of the system, as $t \to \infty$ (resp. $i \to \infty$) the trajectory can converge toward a point, the limit cycle, or have other behaviors (see Figure (1-1)). When the system is chaotic, $u$ converges toward $\Lambda$, a fractal set called a strange attractor (see Figure (1-2) for an example of a strange attractor). On the strange attractor, the trajectory does not follow any periodic pattern. What causes this behavior is the butterfly effect, which stipulates that two trajectories that are very close to each other at $t = 0$ diverge from each other in a very short lapse of time. In other words, the trajectories are extremely sensitive to
the initial conditions and any tiny perturbation in the initial conditions has a big impact on the trajectory of $u$ in the near future.

The quantity of interest is the time average of the instantaneous output $J(u(t), s)$:

$$\langle J \rangle(s) = \lim_{T \to +\infty} \frac{1}{T} \int_{0}^{T} J(u(t), s) dt,$$  \hspace{1cm} (1.3)

or

$$\langle J \rangle(s) = \lim_{N \to +\infty} \frac{1}{N} \sum_{i=0}^{N} J(u_i, s),$$  \hspace{1cm} (1.4)

if the system is discrete. The butterfly effect makes a small neighborhood of $u$ at $t = 0$ spread all over the attractor after a sufficiently large integration time $T$. This leads us to the ergodicity assumption: when $T \to \infty$ the initial small neighborhood of $u$ at $t = 0$ settles into a cloud covering all of the attractor $\Lambda$. It has been shown that in many of the practical examples listed previously, the quantities of interest exhibit ergodic properties, popularly known as chaotic hypothesis [15],[16].

We define $\rho(u, s)$, the SRB or invariant measure of the system to be the 'density' of the steady-state cloud [17],[18]. The regions of $\Lambda$ with high $\rho(u, s)$ correspond to the areas that are 'frequently visited' by trajectories, while regions with low $\rho(u, s)$ are rarely visited. For such ergodic systems, the long-time average converges to the
ensemble average:

\[ \langle J \rangle(s) = \lim_{T \to +\infty} \frac{1}{T} \int_0^T J(u(t), s) dt = \int \lambda J(u, s) \rho(u, s) du. \]  

(1.5)

Indeed, the ergodicity assumption can be understood as a memoryless assumption: no matter what the initial condition \( u(0) \) is, after a long integration time \( T \), the "probability of presence" of \( u \) in any region of the attractor will converge to \( \rho(u, s) \). Consequently, the quantity of interest \( \langle J \rangle \) only depends on the parameter \( s \) and not on the initial condition, making the problem much more tractable.

As for its differentiability, Ruelle has proven that \( \frac{d\langle J \rangle}{ds} \) exists for ergodic systems [19]: our search for this quantity is consequently a well-defined problem.

1.2 Break down of conventional methods

Conventional methods try to compute \( \frac{d\langle J \rangle}{ds} \) by solving the so-called tangent linear equations:

\[
\begin{aligned}
\frac{dv}{dt} &= \frac{\partial f}{\partial u} v + \frac{\partial f}{\partial s}, \\
v(0) &= 0,
\end{aligned}
\]

(1.6)

where \( v(t) \) shows how the trajectory \( \{u(t), t \in \mathbb{R}\} \) would change if the parameter \( s \) becomes \( s + \epsilon \) with \( \epsilon \) infinitesimal and adding the constraint that both the old trajectory \( \{u(t)\} \) and perturbed trajectory \( \{u(t) + \epsilon v(t)\} \) begin at the same point \( u(0) \). Thus, computing \( \frac{d\langle J \rangle}{ds} \) would resume to:

\[
\begin{aligned}
\frac{d\langle J \rangle}{ds} &= \lim_{\epsilon \to 0} \frac{1}{T} \int_0^T \frac{J(u(t, s + \epsilon), s + \epsilon) - J(u(t, s), s)}{\epsilon}, \\
&= \lim_{\epsilon \to 0} \frac{1}{T} \int_0^T \frac{\partial J}{\partial u} v + \frac{\partial J}{\partial s}, \\
&= \lim_{T \to \infty} \int_0^T \frac{\partial J}{\partial u} v + \frac{\partial J}{\partial s}.
\end{aligned}
\]

(1.7, 1.8, 1.9)
Unfortunately, for chaotic systems, \( \lim_{\epsilon \to 0} \frac{u(.\cdot + t) - u(.\cdot)}{\epsilon} \) does not converge uniformly to \( v(.\cdot, s) \), which does not allow us to permute the order of the limits (\( \epsilon \to 0 \) and \( T \to \infty \)). Not only do we have \( \frac{d(J)}{ds} \neq \lim_{T \to \infty} \int_0^T \frac{\partial J}{\partial u} v + \frac{\partial J}{\partial s} \) but \( \lim_{T \to \infty} \int_0^T \frac{\partial J}{\partial u} v + \frac{\partial J}{\partial s} \) itself is not well defined. Actually,

\[
\left| \int_0^T \frac{\partial J}{\partial u} v + \frac{\partial J}{\partial s} dt \right| \xrightarrow{T \to \infty} \infty,
\]

at a very fast rate. This divergence is due to the fact that the solution to the tangent linear system (1.6) \( v(t) \) grows exponentially with time for chaotic systems. Least Squares Shadowing (LSS) replaces the constraint \( v(0) = 0 \) by a minimization problem that produces a much better behaved \( v(t) \), as we will see in the next chapter. Other algorithms have been developed to overcome this failure. Lea et al. proposed the ensemble adjoint method, which applies the adjoint method to many random trajectories, then averages the computed derivatives [7], [20]. However, the algorithm is computationally expensive even for small dynamical system such as Lorenz’s system. Based on the fluctuation dissipation theorem, Abramov and Majda provided an algorithm that successfully computes the desired derivative [21]. Nonetheless, this algorithm assumes the dynamical system to have an equilibrium distribution similar to the Gaussian distribution, an assumption often violated in very dissipative systems.

Recent work by Cooper and Haynes has alleviated this limitation by introducing a nonparametric method to estimate the equilibrium distribution [22]. Compared with these algorithms, the advantages of LSS are:

- its **simplicity** because the least squares problem can easily be formulated and efficiently solved as a linear system,

- it is **less sensitive** to the dimension of the dynamical system,

- it **does not require any explicit knowledge** of its steady-state distribution in phase space.
1.3 Lorenz 63 numerical example

One of the most famous test cases and examples of chaotic dynamical systems is the Lorenz 63 differential equation, used to model atmospheric convection. It is a three-dimensional autonomous differential equation parameterized by \( \sigma, \beta, \rho \), and the dynamics happen to be chaotic when the parameters belong to a certain range of values. The governing equations are the following:

\[
\begin{align*}
\frac{dx}{dt} &= \sigma(y - x), \\
\frac{dy}{dt} &= x(\rho - z) - y, \\
\frac{dz}{dt} &= xy - \beta z.
\end{align*}
\]

The quantity of interest in this example is \( \langle z \rangle = \lim_{T \to \infty} \frac{1}{T} \int_{-T}^{T} z(t) dt \), the time average of the component \( z \), and the algorithm is used to compute \( \frac{d\langle z \rangle}{dp} \), its derivative with respect to \( \rho \). The other two parameters are set to \( \sigma = 10 \) and \( \beta = \frac{8}{3} \). It has been shown that \( \frac{d\langle z \rangle}{dp} \) is approximately equal to 0.96 for a wide range of values of \( \rho \) [7]. Our numerical applications will stay in this range as we can notice from Figure (1-3). The graphs (1-4) show that a conventional adjoint method gives us unrealistic values for \( \frac{d\langle z \rangle}{dp} \) while LSS computes an accurate and useful estimation of this derivative. If we zoom in the graph of \( \langle z \rangle \) (Figure (1-3), right), we notice that \( \langle z \rangle \) has steep low-amplitude oscillations at a local level. This is due to the fact that we approximate computationally \( \langle z \rangle \) by \( \frac{1}{T} \int_{-T}^{T} z(t) dt \) with a large but finite \( T \). As \( T \) goes to infinity, the oscillations become steeper and their amplitude decreases. In the 'theoretical' limit, the oscillations disappear and we obtain a smooth graph with slope \( \approx 1 \). Conventional methods compute the value of the 'local' slope instead of the useful macroscopic slope, which explains the very high values obtained in the left graph of (1-4).

Throughout this thesis, I will be presenting the theoretical foundation of LSS as well as some improvements to the original method. The following chapter is dedicated to the presentation of the algorithm as well as its theoretical foundation. Indeed, we will show that it gives a useful estimation of \( \frac{d\langle z \rangle}{ds} \) for a particular case of uniformly
Figure 1-2: Strange attractor for the Lorenz 63 dynamical system

Figure 1-3: $\langle z \rangle$ with respect to $\rho$
Figure 1-4: Computing $\frac{d(x)}{dp}$ using the conventional adjoint and LSS hyperbolic dynamical systems. In the next chapter, a lighter and faster version of LSS will be presented. We can eliminate some correction terms by introducing a windowing procedure. Finally, we will introduce a new and more robust variant of LSS called LSS with reconnections (LSSR).
Chapter 2

Convergence of LSS

In this chapter, we will present the mathematical foundation of LSS and prove that it gives us the right estimation of the sensitivity for the class of uniformly hyperbolic differential equations. For dynamical maps, a proof of convergence conceived by Wang can be consulted [23]. We consider again the differential equation parameterized by \( s \in \mathbb{R} \) and governing \( u(t) \in \mathbb{R}^m \):

\[
\begin{cases}
\frac{du}{dt} = f(u, s), \\
u(0) = u_0, \quad u_0 \in \mathbb{R}^m.
\end{cases}
\] (2.1)

As we said, the differential equation is assumed to be uniformly hyperbolic (details in Section 2.2). We are also given a \( C^1 \) cost function \( J(u, s) : \mathbb{R}^m \times \mathbb{R} \to \mathbb{R} \) and assume that the system is ergodic, i.e., the infinite time average:

\[
\langle J \rangle(s) = \lim_{T \to +\infty} \frac{1}{T} \int_0^T J(u(t), s) dt,
\] (2.2)

depends on \( s \) but does not depend on the initial condition \( u(0) \).

First, we will explain what we mean by "the algorithm converges to \( \frac{d\langle J \rangle}{ds} \)" in the form of a theorem. Then, I will go through the essential notions of uniform hyperbolicity and time dilation, both relative to the differential equation, because they are necessary to understand the proof of the theorem. The following sections constitute the proof. It is divided into three major parts:
First, we show that there exists a 'well-behaved' perturbation \( \{v(t)\} \) of the trajectory \( \{u(t)\} \) that is well suited for the permutation of the limits in the expression (1.7). This perturbation is called a shadowing direction.

The existence of a shadowing direction is a theoretical result. Nevertheless, we prove that if we had access to it then we could compute \( \frac{d\langle J \rangle}{ds} \).

Finally, we propose an approach to approximate the shadowing direction and show that we can estimate \( \frac{d\langle J \rangle}{ds} \) with this approximation. This concludes the proof of the theorem, which states that the estimation of \( \frac{d\langle J \rangle}{ds} \) converges to its real value when we refine our approximation of the shadowing direction (i.e., we increase the size of our least squares problem).

### 2.1 Discretizing the problem and the LSS theorem

To obtain an algorithm of practical relevance, a discrete version of the above problem should be formulated. First, we replace the differential equation (2.1) parameterized by \( s \) by a family of operators: let \( \varphi_s(u, h) : \mathbb{R}^m \times \mathbb{R}^+ \rightarrow \mathbb{R}^m \) be the family of maps parameterized by \( s \in \mathbb{R} \) such that it is a 'discretization' of the differential equation using a uniform time step size of \( h \). In other words, if \( \{u(t), t \in (-\infty, +\infty)\} \) is a trajectory satisfying the initial differential equation (2.1) for a particular \( s \in \mathbb{R} \), we have:

\[
\varphi_s(u(t), h) = u(t + h) \quad \forall t \in \mathbb{R}.
\]

In this case, \( \varphi_s(\cdot, h) \) corresponds to a perfect numerical integration scheme with a step size of \( h \). We ask for the differential equation to be 'smooth' enough so that the maps \( \varphi(\cdot, \cdot) \) are \( C^2 \).

Then, assuming that all trajectories \( \{u(t), t \in \mathbb{R}\} \) belong to a compact set \( \Lambda \) and that \( s \) also lies in a compact set \( S \subseteq \mathbb{R} \), we can approximate \( \frac{1}{T} \int_0^T J(u(t), s)dt \) with a
Riemann sum and have the following bound on the integration error:

\[
\left| \frac{1}{T} \left( \int_0^T J(u(t), s) dt - \sum_{i=0}^{\lfloor \frac{T}{h} \rfloor} h J(\varphi_s(u(0), ih), s) \right) \right| \leq h \sup_{s \in S} \left( \|DJ(\cdot, s)\|_\infty \right) \sup_{s \in S} \left( \|f(\cdot, s)\|_\infty \right),
\]

(2.3)

where \( \varphi_s(u(0), 0) = u(0) \) and \( \|f(\cdot, s)\|_\infty \), \( \|DJ(\cdot, s)\|_\infty \) are the infinity norms of \( f(\cdot, s) \) and the derivative of \( J(\cdot, s) \) with respect to the first variable on the compact set \( \Lambda \).

Because the bound does not depend on \( T \), we finally have:

\[
\lim_{T \to \infty} \frac{1}{T} \sum_{i=0}^{\lfloor \frac{T}{h} \rfloor} h J(\varphi_s(u(0), ih), s) = O(h).
\]

(2.4)

To simplify the expressions, we introduce the new notation \( \varphi_s(u(0), ih) = u_i^{s,h,T} \) or even \( \varphi_s(u(0), ih) = u_i^{h,T} = u_i^s = u_i \) depending on which parameter is fixed and when there is no ambiguity.

For a sequence \( \{u_i, i = 1, \ldots, \lfloor \frac{T}{h} \rfloor \} \) satisfying \( u_{i+1} = \varphi_s(u_i, h) \), the Least Squares Shadowing method attempts to compute the derivative \( \frac{dJ}{ds} \) via

**Theorem 2.1.1 (THEOREM LSS)** Under ergodicity and hyperbolicity assumptions,

\[
\frac{d\langle J \rangle}{ds}(s) = \lim_{T \to \infty} \lim_{h \to 0} \frac{1}{T} \sum_{i=1}^{\lfloor \frac{T}{h} \rfloor} \left[ (DJ(u_i, s))v_i^{h,T} + \partial_s J(u_i, s) + \left( \eta_i^{h,T} (J(u_i, s) - \langle J \rangle(s)) \right) \right],
\]

\[
= \lim_{T \to \infty} \lim_{h \to 0} \frac{1}{T} \sum_{i=1}^{\lfloor \frac{T}{h} \rfloor} \left[ (DJ(u_i, s))v_i^{h,T} + \partial_s J(u_i, s) + \left( \eta_i^{h,T} (J(u_i, s) - \langle J \rangle(s)) \right) \right],
\]

where \( (v_i^{h,T}, \eta_i^{h,T}) \in \mathbb{R}^m \times \mathbb{R} \), \( i = 1, \ldots, \lfloor \frac{T}{h} \rfloor \) is the solution to the constrained least squares problem:

\[
\min \sum_{i=1}^{\lfloor \frac{T}{h} \rfloor} (\|v_i^{h,T}\|^2 + \alpha(\eta_i^{h,T})^2),
\]

s.t. \( v_{i+1}^{h,T} = (D\varphi_s(u_i, h))v_i^{h,T} + \partial_s \varphi_s(u_i, h) + h\eta_i^{h,T} \partial_h \varphi_s(u_i, h) \),

where \( \alpha \) is any positive constant and \( \|\cdot\| \) is the Euclidean norm in \( \mathbb{R}^m \).
Here, the linearized operators are defined as:

\[
(DJ(u, s))v := (DvJ)(u, s) := \lim_{\epsilon \to 0} \frac{J(u + \epsilon v, s) - J(u, s)}{\epsilon},
\]

\[
(D\varphi_s(u, h))v := (D\varphi_s)(u, h) := \lim_{\epsilon \to 0} \frac{\varphi_s(u + \epsilon v, h) - \varphi_s(u, h)}{\epsilon},
\]

\[
\partial_s J(u, s) := \lim_{\epsilon \to 0} \frac{J(u, s + \epsilon) - J(u, s)}{\epsilon},
\]

\[
\partial_s \varphi_s(u, h) := \lim_{\epsilon \to 0} \frac{\varphi_{s+\epsilon}(u, h) - \varphi_s(u, h)}{\epsilon},
\]

\[
\partial_h \varphi_s(u, h) := \lim_{\epsilon \to 0} \frac{\varphi_s(u, h + \epsilon) - \varphi_s(u, h)}{\epsilon} = f(\varphi_s(u, h)).
\]  

(DJ), (∂s J), (Dφs), (∂s φs) and (∂h φs) are a 1 × m vector, a scalar, an m × m matrix, an m × 1 vector, and an m × 1 vector, respectively, representing the partial derivatives.

### 2.2 Uniform hyperbolicity

Let us now proceed to the presentation of the uniform hyperbolicity property, which is at the origin of the butterfly effect. We say that the dynamical system (2.1) has a compact, global, uniformly hyperbolic attractor Λ ⊂ Rm at s if for all t the map φs(·, t) satisfies:

1. For all u₀ ∈ Rm, dist(Λ, u(t)) \( t \to \infty \) 0 where dist is the Euclidean distance in Rm.

2. There is a C ∈ (0, +∞) and λ ∈ (0, 1), such that for all u ∈ Λ, there is a splitting of Rm representing the space of perturbations around u:

\[
R^m = V^+(u) \oplus V^-(u) \oplus V^0(u),
\]

(2.7) where the subspaces are:
• \( V^+(u) := \{ v \in \mathbb{R}^m / \| (D\varphi_s(u,t))v \| \leq C\lambda^{-t}\|v\|, \forall t < 0 \} \) is the \textit{unstable} subspace at \( u \),

• \( V^-(u) := \{ v \in \mathbb{R}^m / \| (D\varphi_s(u,t))v \| \leq C\lambda^t\|v\|, \forall t > 0 \} \) is the \textit{stable} subspace at \( u \),

• \( V^0(u) := \{ \alpha f(u,s), \forall \alpha \in \mathbb{R} \} = \{ \alpha \partial_h \varphi_s(u_{i-1}, h), \forall \alpha \in \mathbb{R} \} \) is the \textit{neutral} subspace at \( u \).

\( V^-(u), V^+(u) \) and \( V^0(u) \) are all continuous with respect to \( u \).

If \( r = r^+ + r^- + r^0 \) with \( r^+ \in V^+(u), r^- \in V^-(u), r^0 \in V^0(u) \) and \( u \in \Lambda \), the continuity of the three subspaces and the compactness of \( \Lambda \) implies that:

\[
\inf_{u, r^+, r^-, r^0} \frac{\| r^+ + r^- + r^0 \|}{\max(\| r^+ \|, \| r^- \|, \| r^0 \|)} = \beta > 0.
\] (2.8)

This is because if \( \beta = 0 \), then by the continuity of \( V^+(u), V^-(u), V^0(u) \) and the compactness of \( \{(u, r^+, r^-, r^0) \in \Lambda \times \mathbb{R}^m \times \mathbb{R}^m \times \mathbb{R}^m / \max(\| r^+ \|, \| r^- \|, \| r^0 \|) = 1 \} \), there must be a \( (u, r^+, r^-, r^0) \) such that \( \max(\| r^+ \|, \| r^- \|, \| r^0 \|) = 1 \) and \( r^+ + r^- + r^0 = 0 \), which contradicts assumption (2.7). Thus:

\[
\| r^+ \| \leq \frac{\| r \|}{\beta} \quad \| r^- \| \leq \frac{\| r \|}{\beta} \quad \| r^0 \| \leq \frac{\| r \|}{\beta}.
\] (2.9)

The \textit{stable}, \textit{unstable}, and \textit{neutral subspaces} are also \textit{invariant} under the differential of the map \( \varphi_s(\cdot, h) \), i.e., if \( u_{i+1} = \varphi_s(u_i, h) \) and \( v_{i+1} = (D\varphi_s(u_i, h))v_i \), then

\[
\begin{align*}
& v_i \in V^+(u_i) \iff v_{i+1} \in V^+(u_{i+1}), \\
& v_i \in V^-(u_i) \iff v_{i+1} \in V^-(u_{i+1}), \\
& v_i \in V^0(u_i) \iff v_{i+1} \in V^0(u_{i+1}).
\end{align*}
\] (2.10)

Because of their relative simplicity, studies of uniformly hyperbolic dynamical systems (also known as 'ideal chaos') have provided a lot of insight into the properties...
of chaotic dynamical systems [24]. Although most real-life dynamical systems are not uniformly hyperbolic, they can be classified as quasi-hyperbolic; results obtained on hyperbolic systems can often be generalized to them [25]. This proof covers the convergence of LSS for uniform hyperbolic flows; nevertheless, numerical results have shown that the algorithm also works for nonideal chaos [26].

2.3 Neutral subspace and nonuniform discretization of trajectories

One should bear in mind that the dynamical system is continuous, which means that a solution \( \{u(t), t \in \mathbb{R}^+\} \) to equation (2.1) forms a continuous trajectory in phase space. Thus, the sequence \( \{u_i^{(h, \infty)}, i \in \mathbb{N}\} \) is no more than a sequence of sample points on the continuous trajectory, the time step size between two consecutive points being \( h \). The neutral subspace \( V^0(u_i) \), which is one dimensional, is constituted by the line tangent to the continuous trajectory at the sampling point \( u_i \). Consequently, a perturbation in the direction of the neutral subspace around the point \( u_i \) can be interpreted as a time shift. This means that for \( i \in \mathbb{N}^* \) and \( \epsilon \) infinitesimal, if \( u(t_i) = u_i \):

\[
\begin{align*}
u(t_i + \epsilon) &= u_i + \epsilon f(u_i, s),
\end{align*}
\]

and

\[
\begin{align*}
u(t_i + \epsilon) &= \varphi_s(u_{i-1}, h + \epsilon) = \varphi_s(u_{i-1} + \epsilon f(u_{i-1}, s), h),
\end{align*}
\]

, which implies:

\[
\begin{align*}
\varphi_s(u_{i-1} + \epsilon f(u_{i-1}, s), h) &= u_i + \epsilon f(u_i, s),
\end{align*}
\]
i.e.

\[ (D\varphi_s(u_{i-1}, t))f(u_{i-1}, s) = f(u_i, s). \]  \hspace{1cm} (2.14)

Because \( \|f(u_i, s)\| \leq \sup_{s \in S} \|f(\cdot, s)\|_\infty \) < \( \infty \) for all \( i \in \mathbb{N}^* \), then (2.14) implies that a small perturbation in the direction of the neutral subspace remains bounded under the action of forward or backward iterations. In contrast, a small perturbation in the stable or unstable subspace gets amplified exponentially under the action of backward or forward iterations.

The second point to be discussed in this section is the fact that the discretization of a continuous trajectory does not have to respect a uniform step sizing. A better way to discretize a trajectory would be the following: \( \{(u_i, \tau_i), i \in \mathbb{N}\} \) is a sampling of a continuous trajectory if \( u_i = \varphi_s(u_{i-1}, h\tau_i) \) where \( \tau_i \in \mathbb{R} \). To have:

\[ \lim_{T \to +\infty} \sum_{i=0}^{\lfloor T \rfloor} \frac{\tau_i J(u_i, s)}{\sum_j \tau_j^p} = O(h), \]  \hspace{1cm} (2.15)

we only need \( \sup(h\tau_i) \to 0 \) as \( h \to 0 \), which actually happens if, for example, the time dilation factors \( \tau_i \) are bounded (\( \sum_j \) means \( \sum_{j=1}^{\lfloor T \rfloor} \) in the above expression). From now on, a discretization of a trajectory is a sequence of couples \((u_i, \tau_i)\).

2.4 Structural stability and the shadowing direction

Now, we will prove a variant of the shadowing lemma for the purpose of defining the shadowing direction and proving its existence and uniqueness.

The hyperbolic structure ensures the structural stability of the attractor \( \Lambda \) under a perturbation in \( s \) [27], [28]. Without loss of generality, we will assume that \( s = 0 \) and
choose a sequence \( \{u_i^0, i \in \mathbb{Z}\} \) such that:

\[
u_{i+1}^0 = \varphi_0(u_i^0, h).
\]

In this case, the superscript in \( u_i^0 \) is the value of the parameter \( s \). \( h \) and \( T = \infty \) are fixed so they do not appear in the notation.

**Theorem 2.4.1 (Shadowing trajectory)** If the system is uniformly hyperbolic and \( \varphi_s \) continuously differentiable with respect to \( s \) and \( u \), then for all sequences \( \{u_i^0, i \in \mathbb{Z}\} \subset \Lambda \) satisfying \( u_i^0 = \varphi_0(u_{i-1}^0, h) \), there is an \( M > 0 \) such that for all \( |s| < M \) there is a sequence \( \{(u_i^s, \tau_i^s), i \in \mathbb{Z}\} \subset \mathbb{R}^m \) satisfying \( ||u_i^s - u_i^0|| < M, ||\tau_i^s|| < M \) and \( u_i^s = \varphi_s(u_{i-1}^s, h\tau_i^s) \) for all \( i \in \mathbb{Z} \). Furthermore, \( u_i^s \) and \( \tau_i^s \) are \( i \)-uniformly continuously differentiable to \( s \).

The \( i \)-uniform continuous differentiability of \( u_i^s \) means that for all \( s \in (-M, M) \) and \( \epsilon > 0 \) there is a \( \delta > 0 \) such that if \( |s - s'| < \delta \) then \( \| \frac{du_i^s}{ds}(s) - \frac{du_i^{s'}}{ds}(s') \| < \epsilon \) and \( |\frac{d\tau_i^s}{ds}(s) - \frac{d\tau_i^{s'}}{ds}(s')| < \epsilon \) for all \( i \).

To prepare for the proof, let \( B \) be the space of bounded sequences in \( \mathbb{R}^m \) and \( V_i \) the hyperplane of \( \mathbb{R}^m \) defined by \( V_i = V^+(u_i^0) \oplus V^-(u_i^0) \). We introduce \( V \) as the space of bounded sequences \( \{v_i, i \in \mathbb{Z}\} \) such that \( v_i \in V_i \) for all \( i \in \mathbb{Z} \) (\( v_i \) has no components in the neutral subspace). In other words:

\[
V = (\prod_{i \in \mathbb{Z}} V_i) \cap B.
\]

Finally, by considering the space \( T \) of bounded sequences of \( \mathbb{R} \), we denote \( A \) the product of \( V \) by \( T \):

\[
A = V \times T.
\]
We then introduce the notation \((v, \tau) = \{(v_i, \tau_i), i \in \mathbb{Z}\} \in A\) where \(v \in V\), \(\tau \in T\) and define the norm:

\[
\|(v, \tau)\|_A = \sup_{i \in \mathbb{Z}} \|v_i\| + \sup_{i \in \mathbb{Z}} |\tau_i| = \|v\|_\infty + \|\tau\|_\infty.
\]

As defined above, the space \(A\) is a Banach space. We can now define the map \(F\):

\[
A \times \mathbb{R} \to B \quad \forall(v, \tau) \in A, \forall s \in \mathbb{R}, \quad F((v, \tau), s) = \{u_i^0 + v_i - \varphi_s(u_i^{0} + v_{i-1}, h\tau_{i-1}), i \in \mathbb{Z}\}.
\]

For a given \(s\), \(F((v, \tau), s) = 0\) if and only if \(\{(u_i^0 + v_i), i \in \mathbb{Z}\}\) samples, with time steps \(\{h\tau_i, i \in \mathbb{Z}\}\), a continuous trajectory satisfying (2.1). We use the implicit function theorem to complete the proof, which requires \(F\) to be differentiable with respect to \((v, \tau)\) and its derivative to be non-singular at \(v = 0, \tau = 1\) and \(s = 0\).

**Lemma 2.4.2** Under the conditions of theorem 2.4.1, \(F\) has Fréchet derivative at all \((v, \tau) \in A\) and \(|s| < M\):

\[
(DF((v, \tau), s))(w, \epsilon) = \left\{ \frac{w_i}{\|(w, \epsilon)\|_A} - \frac{\varphi_s(u_i^{0} + v_{i-1}, h\tau_{i-1}) - \varphi_s(u_i^{0} + v_{i-1}, h\tau_{i-1})}{\|(w, \epsilon)\|_A} \right\} (2.16)
\]

\[
- h\epsilon_{i-1}\partial_{h}\varphi_s(u_i^{0} + v_{i-1}, h\tau_{i-1}), i \in \mathbb{Z}, \}
\]

where \((w, \epsilon) \in A\).

**Proof** We have:

\[
\frac{F((v + w, \tau + \epsilon), s) - F((v, \tau), s)}{\|(w, \epsilon)\|_A} = \left\{ \frac{w_i}{\|(w, \epsilon)\|_A} - \left( \frac{D\varphi_s(u_i^{0} + v_{i-1}, h\tau_{i-1})}{\|(w, \epsilon)\|_A} \right) (w_{i-1}) \right\} (2.17)
\]

\[
- \frac{h\epsilon_{i-1}\partial_{h}\varphi_s(u_i^{0} + v_{i-1}, h\tau_{i-1})}{\|(w, \epsilon)\|_A} (2.20)\]

(2.21)
in the $A$ norm thanks to the uniform continuity of $D\varphi$ and $\partial_h\varphi$ on the compact set $\Lambda$. Now, we only need to prove that the linear map we obtained is bounded. Because $D\varphi$ and $\partial_h\varphi$ are continuous, they are uniformly bounded in the compact set $\Lambda$. Thus, the norm of the linear map is less than $(1 + \|D\varphi\|_\infty + \|\partial_h\varphi\|_\infty)$. 

**Lemma 2.4.3** Under the conditions of theorem 2.4.1, the Fréchet derivative of $F$ at $(v, \tau) = (0, 1)$ and $s = 0$ is a bijection.

**Proof** The Fréchet derivative of $F$ at $(v, \tau) = (0, 1)$ and $s = 0$ in the direction $(w, \epsilon)$ is:

$$
(DF((0, 1), 0))(w, \epsilon) = \{w_i - (D\varphi_0(u^0_{i-1}, h))w_{i-1} - h\epsilon_{i-1}\partial_h\varphi_0(u^0_{i-1}, h), i \in \mathbb{Z}\}.
$$

To prove its bijectivity, we only need to show that for any $r = \{r_i\} \in B$ there is a unique $(w, \epsilon) \in A$ such that $(DF((0, 1), 0))(w, \epsilon) = r$.

In this case, we can find an analytical expression for the pre-image of $r$. Let $(w, \epsilon)$ be defined as:

$$
(w_i, \epsilon_i) = \left(\sum_{j=0}^{\infty}(D\varphi_0(u^0_{i-j}, jh))r_{i-j}^+ - \sum_{j=1}^{\infty}(D\varphi_0(u^0_{i+j}, -jh))r_{i+j}^+, \frac{1}{h}\langle r_{i+1}^+; \partial_h\varphi_0(u^0_i, h)\rangle, \frac{1}{h}\langle r_{i}^--; \partial_h\varphi_0(u^0_i, h)\rangle\right).
$$

(2.22)

We can verify that $w_i - (D\varphi_0(u^0_{i-1}, h))(w_{i-1}) - h\epsilon_{i-1}\partial_h\varphi_0(u^0_{i-1}, h) = r_i$ for all $i$.\(^1\)

We still have to ensure that $(w, \epsilon)$ belongs to $A$. Based on (2.10), we notice that the $w_i$ we have just defined belongs to $V_i = V^+(u^0_i) \oplus V^-(u^0_i)$. Then, thanks to (2.7), we can write $r_i = r_{i-}^+ + r_{i-}^+ + r_{i0}^0$ where $r_{i-}^+ \in V^+(u^0_i)$, $r_{i-}^+ \in V^-(u^0_i)$ and $r_{i0}^0 \in V^0(u^0_i)$. Because $V^+(u)$, $V^-(u)$ and $V^0(u)$ are continuous with respect to $u$ and $\Lambda$ is compact:

$$
\max(\|r_{i-}^+\|, \|r_{i-}^+\|, \|r_{i0}^0\|) \leq \frac{\|r_i\|}{\beta} \leq \|r\|_{\mathbb{B}} \beta \text{ for all } i,
$$

(2.23)

where $\beta > 0$.

\(^1\)Based on the fact that $D\varphi_0(u^0_{i-1}, h)D\varphi_0(u^0_{i-j-1}, jh) = D\varphi_0(u^0_{i-j-1}, (j + 1)h)$ and $D\varphi_0(u^0_{i-1}, h)D\varphi_0(u^0_{i-1+j}, -jh) = D\varphi_0(u^0_{i-1+j}, (-j + 1)h)$.  

28
Consequently, for all $i$:

$$
\|w_i\| \leq \sum_{j=0}^{\infty} \|(D\varphi_0(u^0_{i-j}, jh))r^+_{i-j}\| + \sum_{j=1}^{\infty} \|(D\varphi_0(u^0_{i+j}, -jh))r^+_{i+j}\|,
$$

(2.24)

$$
\leq \sum_{j=0}^{\infty} C\lambda^j \|r^+_{i-j}\| + \sum_{j=1}^{\infty} C\lambda^j \|r^+_{i+j}\|,
$$

(2.25)

$$
\leq \frac{2C}{1 - \lambda^i} \|r\|_B\beta,
$$

(2.26)

because $V^+$ and $V^-$ are invariant under $D\varphi_0$ (property (2.10)). Thus, $w_i$ is uniformly bounded and $w \in V$. In the same way, we show that for all $i$:

$$
\epsilon_i \leq \frac{1}{h} \frac{||r^0_{i+1}||}{\|\partial_h\varphi_0(u^0_i, h)\|^2} \leq \frac{\|r^0_{i+1}\|}{h\|\partial\varphi_0(u^0_i, h)\|^2},
$$

(2.27)

$$
\leq \frac{\|r\|_B}{h\beta m},
$$

(2.28)

where $m = \inf_{u\in\Lambda} \{ f(u, 0) \} > 0$. Consequently, $\epsilon_i$ is uniformly bounded, which leads to $\epsilon \in T$ and $(w, \epsilon) \in A$.

Because of linearity, the uniqueness of $(w, \epsilon)$ such that $(DF((0, 1), 0))(w, \epsilon) = r$ only needs to be proved for $r = 0$. Because $R^m = V^+(u^0_0) \oplus V^-(u^0_0) \oplus V^0(u^0_0)$, $r_i = 0$ is equivalent to $r^+_i = r^-_i = r^0_i = 0$. Thanks to property (2.10), by splitting $w_i = w^+_i + w^-_i$ and knowing that $\epsilon r_{i-1} \partial_h\varphi_0(u^0_{i-1}, h) \in V^0(u^0_i)$, we have:

$$
0 = r^+_i + r^-_i = (w^+_i - (D\varphi_h(u^0_{i-1}, 0))w^+_i) + (w^-_i - (D\varphi_h(u^0_{i-1}, 0))w^-_i),
$$

(2.29)

where the two parentheses are in $V^+(u^0_0)$ and $V^-(u^0_0)$. Again knowing that $R^m = V^+(u^0_0) \oplus V^-(u^0_0) \oplus V^0(u^0_0)$, both parentheses should be equal to zero. This is true for all $i$, so we obtain:

$$
w^+_i = (D\varphi_0(u^0_{i-1}, h))w^+_i = \cdots = (D\varphi^{(r-j)}_0(u^0_j, h))w^+_j,
$$

(2.30)

$$
w^-_i = (D\varphi_0(u^0_{i-1}, h))w^-_i = \cdots = (D\varphi^{(r-j)}_0(u^0_j, h))w^-_j,
$$

(2.31)

for all $j < i$. Based on the properties of uniform hyperbolicity, $\|w^+_j\| \leq C\lambda^{h(i-j)}\|w^+_i\|$
and $\|w_i^\pm\| \leq C \lambda^{h(i-j)} \|w_j^\pm\|$. If for some $j$ we have $w_j^+ \neq 0$, then:

$$\frac{\|w_i\|}{\beta} \geq \|w_j^+\| \geq \frac{\lambda^{h(j-i)}}{C} \|w_j^+\| \quad \text{for all} \quad i > j,$$

(2.32)

which means that $\{w_i, i \in \mathbb{Z}\}$ is unbounded ($0 < \lambda < 1$). Similarly, if $w_i^- \neq 0$ for some $i$ then:

$$\|w_j^+\| \geq \|w_j^\pm\| \geq \frac{\lambda^{h(j-i)}}{C} \|w_j^\pm\| \quad \text{for all} \quad j < i,$$

(2.33)

and $\{w_i, i \in \mathbb{Z}\}$ is also unbounded. Consequently, for $\{w_i\}$ to be bounded we must have $w_i = w_i^+ + w_i^- = 0$ for all $i$.

On the other hand, showing that $\epsilon_i = 0$ is trivial:

$$0 = r^0_i = -h\epsilon_{i-1} \partial_h \varphi_0(u^0_i, h).$$

(2.34)

Because $\|\partial_h \varphi_0(u^0_i, h)\| \geq m > 0$ then $\epsilon_{i-1} = 0$. This is true for all $i$, which means that $\epsilon = 0$. This proves the uniqueness of $(w, \epsilon)$ for $r = 0$.

**Proof (of theorem 2.4.1)** Because $F((0,1), 0) = \{u^0_0 - \varphi_0(u^0_{i-1}, h)\} = 0$, $(0,1)$ is a zero point of $F$ at $s = 0$. Based on this information and on the two previous lemmas, the implicit function theorem states that there exist $M > 0$ such that for all $|s| < M$ there is a unique $(v^s, \tau^s)$ satisfying $\|(v^s, \tau^s)\|_A < M$ and $F((v^s, \tau^s), s) = 0$. Furthermore, this $(v^s, \tau^s)$ is continuously differentiable to $s$, i.e., $\frac{d(v^s, \tau^s)}{ds} \in A$ is continuous with respect to $s$ in the $A$ norm. By the definition of derivatives (in $A$),

$$\frac{d(v^s, \tau^s)}{ds} = \left\{\left(\frac{dv^s_i}{ds}, \frac{d\tau^s_i}{ds}\right)\right\}.$$  

Continuity of $\frac{d(v^s, \tau^s)}{ds}$ in $A$ then implies that $\frac{dv^s_i}{ds}$ and $\frac{d\tau^s_i}{ds}$ are $i$-uniformly continuous with respect to $s$. By defining:

$$\{(u^s_i, \tau^s_i), i \in \mathbb{Z}\} = \{(u^0_i + v^s_i, \tau^s_i), i \in \mathbb{Z}\},$$

(2.35)

we finally obtain the results of theorem (2.4.1).

If we return to the expanded notation of $u_i^s$, this theorem states that for a discretization $\{(u^0_i, \infty), 1\}$ of a continuous trajectory satisfying (2.1) for $s = 0$, there is a
series \{ (u^s_i^{(h,\infty)}, \tau_i^{s(h,\infty)}) \} also being a discretization of a continuous trajectory at nearby values of \( s \). In addition, \{ (u^s_i^{(h,\infty)}, \tau_i^{s(h,\infty)}) \} shadows \{ (u^{0(h,\infty)}_i, 1) \} meaning that \{ (u^s_i^{(h,\infty)}, \tau_i^{s(h,\infty)}) \} is close to \{ (u^{0(h,\infty)}_i, 1) \} when \( s \) is close to 0. In addition, \{ \left( \frac{du_i^{s(h,\infty)}}{ds}, \frac{d\tau_i^{s(h,\infty)}}{ds} \right) \} exists and is \( i \)-uniformly bounded.

The shadowing direction \((v_i^{(h,\infty)}, \eta_i^{(h,\infty)})\) is defined as the uniformly bounded series:

\[
\left\{ (v_i^{(h,\infty)}, \eta_i^{(h,\infty)}) \right\} := \left\{ \left( \frac{du_i^{s(h,\infty)}}{ds}, \frac{d\tau_i^{s(h,\infty)}}{ds} \right) \right\} \in \mathbf{A}. \tag{2.36}
\]

In addition, we can find two constants \( \|v^{(\infty)}\| \) and \( \|\eta^{(\infty)}\| \) independent of \( h \) such that for all \( i \):

\[
v_i^{(h,\infty)} \leq \|v^{(\infty)}\| \quad \text{and} \quad \eta_i^{(h,\infty)} \leq \|\eta^{(\infty)}\|. \tag{2.37}
\]

Please refer to appendix A.1 to see how these constants are built.

### 2.5 A simpler result

In this section, we prove an easier version of Theorem LSS in which we replace the solution \{ \((v_i^{(h,T)}, \eta_i^{(h,T)}), i = 1, ..., \left[ \frac{T}{h} \right] \) \} to the constrained least squares problem (2.5) by the shadowing direction we found earlier \{ \((v_i^{(\infty)}, \eta_i^{(\infty)}), i = 1, ..., \left[ \frac{T}{h} \right] \) \}, which can be written \{ \((v_i^{(h,\infty)}, \eta_i^{(h,\infty)}), i = 1, ..., \left[ \frac{T}{h} \right] \) \} if \( h \) is to be displayed explicitly.

**Theorem 2.5.1** If uniform hyperbolicity holds and \( \varphi_s(\cdot, h) \) is continuously differentiable for all \( h \), then for all continuously differentiable functions \( J : \mathbf{R}^m \times \mathbf{R} \to \mathbf{R} \) whose infinite time average:

\[
\langle J \rangle(s) = \lim_{T \to +\infty} \frac{1}{T} \int_0^T J(u(t), s)dt \quad \text{where} \quad \frac{du}{dt} = f(u, s) \quad \text{and} \quad u(0) = u_0, \tag{2.38}
\]

is independent of the initial state \( u_0 \), let \{ \((v_i^{(h,\infty)}, \eta_i^{(h,\infty)}), i = 1, ..., \left[ \frac{T}{h} \right] \) \} be the se-
sequence of shadowing directions, then:

\[
\frac{d(J)}{ds} = \lim_{h \to 0} \lim_{T \to \infty} \frac{h}{T} \sum_{i=1}^{[\frac{T}{h}]} \left[ (DJ(u_i, 0))v_i^{(h, \infty)} + (\partial_s J(u_i, 0)) + (\eta_i^{(h, \infty)}(J(u_i, 0) - \langle J \rangle(0))) \right],
\]

(2.39)

\[
= \lim_{T \to \infty} \lim_{h \to 0} \frac{h}{T} \sum_{i=1}^{[\frac{T}{h}]} \left[ (DJ(u_i, 0))v_i^{(h, \infty)} + (\partial_s J(u_i, 0)) + (\eta_i^{(h, \infty)}(J(u_i, 0) - \langle J \rangle(0))) \right].
\]

(2.40)

\textbf{Proof} The proof is essentially an exchange of limits through uniform convergence. Because \(\langle J \rangle\) is independent of \(u_0\), we set \(u_0 = u_0^{(h, \infty)}\) as defined in the previous section and we know that \(u_i^{(h, \infty)} = \varphi_i(u_i^{(h, \infty)}, h\tau_i^{(h, \infty)})\). To simplify the notations, \(u_i^{(h, \infty)}\) and \(\tau_i^{(h, \infty)}\) will be expressed as \(u_i^s\) and \(\tau_i^s\) in what follows. The integral could be discretized into an infinite summation that involves the time dilation factors:

\[
\langle J \rangle(s) = \lim_{T \to +\infty} \frac{1}{T} \int_0^T J(u(t), s) \, dt = \lim_{h \to 0} \lim_{T \to +\infty} \frac{1}{T} \sum_{i=1}^{[\frac{T}{h}]} \frac{\tau_i^s J(u_i^s, s)}{\tau_i^s}.
\]

(2.41)

\[
= \lim_{T \to +\infty} \lim_{h \to 0} \frac{1}{T} \sum_{i=1}^{[\frac{T}{h}]} \frac{\tau_i^s J(u_i^s, s)}{\tau_i^s}.
\]

(2.42)

The two limits can be permuted at will, but we will only keep one notation for the
remainder of the proof. We can write:

\[
\frac{d\langle J \rangle}{ds}_{s=0} = \lim_{s \to 0} \frac{\langle J(s) - \langle J \rangle(0) \rangle}{s},
\]

\[
= \lim_{s \to 0} \lim_{h \to 0} \lim_{T \to +\infty} \left( \frac{1}{s} \sum_{i=1}^{[\frac{1}{h}]} \frac{h \tau^*_i J(u^*_i, s) - h J(u^*_i, 0)}{s} \right),
\]

\[
= \lim_{s \to 0} \lim_{h \to 0} \lim_{T \to +\infty} \left( \frac{1}{s} \sum_{i=1}^{[\frac{1}{h}]} \frac{h \tau^*_i J(u^*_i, s) - h J(u^*_i, 0)}{s} - \frac{h J(u^*_i, 0) - h J(u^*_i, 0)}{T} \right),
\]

\[
= \lim_{s \to 0} \lim_{h \to 0} \lim_{T \to +\infty} \left( \frac{1}{s} \sum_{i=1}^{[\frac{1}{h}]} \frac{h J(u^*_i, s) - J(u^*_i, 0) + (\tau^*_i - 1) J(u^*_i, s)}{s} \right),
\]

\[
- \frac{(h \sum_j (\tau^*_j - 1)) \times h J(u^*_i, 0)}{T(h \sum_j \tau^*_j)},
\]

\[
= \lim_{s \to 0} \lim_{h \to 0} \lim_{T \to +\infty} \left( \frac{1}{s} \sum_{i=1}^{[\frac{1}{h}]} \frac{h J(u^*_i, s) - J(u^*_i, 0) + (\tau^*_i - 1) J(u^*_i, s)}{T + h \sum_j (\tau^*_j - 1)} \right),
\]

\[
- \frac{(h \sum_j (\tau^*_j - 1)) \times h J(u^*_i, 0)}{T(T + h \sum_j (\tau^*_j - 1))},
\]

\[
= \lim_{s \to 0} \lim_{h \to 0} \lim_{T \to +\infty} \left( \frac{h \sum_{i=1}^{[\frac{1}{h}]} (J(u^*_i, s) - J(u^*_i, 0))}{s} + O(s) \right),
\]

\[
+ \lim_{s \to 0} \lim_{h \to 0} \lim_{T \to +\infty} \left( \frac{h \tau^*_i}{T} \sum_{i=1}^{[\frac{1}{h}]} J(u^*_i, s) - \frac{1}{T} \sum_j h J(u^*_i, 0)) + O(s) \right).
\]

Let us eliminate \( \lim_{s \to 0} \) in the first term. We define:

\[
\gamma_i^s = \frac{dJ(u^*_i, s)}{ds} = (D J(u^*_i, s)) \frac{du^*_i}{ds} + \partial s J(u^*_i, s).
\]

(2.43)

Then, thanks to the mean value theorem, for all \( i \) there exist a \( \xi_i(s) \in [0, s] \) such that:

\[
\frac{(J(u^*_i, s) - J(u^*_i, 0))}{s} = \gamma_i^s(s).
\]

(2.44)

Consequently:

\[
\lim_{s \to 0} \lim_{h \to 0} \lim_{T \to +\infty} \left( \frac{h \sum_{i=1}^{[\frac{1}{h}]} (J(u^*_i, s) - J(u^*_i, 0))}{s} \right) = \lim_{s \to 0} \lim_{h \to 0} \lim_{T \to +\infty} \left( \frac{h \sum_{i=1}^{[\frac{1}{h}]} \gamma_i^s(s)}{s} \right).
\]

(2.45)

We can choose a neighborhood of \( \Lambda \times \{0\} \) that contains \( (u^*_i, s) \) for all \( i \) (for \( s \) sufficiently
small) and in which both \((DJ(u, s))\) and \(\partial_s J(u, s)\) are uniformly continuous. Because the \(\frac{du^i}{ds}\) are \(i\)-uniformly continuous and bounded, for all \(\epsilon > 0\) there exists \(M > 0\) such that for all \(|\xi| < M:\)

\[
\|\gamma_i^\xi - \gamma_i^0\| < \epsilon \quad \forall i.
\]

Thus, for all \(|s| < M, |\xi_i(s)| \leq |s| < M\) for all \(i\), therefore for all \(h, T\) \((h << T)\):

\[
\left\| \frac{h}{T} \sum_{i=1}^{\frac{k}{h}} \gamma_i^\xi(s) - \frac{h}{T} \sum_{i=1}^{\frac{k}{h}} \gamma_i^0 \right\| \leq \frac{h}{T} \sum_{i=1}^{\frac{k}{h}} \|\gamma_i^\xi(s) - \gamma_i^0\| < \epsilon. \tag{2.46}
\]

Hence,

\[
\left\| \lim_{h \to 0} \lim_{T \to +\infty} \left( \frac{h}{T} \sum_{i=1}^{\frac{k}{h}} \gamma_i^\xi(s) \right) - \lim_{h \to 0} \lim_{T \to +\infty} \left( \frac{h}{T} \sum_{i=1}^{\frac{k}{h}} \gamma_i^0 \right) \right\| \leq \epsilon. \tag{2.47}
\]

Finally,

\[
\lim_{s \to 0} \lim_{h \to 0} \lim_{T \to +\infty} \left( \frac{h}{T} \sum_{i=1}^{\frac{k}{h}} \gamma_i^\xi(s) \right) = \lim_{h \to 0} \lim_{T \to +\infty} \left( \frac{h}{T} \sum_{i=1}^{\frac{k}{h}} \gamma_i^0 \right), \tag{2.48}
\]

which gives us the desired result for the first term via the definition of \(\gamma_i^0\).

For the second term, \(J\) is continuously differentiable thus continuous and the \((u^i_s, \tau^i_s)\) are \(i\)-uniformly continuously differentiable and bounded. Based on that, for \(s\) sufficiently small, we can find a compact neighborhood of \(\Lambda \times \{0\}\) that contains \((u^i_s, s)\) for all \(i \in \mathbb{Z}\) and in which \(J(u, s)\) will be uniformly continuous. Consequently, the sequence \(\left\{ \frac{h(\tau^i_s - 1)}{T_s} J(u^i_s, s), i \in \mathbb{Z} \right\}\), which can be written \(\left\{ \frac{h(\tau^i_s - 0)}{T_s} J(u^i_s, s), i \in \mathbb{Z} \right\}\) converges uniformly to \(\left\{ \frac{h}{T} J(u^0_s, s), i \in \mathbb{Z} \right\}\) when \(s\) goes to 0. Because the term \(\frac{1}{T} \sum_j hJ(u^0_i, 0)\) does not depend on \(s\) at all, we finally have:

\[
\lim_{s \to 0} \lim_{h \to 0} \lim_{T \to +\infty} \left( \frac{h(\tau^i_s - 1)}{T_s} \left( J(u^i_s, s) - \frac{1}{T} \sum_j hJ(u^0_i, 0) \right) \right) = \lim_{h \to 0} \lim_{T \to +\infty} \left( \frac{h}{T} - \frac{1}{T} (J(u^0_i, 0) - \langle J \rangle(0)) \right),
\]

which concludes the proof.
### 2.6 Computational approximation of the shadowing direction

The main task of this section is to provide a bound for:

\[
\varepsilon_i^{\{h,T\}} = v_i^{\{h,T\}} - v_i^{\{h,\infty\}},
\]

\[
\varepsilon_i^{\{h,T\}} = \eta_i^{\{h,T\}} - \eta_i^{\{h,\infty\}},
\]

for \(i = 1, \ldots, \frac{T}{h}\), where the \(v_i^{\{h,T\}}, \eta_i^{\{h,T\}}\) are the solution to the least squares problem:

\[
\min \sum_{i=1}^{\left\lfloor \frac{T}{h} \right\rfloor} (||v_i^{\{h,T\}}||^2 + \alpha(\eta_i^{\{h,T\}})^2),
\]

s.t. \(v_i^{\{h,T\}} = (D\varphi_s(u_i, h))v_i^{\{h,T\}} + (\partial_s\varphi_s(u_i, h)) + h\eta_i^{\{h,T\}}\partial_h\varphi_s(u_i, h).\) \hspace{1cm} (2.52)

The shadowing lemma guarantees the existence of a shadowing trajectory, but provides no clear way to compute \(\{(v_i^{\{h,\infty\}}, \eta_i^{\{h,\infty\}})\}\). This section suggests that the solution to the least squares problem gives a useful approximation of the shadowing trajectory allowing us to compute \(\frac{d(J_s)}{ds}\). Without loss of generality, we consider that \(s = 0\) in (2.52). By definition, the shadowing trajectory satisfies:

\[
u_i^{s\{h,\infty\}} = \varphi_s(u_i^{s\{h,\infty\}}, h\tau_i^{s\{h,\infty\}}).
\]

(2.53)

After taking the derivative to \(s\) on both sides for \(s = 0\), we obtain:

\[
v_i^{\{h,\infty\}} = (D\varphi_0(u_i, h))v_i^{\{h,\infty\}} + \frac{\partial \varphi_0}{\partial s}(u_i, h) + h\eta_i^{\{h,\infty\}}\partial_h\varphi_0(u_i, h).
\]

(2.54)

Thus, the shadowing direction satisfies the constraint in equation (2.51) and:

\[
\sum_{i=1}^{\left\lfloor \frac{T}{h} \right\rfloor} (||v_i^{\{h,T\}}||^2 + \alpha(\eta_i^{\{h,T\}})^2) \leq \sum_{i=1}^{\left\lfloor \frac{T}{h} \right\rfloor} (||v_i^{\{h,\infty\}}||^2 + \alpha(\eta_i^{\{h,\infty\}})^2) \leq \frac{T}{h} (||v^{\{\infty\}}||^2 + \alpha||\eta^{\{\infty\}}||^2).
\]

(2.55)
Consequently:

\[
\max_i ||\eta_i^{(h,T)}|| \leq \sqrt{\frac{T}{h}} \left( \frac{||v^{(\infty)}||^2_B}{\alpha} + ||\eta^{(\infty)}||^2 \right)^{\frac{1}{2}},
\]

(2.56)

because \(\epsilon_i^{(h,T)} = \eta_i^{(h,T)} - \eta_i^{(h,\infty)}\):

\[
\max_i ||\epsilon_i^{(h,T)}|| \leq \sqrt{\frac{T}{h}} \left( \frac{||v^{(\infty)}||^2_B}{\alpha} + ||\eta^{(\infty)}||^2 \right)^{\frac{1}{2}} + ||\eta^{(\infty)}||.
\]

(2.57)

We can get a similar bound for \(\max_i ||\epsilon_i^{(h,T)0}||\):

\[
\max_i ||\epsilon_i^{(h,T)0}|| \leq \sqrt{\frac{T}{h}} \left( \frac{||v^{(\infty)}||^2_B}{\alpha} + \alpha ||\eta^{(\infty)}||^2 \right)^{\frac{1}{2}} + \frac{||v^{(\infty)}||}{\gamma}.
\]

(2.58)

Concerning \(\max_i ||\epsilon_i^{(h,T)+}||\) and \(\max_i ||\epsilon_i^{(h,T)-}||\), combining the constraint equation (2.52) as well as (2.54) we obtain:

\[
\begin{align*}
\epsilon_{i+1}^{(h,T)+} &= D\varphi_0(u, h)\epsilon_i^{(h,T)+} \\
\epsilon_{i+1}^{(h,T)-} &= D\varphi_0(u, h)\epsilon_i^{(h,T)-}
\end{align*}
\]

Thus, because \(\epsilon_i^{(h,T)+} \in V^+(u_i), \epsilon_i^{(h,T)-} \in V^-(u_i)\) and based on the following definition of the unstable and stable subspaces:

\[
V^+(u) := \{v \in \mathbb{R}^m/ \|(D\varphi_0(u, t))v\| \leq C\lambda^{-t}||v||, \forall t < 0\},
\]

(2.59)

\[
V^-(u) := \{v \in \mathbb{R}^m/ \|(D\varphi_0(u, t))v\| \leq C\lambda^t||v||, \forall t > 0\},
\]

(2.60)

we obtain:

\[
\max_i ||\epsilon_i^{(h,T)+}|| \leq \max(1, C)||\epsilon_i^{(h,T)+}||,
\]

(2.61)

\[
\max_i ||\epsilon_i^{(h,T)-}|| \leq \max(1, C)||\epsilon_i^{(h,T)-}||.
\]

(2.62)
In addition to that, \( \varphi_0(u, 0) = u \), which means that \( D\varphi_0(u, 0) = I \) where \( I \) is the identity operator in \( \mathbb{R}^m \). For \( u \in \Lambda, h \in H \) and \( s \in S \) where \( H \) and \( S \) are compact sets containing \( h = 0 \) and \( s = 0 \), we can find a positive constant \( K \) such that:

\[
\| \partial_h D\varphi_0(u, h) \| \leq K, \tag{2.63}
\]

because \( \varphi(\cdot, \cdot) \) is \( C^2 \). \( \partial_h D\varphi_0(u, h) \) belongs to a space of finite dimension so all norms are equivalent and any choice of norm \( \| \cdot \| \) is valid. For a sufficiently small \( h \) such that \( hK < 1 \), we get:

\[
\|(D\varphi_0(u, h))v\| \geq (1 - hK)\|v\|, \tag{2.64}
\]

for all \( v \in \mathbb{R}^m \). Consequently:

\[
\sum_{i=1}^{[\frac{T}{2}]} \|e_i^{(h,T)}\|^2 \geq \sum_{i=1}^{[\frac{T}{2}]} (1 - hK)^2(i-1)\|e_i^{(h,T)}\|^2, \tag{2.65}
\]

\[
\geq \|e_1^{(h,T)}\|^2 \frac{1 - (1 - hK)^2[\frac{T}{2}]}{h(2K - hK^2)}. \tag{2.66}
\]

which means that:

\[
\|e_1^{(h,T)}\|^2 \leq \frac{h(2K - hK^2)}{1 - (1 - hK)^2[\frac{T}{2}]} \sum_{i=1}^{[\frac{T}{2}]} \|e_i^{(h,T)}\|^2, \tag{2.67}
\]

\[
\leq \frac{h(2K - hK^2)}{1 - e^{-2TK}} \sum_{i=1}^{[\frac{T}{2}]} \|e_i^{(h,T)}\|^2 \leq \frac{2hK}{1 - e^{-2TK}} \sum_{i=1}^{[\frac{T}{2}]} \|e_i^{(h,T)}\|^2. \tag{2.68}
\]

For \( T \) sufficiently large, \( e^{-2KT} < \frac{1}{2} \), which means that:

\[
\|e_1^{(h,T)}\|^2 \leq 4hK \sum_{i=1}^{[\frac{T}{2}]} \|e_i^{(h,T)}\|^2. \tag{2.69}
\]

Because \( e_i^{(h,T)} = v_i^{(h,T)} - v_i^{(h,\infty)} \) then:

\[
\|e_i^{(h,T)}\|^2 \leq 2\left(\|v_i^{(h,T)}\|^2 + \|v_i^{(h,\infty)}\|^2\right) \leq \frac{2}{\gamma} \left(\|v_i^{(h,T)}\|^2 + \|v_i^{(h,\infty)}\|^2\right), \tag{2.70}
\]
leading to:

\[
\| e_i^{(h,T)^-} \|^2 \leq \frac{8hK}{\gamma} \sum_{i=1}^{\bar{k}} (\| u_i^{(h,T)} \|^2 + \| v_i^{(h,\infty)} \|^2),
\]

(2.71)

\[
\leq \frac{8hK}{\gamma} \times \frac{T}{h} (2\| \mathbf{v}^{(\infty)} \|_B^2 + \alpha \| \eta^{(\infty)} \|_B^2).
\]

(2.72)

Finally:

\[
\max_i \| e_i^{(h,T)^-} \| \leq \sqrt{T} \times \max(1, C) \times \left( \frac{8K}{\gamma} \times (2\| \mathbf{v}^{(\infty)} \|_B^2 + \alpha \| \eta^{(\infty)} \|_B^2) \right)^{\frac{1}{2}},
\]

(2.73)

\[
\leq E\sqrt{T},
\]

(2.74)

where \( E = \max(1, C) \times \left( \frac{8K}{\gamma} \times (2\| \mathbf{v}^{(\infty)} \|_B^2 + \alpha \| \eta^{(\infty)} \|_B^2) \right)^{\frac{1}{2}} \) is a constant that does not depend on \( h \) nor on \( T \). In the same way we obtain:

\[
\max_i \| e_i^{(h,T)^+} \| \leq E\sqrt{T}.
\]

(2.75)

Even though the bounds we found for \( \eta_i^{(h,T)} \), \( e_i^{(h,T)^0} \), \( e_i^{(h,T)^+} \) and \( e_i^{(h,T)^-} \) may depend on \( T \) and/or \( h \), we will see in the next section that they are strong enough to prove the convergence of the algorithm. Furthermore, experimental simulations have shown that \( e_i^{(h,T)} \) and \( \eta_i^{(h,T)} \) do not necessarily grow when \( h \to 0 \), \( T \to \infty \) and stay bounded [23].

### 2.7 Convergence of least squares shadowing

In this section, we use the results obtained previously to prove our initial theorem:

**Theorem 2.7.1 (THEOREM LSS)** For a \( C^2 \) map \( \varphi(\cdot, \cdot) \) and a \( C^1 \) cost function
\[ \frac{d(J)}{ds} = \lim_{h \to 0} \lim_{T \to \infty} \frac{h}{T} \sum_{i=1}^{\left\lceil \frac{T}{h} \right\rceil} \left[ (DJ(u_i, s))v_i^{(h,T)} + (\partial_s J(u_i, s)) + \left( \eta_i^{(h,T)}(J(u_i, s) - (J)(s)) \right) \right], \]

\[ = \lim_{T \to \infty} \lim_{h \to 0} \frac{h}{T} \sum_{i=1}^{\left\lceil \frac{T}{h} \right\rceil} \left[ (DJ(u_i, s))v_i^{(h,T)} + (\partial_s J(u_i, s)) + \left( \eta_i^{(h,T)}(J(u_i, s) - (J)(s)) \right) \right]. \]

**Proof** Because \( J \) is \( C^1 \) and \( \Lambda \) is compact, \( (DJ(u_i, 0)) \) is uniformly bounded, i.e., there exists a constant \( A \) such that \( \|DJ(u_i, 0)\| < A \) for all \( i \). Let \( e_i^{(h,T)} \) be defined as in the previous section, then:

\[
\left| \frac{h}{T} \sum_{i=1}^{\left\lceil \frac{T}{h} \right\rceil} \left[ (DJ(u_i, s))v_i^{(h,T)} + (\partial_s J(u_i, s)) + \left( \eta_i^{(h,T)}(J(u_i, s) - (J)(s)) \right) \right] \right| \leq T \left( \sum_{i=1}^{\left\lceil \frac{T}{h} \right\rceil} \right) \left\| DJ(u_i, s) \right\| \left\| v_i^{(h,T)} \right\| + \left\| (\partial_s J(u_i, s)) \right\| + \left\| \eta_i^{(h,T)}(J(u_i, s) - (J)(s)) \right\| ,
\]

\[ \leq \frac{h}{T} \sum_{i=1}^{\left\lceil \frac{T}{h} \right\rceil} \left[ (DJ(u_i, s))e_i^{(h,T)} + (e_i^{(h,T)})(J(u_i, s) - (J)(s)) \right], \]

\[ = \frac{h}{T} \sum_{i=1}^{\left\lceil \frac{T}{h} \right\rceil} \left[ (DJ(u_i, s))e_i^{(h,T)} + (e_i^{(h,T)})(J(u_i, s) - (J)(s)) \right], \]

\[ < \frac{h}{T} \sum_{i=1}^{\left\lceil \frac{T}{h} \right\rceil} \left[ (DJ(u_i, s))e_i^{(h,T)} + (e_i^{(h,T)})(J(u_i, s) - (J)(s)) \right] + \frac{h}{T} \sum_{i=1}^{\left\lceil \frac{T}{h} \right\rceil} \left[ (DJ(u_i, s))e_i^{(h,T)} + (e_i^{(h,T)})(J(u_i, s) - (J)(s)) \right]. \]

For the first term:

\[
\left| \frac{h}{T} \sum_{i=1}^{\left\lceil \frac{T}{h} \right\rceil} \left[ (DJ(u_i, s))e_i^{(h,T)} + (e_i^{(h,T)})(J(u_i, s) - (J)(s)) \right] \right| \leq \frac{h}{T} \sum_{i=1}^{\left\lceil \frac{T}{h} \right\rceil} \left\| (DJ(u_i, s)) \right\| \left\| e_i^{(h,T)} \right\| \leq \frac{h}{T} \sum_{i=1}^{\left\lceil \frac{T}{h} \right\rceil} \left\| (DJ(u_i, s)) \right\| \left\| e_i^{(h,T)} \right\| + \frac{h}{T} \sum_{i=1}^{\left\lceil \frac{T}{h} \right\rceil} \left\| (DJ(u_i, s)) \right\| \left\| e_i^{(h,T)} \right\| ,
\]

\[ \leq \frac{h}{T} \sum_{i=1}^{\left\lceil \frac{T}{h} \right\rceil} \left\| (DJ(u_i, s)) \right\| \left\| e_i^{(h,T)} \right\| + \frac{h}{T} \sum_{i=1}^{\left\lceil \frac{T}{h} \right\rceil} \left\| (DJ(u_i, s)) \right\| \left\| e_i^{(h,T)} \right\| . \]
\[
\leq A_h^\frac{h}{T} \left( \sum_{i=1}^{[\frac{T}{h}]} C\lambda_i^{h(i-1)} \|e_i^{(h,T)}\| + \sum_{i=1}^{[\frac{T}{h}]} C\lambda_i^{h(i-1)} \|e_0^{(h,T)}\| \right),
\]
(2.83)
\[
\leq \frac{h}{T} \frac{2AC}{(1 - \lambda^h)} \times E\sqrt{T},
\]
(2.84)
\[
\leq \frac{1}{\sqrt{T}} \times \frac{2AC}{\log(\frac{t}{h})},
\]
(2.85)

which goes to 0 when \( T \) increases. Thus, we notice that, in the stable and unstable subspaces, the difference \( e_i^{(h,T)} \) between the shadowing trajectory \( v_i^{(h,\infty)} \) and its approximation \( v_i^{(h,T)} \) decreases extremely fast so that the whole term \( h \sum_{i=1}^{[\frac{T}{h}]} (DJ(u_i, s))(e_i^{(h,T)} + e_i^{(h,T)}) \) tends to 0.

The situation is more complicated for the second term because there is no reason for \( e_i^{(h,T)} \) and \( e_i^{(h,T)} \) to decrease when \( T \) increases. The cancellation of the second term is the result of the mutual cancellation of the elements in the summation, as we shall see. Based on the sampling points \( \{(u_i, \tau_i, s^{(h,\infty)} + s e_i^{(h,T)})\} \) for the continuous shadowing trajectory found in Section 2.4, we consider the new set of sampling points \( \{(u_i, \tau_i, s^{(h,\infty)} + s e_i^{(h,T)})\} \), which satisfy the following relation:

\[
\lim_{s \to 0} \frac{u_i - u_i}{s} = e_i^{(h,T)}
\]
(2.86)

for all \( i \). We can notice that the new sampling points describe the same continuous trajectory as the old set of values. Assuming that \( e_i^{(h,T)} \) and \( e_i^{(h,T)} \) are bounded, we have for a sufficiently small \( s \):

\[
(J)(s) = \lim_{h \to 0} \lim_{T \to +\infty} \sum_{i=0}^{[\frac{T}{h}]} \frac{h(\tau_i + s e_i^{(h,T)}), J(u_i, s)}{h \sum_j(\tau_j + s e_j^{(h,T)})}.
\]
(2.87)

We would obtain by following the same operations we did in Section 2.5 (but
(upside down this time): 

\[
\lim_{h \to 0} \lim_{T \to \infty} \left( \frac{h}{T} \sum_{i=1}^{[T]} \left( (DJ(u_i, s))e_i^{(h,T)} + \left( e_i^{(h,T)}(J(u_i, s) - \langle J \rangle(s)) \right) \right) \right) 
\]

\[= \lim_{h \to 0} \lim_{T \to \infty} \lim_{s \to 0} \left( \frac{h}{T} \sum_{i=0}^{[T]} \frac{(J(u_i^s, s) - J(u_i^s, s))}{s} \right) \]

\[+ \lim_{h \to 0} \lim_{T \to \infty} \lim_{s \to 0} \left( \frac{h\epsilon_i^{(h,T)}}{T} \left( J(u_i^s, s) - \frac{1}{T} \sum_j hJ(u_i^s, s) \right) \right) \]

\[= \lim_{h \to 0} \lim_{T \to \infty} \lim_{s \to 0} \left( \frac{1}{s} \sum_{i=0}^{[T]} \frac{h(\tau_{i}^s + s\epsilon_i^{(h,T)})J(u_i^s, s)}{h \sum_j (\tau_j^s + s\epsilon_j^{(h,T)})} - \frac{h\tau_{i}^s J(u_i^s, s)}{h \sum_j \tau_j^s} \right) + O(s) \]

\[= \lim_{s \to 0} \lim_{h \to 0} \lim_{T \to \infty} \left( \frac{1}{s} \sum_{i=0}^{[T]} \frac{h(\tau_{i}^s + s\epsilon_i^{(h,T)})J(u_i^s, s)}{h \sum_j (\tau_j^s + s\epsilon_j^{(h,T)})} - \frac{h\tau_{i}^s J(u_i^s, s)}{h \sum_j \tau_j^s} \right) + O(s) \]

\[= \lim_{s \to 0} \frac{\langle J \rangle(s) - \langle J \rangle(s)}{s} + O(s) = 0 \]

However, this is not necessarily true because \(e_i^{(h,T)}\) and \(\epsilon_i^{(h,T)}\) may grow as \(\frac{T}{h}\) increases. Permuting the limits is much more delicate but is still possible. Please refer to Appendix A.2 for further details about how to permute the limits. The idea is to use the relation:

\[
\sum_{i=1}^{[T]} \left( \|v_i^{(h,T)}\|^2 + \alpha(\eta_i^{(h,T)})^2 \right) \leq \sum_{i=1}^{[T]} \left( \|v_i^{(h,\infty)}\|^2 + \alpha(\eta_i^{(h,\infty)})^2 \right) \leq \frac{T}{h} \left( \|v^{(\infty)}\|^2_B + \alpha\|\eta^{(\infty)}\|^2 \right) \]

(2.94)

to show that most \(e_i^{(h,T)}\), \(\epsilon_i^{(h,T)}\) remain bounded and that the contribution of the unbounded terms fades out.
In conclusion:

\[
\frac{d(J)}{ds} - h \sum_{i=1}^{\left\lceil \frac{T}{h} \right\rceil} \left[ (DJ(u_i, s))u_i^{h,T} + (\partial_s J(u_i, s)) + \left( \eta_i^{h,T} (J(u_i, s) - \langle J \rangle(s)) \right) \right],
\]

(2.95)

\[
\leq \left| \frac{d(J)}{ds} - h \sum_{i=1}^{\left\lceil \frac{T}{h} \right\rceil} \left[ (DJ(u_i, s))u_i^{h,\infty} + (\partial_s J(u_i, s)) + \left( \eta_i^{h,\infty} (J(u_i, s) - \langle J \rangle(s)) \right) \right] \right|
\]

(2.96)

\[
+ \frac{h}{T} \sum_{i=1}^{\left\lceil \frac{T}{h} \right\rceil} \left[ (DJ(u_i, s))u_i^{h,T} + (\partial_s J(u_i, s)) + \left( \eta_i^{h,T} (J(u_i, s) - \langle J \rangle(s)) \right) \right]
\]

(2.97)

\[
- \frac{h}{T} \sum_{i=1}^{\left\lceil \frac{T}{h} \right\rceil} \left[ (DJ(u_i, s))u_i^{h,\infty} + (\partial_s J(u_i, s)) + \left( \eta_i^{h,\infty} (J(u_i, s) - \langle J \rangle(s)) \right) \right]
\]

(2.98)

(2.99)

and we have shown that both terms go to 0 as \( T \to \infty \) and \( h \to 0 \). This concludes the proof.

2.8 The algorithm in practice

As we have shown through this chapter, LSS gives us a good estimation for \( \frac{d(J)}{ds} \) when the dynamical system is uniformly hyperbolic. After running a simulation for a given \( s \), an arbitrary initial condition \( u_0 \) and a uniform time step size of \( h \), we obtain a sequence of reference sampling points\(^2\) \( \{u_i^h, i = 1, \ldots, \frac{T}{h}\} \). If we had access to the shadowing direction, we would easily compute:

\[
\frac{d(J)}{ds} \approx \frac{h}{T} \sum_{i=1}^{\left\lceil \frac{T}{h} \right\rceil} \left[ (DJ(u_i^h, s))u_i^{h,\infty} + (\partial_s J(u_i^h, s)) + \left( \eta_i^{h,\infty} (J(u_i^h, s) - \langle J \rangle(s)) \right) \right].
\]

(2.100)

\(^2\)In practice, we can rule out the first hundred sampling points to be sure that we have reached the attractor \( \Lambda \)
However, in real-life problems we usually do not have access to the stable and unstable subspaces around each $u^t$, prohibiting use of the closed form expression of $\nu_i^{(h, \infty)}$ and $\eta_i^{(h, \infty)}$. Thus, we have no other choice than computing an approximation of the shadowing direction. This approximation is given by the solution to the least squares problem:

$$\min \sum_{i=1}^{[\frac{T}{h}]} (\|v_i^{(h,T)}\|^2 + \alpha(\eta_i^{(h,T)})^2)$$

s.t. $v_i^{(h,T)} = (D\varphi_s(u_i^s, h))v_i^{(h,T)} + \partial_s \varphi_s(u_i^s, h) + h\eta_i^{(h,T)} \partial_h \varphi_s(u_i^s, h)$.

After solving this quadratic optimization problem, we estimate $\frac{d(J)}{ds}$ using expression (2.100) again where the $(\nu_i^{(h, \infty)}, \eta_i^{(h, \infty)})$ are replaced by $(\nu_i^{(h,T)}, \eta_i^{(h,T)})$. As we have seen previously, this estimation converges to the real value of $\frac{d(J)}{ds}$ when the time step size $h$ is refined and the integration lapse $T$ increases.
Chapter 3

Simplified Least Squares
Shadowing

In the above version of LSS, corrective time dilation factors $\eta$ have to be introduced to ensure its convergence, but these same terms lead to a heavier and more expensive system of equations to solve. In this chapter, we introduce a modified version of LSS in which the introduction of the time dilation factors is replaced by a simple windowing procedure: the result of the non-corrected system of equations is multiplied by a specific windowing function. This procedure has been used for systems that have a periodic behavior [29], but we will show that the fundamental idea is still valid in our framework and can be transposed to chaotic dynamical systems. Because this "windowing" operation is almost costless, the new algorithm is more efficient than standard LSS.

First, we introduce the new algorithm in both its tangent and adjoint versions. Then, the underlying theory of the algorithm is presented and we prove that the result given by simplified LSS converges to the result given by the original algorithm when the integration time goes to infinity. Finally, the last section is dedicated to a numerical application of the new algorithm using the Lorenz 63 test case dynamical system.
3.1 Tangent and adjoint algorithms of the simplified Least Squares Shadowing method

We consider the family of ergodic dynamical systems satisfying a differential equation parameterized by $s$:

$$\frac{du}{dt} = f(u, s), \quad (3.1)$$

where $f$ is smooth with respect to both $u$ and $s$. The derivative of $\frac{ds}{ds}$ can be approximated by the following three steps:

1. Integrate equation (3.1) until the initial transient behavior has passed. Then further integrate the equation over a period of $T$, which should be a multiple of the longest time scales in its solution. Store the trajectory of the second time integration as $u(t), 0 < t < T$.

2. Find a function $\tilde{v}(t), 0 < t < T$ with the least $L^2$ norm that satisfies the linearized equation

$$\frac{d\tilde{v}}{dt} = f_u \tilde{v} + f_s, \quad (3.2)$$

where the time-dependent Jacobians $f_u := \frac{\partial f}{\partial u}$ and $f_s := \frac{\partial f}{\partial s}$ are based on the trajectory obtained in the previous step. Notice that equation (3.2) does not include the dilation term. Consequently, $\tilde{v}(t)$ is different from the shadowing direction $v(t)$. This $\tilde{v}(t)$ can be found by solving a system of linear equations derived from the KKT conditions of the constrained least squares problem:

$$\begin{cases}
\frac{d\dot{w}}{dt} = f_u \ddot{v} + f_s, \\
\frac{d\tilde{w}}{dt} = -f_u^T \dot{w} + \ddot{v}, \\
\tilde{w}(0) = \tilde{w}(T) = 0.
\end{cases} \quad (3.3)$$

3. Approximate the derivative of $\langle J \rangle(s)$ by computing a windowed time-average:

$$\frac{d\langle J \rangle}{ds} \approx \frac{1}{T} \int_0^T w\left(\frac{t}{T}\right) (DJ\tilde{v} + \partial_s J) dt, \quad (3.4)$$
where \( w \), the window function, is a scalar function in \([0, 1]\) satisfying

(a) \( w \) continuously differentiable,
(b) \( w(0) = w(1) = 0 \),
(c) \( \int_0^1 w(s) \, ds = 1 \).

An example satisfying all three criteria is \( w(s) = 1 - \cos 2\pi s \).

This resulting derivative approximation converges to the true derivative as \( T \to \infty \), as mathematically derived in Section 3.2 and under the same assumptions as the original Least Squares Shadowing method.

In the algorithm above, the cost of solving the constrained least squares problem (3.3) scales with the dimension of \( s \), and is independent of the dimension of \( J \). Such an algorithm, which favors a low-dimensional parameter \( s \) and a high-dimensional quantity of interest \( J \), can be categorized as a tangent method in sensitivity analysis. A corresponding adjoint method can be derived, whose computation cost favors a high-dimensional \( s \) and a low-dimensional \( J \). This adjoint algorithm, also consists of three steps:

1. Obtain a trajectory \( u(t) \), \( 0 \leq t \leq T \) in the same way as Step 1 of the previous algorithm.

2. Solve the system of linear equations

\[
\begin{align*}
\frac{d\hat{w}}{dt} &= f_u \hat{w}, \\
\frac{d\hat{v}}{dt} &= -f_u^T \hat{v} + \hat{w} + w(\frac{t}{T})DJ, \\
\hat{v}(0) &= \hat{v}(T) = 0,
\end{align*}
\]  

(3.5)

where \( w(s) \), \( 0 \leq s \leq 1 \) is a scalar windowing function satisfying the criteria described in Step 3 of the previous algorithm. This system of linear differential equations is the dual of the system in Step 2 of the previous algorithm, derived by combining it with Equation (3.4) and integrating by parts.
3. Approximate the derivative of $(J)(s)$ by the following equation, derived together with Equations (3.5) in Step 2:

$$\frac{d(J)}{ds} \approx \frac{1}{T} \int_0^T \left( DT^T \dot{\phi} + \partial_s J \right) dt.$$  

(3.6)

We can show that this adjoint algorithm produces a consistent approximation to that produced by the tangent algorithm. The approximated $\frac{d(J)}{ds}$ should be the same if the differential equations are solved exactly in both algorithms, and the integrals are evaluated exactly. With such exact numerics, the error in the approximation is solely due to the infeasibility of using an infinite $T$, and should diminish as $T \to \infty$. This error depends on the trajectory $u(t)$, but does not depend on whether the tangent or adjoint algorithm is used. In what follows, we mostly analyze the tangent algorithm, but the conclusions are also valid for the adjoint version because both algorithms approximate the derivative in a consistent way.

### 3.2 How windowing mitigates the effect of time dilation

The new method is similar to the original Least Squares Shadowing method, except for two major differences. The first difference is the use of a smooth windowing function $w$ satisfying

$$w(0) = w(1) = 0 \quad \text{and} \quad \int_0^1 w(s) ds = 1;$$

which averages to 1 and tapers off to 0 at both ends of the interval $[0, 1]$. The second difference is the lack of a time dilation term in Equation (3.3) (Equation (3.5) for the adjoint version). Removal of the time dilation term can simplify the implementation of a chaotic sensitivity analysis capability for many solvers.
With *standard LSS*, the desired derivative is computed as follows:

$$\frac{d\langle J \rangle}{ds} = \langle DJv \rangle + \langle \partial_s J \rangle + \langle \eta J \rangle - \langle \eta \rangle \langle J \rangle,$$

(3.7)

to account for the time dilation effect of $\eta$. *Simplified LSS* avoids time dilation by only computing an approximation of $v$ instead of the uniformly bounded pair $(v, \eta)$. This new quantity, denoted $\tilde{v}_\tau$, is equal to:

$$\tilde{v}_\tau(t) = v(t) - f(t) \int_\tau^t \eta(\tau)d\tau,$$

(3.8)

for some $\tau$, where $f(t)$ denotes $f(u(t; s), s) = \frac{du}{dt}$. In general, $\tilde{v}_\tau$ has linear growth with respect to time due to the second term in equation (3.8). Using the fact that $\frac{df}{dt} = f_u \frac{du}{dt} = f_u f$, we obtain:

$$\frac{d\tilde{v}}{dt} = \frac{dv}{dt} - \frac{df}{dt} \int_\tau^t \eta d\tau - \eta f = f_u \tilde{v} + f,$$

meaning that $\tilde{v}_\tau$ satisfies the simple no time-dilated Equation (3.2).

Because this $\tilde{v}_\tau(t)$ defined by Equation (3.8) is not uniformly bounded, it cannot be directly used to compute the desired derivative by commuting the limit and derivative. Instead, we introduce an approximation that involves a window function $w : [0, 1] \to \mathbb{R}$ to mitigate the linear growth of $\tilde{v}_\tau$. This approximation is

$$\frac{d\langle J \rangle}{ds} \approx \frac{1}{T} \int_0^T w(\frac{t}{T}) \langle DJ\tilde{v}_\tau + \partial_s J \rangle dt,$$

(3.9)

for any $\tilde{\tau} \in [0, T]$. The validity of this approximation is established through the following theorem.

**Theorem 3.2.1** If the following are true:

1. $w$ is continuously differentiable,

2. $w(0) = w(1) = 0$,

3. $\int_0^1 w(s)ds = 1$, and
4. \( \hat{\tau} \) is a function of \( T \) satisfying \( 0 \leq \hat{\tau} \leq T \) and \( \lim_{T \to \infty} \frac{\hat{\tau}}{T} \) exists.

then,

\[
\frac{d}{ds} \lim_{T \to \infty} \frac{1}{T} \int_0^T J(u(t; s), s)dt = \lim_{T \to \infty} \frac{1}{T} \int_0^T w\left(\frac{t}{T}\right)(DJ\hat{v}_\tau + \partial_x J)dt.
\] (3.10)

This equality is nontrivial. To prove that it is true, we first define the following.

**Definition** For any continuous function \( w : [0, 1] \to \mathbb{R} \), the mean of the window is

\[
\overline{w} := \int_0^1 w(s)ds;
\]

the infinitely-long windowed time average of a signal \( x(t) \) is

\[
\langle x \rangle_w := \lim_{T \to \infty} \frac{1}{T} \int_0^T w\left(\frac{t}{T}\right)x(t)dt.
\]

A special case of the window function is \( w \equiv 1 \), called a *square* window. The mean of this window is 1; the infinitely-long windowed time average of a signal \( x(t) \) is simply its ergodic average, which we already denoted as:

\[
\langle x \rangle := \lim_{T \to \infty} \frac{1}{T} \int_0^T x(t)dt.
\]

**Lemma 3.2.2** If \( x(t) \) is bounded and \( \langle x \rangle \) exists, then \( \langle x \rangle_w \) also exists for any continuous \( w \), and the following equality is true:

\[
\langle x \rangle_w = \overline{w} \langle x \rangle.
\]

The proof is given in B.1.

Note that Lemma 3.2.2 does not apply to the windowed average on the right hand side of Equation (3.10) in Theorem 1. This is because the lemma requires \( x(t) \) to be independent of the averaging length \( T \). But in Theorem 1, \( \hat{\tau} \) and thus \( DJ\hat{v}_\tau + \partial_x J \) depend on \( T \). To apply Lemma 3.2.2, we must first decompose \( \hat{v}_\tau \) according to
Equation (3.8). Lemma 3.2.2 can then be applied to all but one of the components:

\[
\lim_{T \to \infty} \frac{1}{T} \int_0^T w(\frac{t}{T}) (DJ \tilde{\varphi} + \partial_s J) dt
\]

\[
= (DJ_v)_w + (\partial_s J)_w - \lim_{T \to \infty} \frac{1}{T} \int_0^T w(\frac{t}{T}) DJ f(t) (f_t^* \eta(t) d\tau) dt,
\]

(3.11)

\[
= (DJ_v) + (\partial_s J) - \lim_{T \to \infty} \frac{1}{T} \int_0^T w(\frac{t}{T}) \left( \int_0^t \eta(t) d\tau \right) \frac{dJ}{dt} dt,
\]

if \( w = 1 \). Here we used the fact that:

\[
\frac{dJ}{dt} = DJ \frac{du}{dt} + \partial_s J \frac{dJ}{dt} = DJ f.
\]

We then apply integration by parts to the remaining windowed average, and use the assumption that \( w(0) = w(1) = 0 \) in Theorem 1, to obtain:

\[
- \lim_{T \to \infty} \frac{1}{T} \int_0^T w(\frac{t}{T}) \left( \int_0^t \eta(t) J(t) dt \right) \frac{dJ}{dt} dt
\]

\[
= \lim_{T \to \infty} \frac{1}{T} \int_0^T w(\frac{t}{T}) \eta(t) J(t) dt + \frac{1}{T} \int_0^T \frac{d}{dt} w(\frac{t}{T}) \left( \int_0^t \eta(t) d\tau \right) J(t) dt,
\]

(3.12)

\[
= (\eta J) + \lim_{T \to \infty} \frac{1}{T} \int_0^T w'(\frac{t}{T}) \frac{1}{T} \left( \int_0^t \eta(t) d\tau \right) J(t) dt
\]

Here \( w' \) is the derivative of the window function \( w \). By substituting Equation (3.12) into Equation (3.11), then comparing with Equation (3.7), we see that we can prove Theorem 1 by proving the equality

\[
\lim_{T \to \infty} \frac{1}{T} \int_0^T w'(\frac{t}{T}) \frac{1}{T} \left( \int_0^t \eta(t) d\tau \right) J(t) dt = - \langle \eta \rangle \langle J \rangle.
\]

(3.13)

We now establish this equality, thereby proving Theorem 1, through two lemmas:

**Lemma 3.2.3** If \( \eta \) is bounded and \( \langle \eta \rangle \) exists, then

\[
\lim_{T \to \infty} \left( \sup_{\tau,t \in [0,T]} \left( \frac{1}{T} \left( \int_0^t \eta(t) d\tau \right) - \langle \eta \rangle \frac{t-\tau}{T} \right) \right) = 0.
\]
The proof of this lemma is given in B.2. This lemma establishes the equality that

$$\lim_{T \to \infty} \frac{1}{T} \int_0^T w'(\frac{t}{T}) \left( J(t) \eta(t) + \frac{1}{T} \int_0^t J(\tau) \eta(\tau) d\tau \right) J(t) dt = \langle \eta \rangle \lim_{T \to \infty} \frac{1}{T} \int_0^T w'(\frac{t}{T}) \frac{t - \frac{T}{2}}{T} J(t) dt.$$  

The remaining task in proving Equation (3.13) is achieved by the following lemma:

**Lemma 3.2.4** If $J$ is bounded, $w \in C^1[0,1]$, $w(0) = w(1) = 0$, and $\lim_{T \to \infty} \frac{\tilde{J}}{T}$ exists, then

$$\lim_{T \to \infty} \frac{1}{T} \int_0^T w'(\frac{t}{T}) \frac{t - \frac{T}{2}}{T} J(t) dt = -\overline{w}(J).$$

**Proof** Let $\hat{s} = \lim_{T \to \infty} \frac{\tilde{J}}{T}$. Because both $J$ and $w'$ are bounded ($w$ is continuously differentiable in a closed interval),

$$\lim_{T \to \infty} \frac{1}{T} \int_0^T w'(\frac{t}{T}) \frac{t - \frac{T}{2}}{T} J(t) dt = \lim_{T \to \infty} \frac{1}{T} \int_0^T w'(\frac{t}{T}) \left( \frac{t}{T} - \hat{s} \right) J(t) dt.$$

Define $w_s(s) = w'(s)(s - \hat{s})$, then Lemma 2 can turn the equality above into

$$\lim_{T \to \infty} \frac{1}{T} \int_0^T w'(\frac{t}{T}) \frac{t - \frac{T}{2}}{T} J(t) dt = \langle J \rangle w_s = \overline{w_s}(J),$$

in which

$$\overline{w_s} := \int_0^1 w'(s)(s - \hat{s}) ds = \int_0^1 \frac{d}{ds} w(s) ds \bigg|_{0}^{1}$$

In our case, not only $\lim_{T \to \infty} \frac{\tilde{J}}{T}$ exists but we even have $\lim_{T \to \infty} \frac{\tilde{J}}{T} \to \frac{1}{2}$, as shown in B.3. This result comes from the fact that the computed $\hat{v}_\tilde{J}$ is the one with minimal $L^2$ norm.

Lemma 3.4 combines to prove Equation (3.13), which combines with (3.11) and (3.12) to:

$$\lim_{T \to \infty} \frac{1}{T} \int_0^T w'(\frac{t}{T})(DJ\hat{v}_\tilde{J} + \partial_s J) dt = \langle DJ\hat{v}_\tilde{J} + \langle \partial_s J \rangle + \langle \eta J \rangle - \langle \eta \rangle \langle J \rangle.$$  

(3.14)

This, together with Equation (3.7), proves that the desired derivative $\frac{d(J)}{ds}$ can be computed via a windowed average of $DJ\hat{v}_\tilde{J} + \partial_s J$, where $\hat{v}$ is a solution to the tangent
equation without time dilation.

\section*{3.3 Numerical results}

Now, we are going to apply simplified LSS to the Lorenz 63 test case. The chosen windowing functions for this test case are (see Figure 3-1):

- **Square window:**
  \[ w(t) = 1, \quad t \in [0, 1]. \]

- **Sine window:**
  \[ w(t) = \sin(\pi t), \quad t \in [0, 1]. \]

- **Sine squared window:**
  \[ w(t) = \sin^2(\pi t), \quad t \in [0, 1]. \]

- **Sine to the power four, also known as the Hann-squared window:**
  \[ w(t) = \sin^4(\pi t), \quad t \in [0, 1]. \]

- **Bump window:**
  \[ w(t) = \exp\left(\frac{-1}{t-t^2}\right), \quad t \in [0, 1], \]
  defined up to normalization constants.

All windows respect the criteria of theorem 1 with the exception of the square window, which is equivalent to not using any window. The major difference between the last four functions is their Taylor expansion in the neighborhood of \( t = 0 \) and \( t = 1 \). Actually, we can expect the areas around the extremities to be the most 'sensible' ones, leading to the biggest error terms in the approximation of \( \frac{d\phi}{d\tau} \) because \( \tilde{v}_r \) is maximal in these areas. Thus, choosing a windowing function that collapses quite fast on the extremities is expected to be the more accurate. The simple sine has
nonzero derivatives on the extremities, the squared sine has a zero derivative on both sides, the Hann-squared function has zero coefficients until the third-order derivative while the bump function has zero coefficients for all derivative orders. A deep and rigorous analysis of this intuitive idea has been carried out by Krakos et al. for the periodic case (periodic dynamical system) [29].

For all simulations, the equations were discretized using a second-order scheme and a uniform time step of $\Delta t = 0.02$. The burn-in period for computing $u(t)$ was set to 10 time units.

First, Figure 3-2 shows the norm of the computed $\tilde{v}_\tau$ with respect to $t$ where $\rho = 28$ and the time integration length is $T = 100$. We can clearly notice the linear growth of the 'envelope' of $\tilde{v}_\tau$ as $t$ increases or decreases, as predicted in Equation (3.8):

$$\tilde{v}_\tau(t) = v(t) - f(t) \int_{\tau}^{t} \eta(\tau)d\tau.$$  

Furthermore, $\tilde{v}_\tau$ is minimal around $t = \frac{T}{2} = 50$, which is in agreement with the following result:

$$\lim_{T \to \infty} \frac{\tilde{\tau}}{T} \to \frac{1}{2}$$  

It is worth noting that both the integration scheme for $u(t)$ and discretization of equations (3.3) should have the same accuracy order for stability reasons.
Then, we have computed $\frac{d(z)}{dp}$ for $p \in [25, 35]$ and $T = 50$ using different windowing functions as well as the original Least Squares Shadowing algorithm (Figure 3-3). In this range of the parameter $p$, the dynamical system is known to be quasi-hyperbolic and the analysis we carried out in the previous section remains valid.

Knowing that the analytical value of $\frac{d(z)}{dp}$ is around 0.96, we conclude that the original LSS as well as the windowed algorithms give consistent and very similar results except for the square window. This is quite reassuring because the square window is, de facto, not a valid windowing function ($w(0) = w(1) = 1 \neq 0$) and, above all, it confirms that the other windows are efficiently "correcting" the error coming from the unboundedness of $\tilde{v}_s$.

Nevertheless, all windows do not seem to have the same performance: the results obtained with the Hann-squared and the bump window are smoother and more self-consistent than the results coming from the sine squared and much smoother than the results given by the simple sine window. To point out this phenomenon, a complementary analysis has been performed: for $p = 28$, $p = 50$ and integration time lengths of $T = 25$, $T = 50$, and $T = 100$, 2000 simulations (each one with a different initial condition) were run to compute a 95% confidence interval of the standard deviation of $\frac{d(z)}{dp}$ for each one of the windows (see Figure 3-4). The results confirm
Figure 3-3: $\frac{d(z)}{dp}$ using different windowing functions and original LSS for integration time $T = 50$

our previous remark: for a fixed $T$ and $\rho = 28$, the Hann-squared and bump windows have the lowest standard deviations, meaning they are more robust than the other windows. Among the valid windowing functions, the simple sine gives the worst results. Then, for a fixed window, we notice that increasing the time integration length decreases the standard deviation, which is an intuitive result because when $T$ gets bigger the influence of the initial condition on the dynamical system fades out (due to ergodicity). Finally, for $\rho = 50$, all windows give bad results (standard deviation of order 1), which can be explained by the fact that the dynamical system is no longer quasihyperbolic for this value of $\rho$. The theory we have developed does not hold any more and there is no reason for simplified LSS to converge to the true value of $\frac{d(z)}{dp}$ (for $T = 100$, the confidence intervals were so big and uninformative that we only represented the standard deviation estimator).
Figure 3-4: Standard deviation confidence intervals for $\rho = 28$ (upper graph) and $\rho = 50$ (lower graph) using different windowing functions
Chapter 4

LSS with reconnections

4.1 An approach involving the invariant density

In this final chapter, we will present a major improvement to the robustness of LSS. The new algorithm, called LSS with reconnections or LSSR, incorporates some traits of the probability density adjoint method [30]. Till now, we have supposed that the system is perfectly ergodic, meaning that LSS can be performed for any trajectory in phase space no matter what its initial condition is. Although this hypothesis seems to be satisfied for most real-life applications, it is not always the case. For some particular initial conditions, the computed trajectory does not reflect the attractor’s properties: values computed using time averages do not reflect the values using ensemble averages. LSS has a single trajectory \( \{u_1, \cdots, u_n\} \) for input so it can be sensitive to this kind of error. On the opposite side, density adjoint algorithms compute how the density and shape of the attractor changes when the parameter is changed, making them very robust. However, they may be more expensive and above all, very hard if not impossible to implement for high-dimensional systems because they require an explicit knowledge of the attractor (shape, dimension, ...). LSSR comes in the middle of this spectrum. A more in-depth explanation of its fundamentals can be found in [31]. Intuitively, it takes a sequence of points \( \{u'_1, \cdots, u'_n\} \) (not necessarily a trajectory), computes a shadowing direction for these points as LSS but uses a set of constraints that takes into account the invariant properties of the
steady-state density. Namely, the minimization problem is the following:

\[
\min_v \sum_{y \in \Lambda} \|v(y)\|^2 \\
\text{s.t. } v(y) = \sum_{u \in f^{-1}(y, s)} \frac{\rho(u, s)}{\rho(y, s)|f_u|} (f_u v + f_s),
\] (4.1)

where \(\rho(., s)\) is the invariant measure on the attractor \(\Lambda\) for a design parameter \(s\) and \(|f_u|\) is the absolute value of the determinant of the Jacobian matrix \(f_u\). The \(v\) presented here is not, \textit{a priori}, the shadowing direction as defined previously and, if we want to be rigorous, the summation on the left is actually an integral over the attractor with respect to the invariant measure and should be written \(\int_{y \in \Lambda} \|v(y)\|^2 d\rho\).

The vector \(v\) should be interpreted as the local displacement of the attractor when \(s\) changes. As in continuum mechanics, we identify the probability density \(\rho\) to a mass density: when \(s\) is perturbed, \(v\) shows how the total "mass" (probability of presence) is translated and/or distorted in phase space. As a real mass, the probability of presence is a conservative quantity \((\text{div}(\rho v) + \frac{\partial \rho}{\partial y} = 0)\) and is equal to 1 for all \(s\). Furthermore, the steady-state distribution \(\rho\) is, by definition, time invariant. In other words, if \(X\) is a random variable with density \(\rho\) then \(f(X)\) also has density \(\rho\). By combining the time-invariance and mass-conservation properties we obtain the set of equations (4.1).

A detailed derivation of this minimization problem can be found in [31]. If we look at the constraint, it means that \(v(y)\) is a prorated combination of all the perturbations of its pre-images by \(f\). The impact of a pre-image on \(y\) is proportional to how much of \(y\)'s "probability mass" comes from this pre-image. Clearly, pre-images with high probability density will have more impact on \(y\). In the same way, the probability mass around a pre-image with a low \(|f_u|\) will stay "concentrated" and be sent to a small neighborhood of \(y\). Thus, no mass is "lost" and a pre-image with a low \(|f_u|\) will have a great impact on \(y\) as well.

Through a more intuitive rather than rigorous explanation, let us now relate this newly defined \(v\) to the \textit{shadowing direction} we already know and see how we can incorporate this result to \textit{LSS}. For a hypothetical infinitely long trajectory on the attractor \(\Lambda\), all points of \(\Lambda\) will at some point be reached\(^1\) and the proportion of time

\(^1\)The infinite trajectory is dense in \(\Lambda\) so will come as close as we want from any point in the attractor (almost surely with respect to \(\rho\)).
spent in each area of the attractor converges to the probability determined by the invariant measure. Thus, an infinitely long trajectory can be seen as the attractor itself with its weighting probability density. If $s$ is perturbed, this infinitely long trajectory will follow the shadowing direction. The perturbed infinitely long trajectory (at $s + \delta s$) is nothing else than the attractor for $s = s + \delta s$. Thus, the shadowing direction can be interpreted as the displacement of the attractor $v$ introduced above and the two concepts match. Thus, imposing this new set of constraints gives to the shadowing direction characteristics specific to a probability density displacement (such as making $v$ smoother). In some sense, we are forcing the shadowing direction to behave as if it represented the displacement of the attractor itself and, as we will see, this approach will make our algorithm more robust.

4.2 The algorithm in practice

In practice, we do not have access to the invariant measure $\rho$ but we can simulate samples $\{x_1, \ldots, x_N\}$ following this distribution. In fact, for a sufficiently long trajectory $\{u_1, \ldots, u_N\}$, these points can be considered our samples because the system is ergodic. This procedure is similar to a Markov Chain Monte Carlo method and, by taking nonsequential points we can make our samples almost independent (Monte Carlo sampling). Then, we should find a discrete version for the set of constraints in (4.1). Because we have a finite number of samples, we will never have all the pre-images of a specific $u_i \in \Lambda$ in our sample. Consequently, we should be more flexible and consider a new criterion for 'being a pre-image of $u_i$' such that: we say that $u_j$ is a pre-image of $u_i$ if $|u_i - f(u_j)| < \epsilon$ for a certain $\epsilon > 0$. Consequently, the new set of equations would be:

$$v(u_i) = \frac{1}{\sum_{j=1}^{N} 1_{\epsilon}(|u_i - f(u_j)|)} \sum_{j=1}^{N} 1_{\epsilon}(|u_i - f(u_j)|) \left( f_u v(u_j) + f_s \right),$$

(4.2)

where $1_{\epsilon}(x) = 1$ if $0 \leq x < \epsilon$, 0 otherwise. Notice that the denominator acts as a normalization factor and we will show that, as $N \to \infty$ and $\epsilon \to 0$, $\frac{\sum_{k=1}^{N} 1_{\epsilon}(|u_i - f(u_k)|)}{\sum_{k=1}^{N} 1_{\epsilon}(|u_i - f(u_k)|)}$
will converge to $\frac{\rho(u_{j+1}, s)}{\rho(u_j, s)}$. Compared with the original LSS formulation, the shadowing direction at $u_i$ not only depends on the previous point $u_{i-1}$ but potentially on any other sample, which explains the name LSS with reconnections for the new algorithm. Actually, there is no need to implement a cut-off threshold $\epsilon$, the "weight function" $1_\epsilon$ is only one possible example. Intuitively, the main idea of this procedure is to give more importance to points $u_j$ such that their image $f(u_j)$ is close to $u_i$. As the number of sample points increases, we can narrow down the area of influence of our weight ($\epsilon \to 0$). Thus, a valid weight would be any normalized family of nonnegative functions $\{w_\epsilon\}_{\epsilon>0}$ such that for $\delta > 0$ and $y \in \Lambda$:

$$
\lim_{\epsilon \to 0} \int_{B(y, \delta)} w_\epsilon(y - x) d\rho = \lim_{\epsilon \to 0} \int_\Lambda w_\epsilon(y - x) d\rho = \rho(y), \quad (4.3)
$$

$B(y, \delta)$ being the ball around $y$ with radius $\delta$. In other words, $\{w_\epsilon\}_{\epsilon>0}$ is an approximation of the Dirac distribution and all of the weight gets concentrated in a neighborhood of $0$ as small as we want when $\epsilon$ approaches 0. For example, the weight functions could be (see Figure 4-1):

- **Cut-off**:
  $$
  w_\epsilon^c(x) = 1 \times C_\epsilon^c \quad \text{if } 0 \leq x < \epsilon, \quad 0 \quad \text{otherwise.} \quad (4.4)
  $$

- **Cauchy function**:
  $$
  w_\epsilon^{ca}(x) = \frac{C_\epsilon^{ca}}{(\frac{x}{\epsilon})^2 + 1} \quad (4.5)
  $$

- **Gaussian**
  $$
  w_\epsilon^g(x) = C_\epsilon^g \exp\left(-\left(\frac{x}{\epsilon}\right)^2\right) \quad (4.6)
  $$

where $C_\epsilon^c, C_\epsilon^{ca}$ and $C_\epsilon^g$ are the normalization constants.
4.3 Convergence of the constraint approximation

Let \{u_1, \cdots, u_N\} be a set of points belonging to the attractor \Lambda such that they have been sampled following the distribution \rho. For any \( y \in \{u_1, \cdots, u_N\} \), we define \{x_1, \cdots, x_m\} to be the set of its predecessors:

\[
y = f(x_1) = \cdots = f(x_m).
\]

Notice that, in general, the \( x_i \) do not belong to the set of sampled points \{u_1, \cdots, u_N\}. For reasons of simplicity, we define \( v_u \) to be the shadowing direction at \( u \in \Lambda \). Theoretically, the computed shadowing directions should respect:

\[
v_y = \sum_{i=1, \cdots, m} \frac{\rho(x_i)}{\rho(y) f_u(x_i)} (f_u v_{x_i} + f_s),
\]

(4.7)

for all \( y \in \Lambda \). With LSSR, after sampling the points \{u_1, \cdots, u_N\} and choosing a weight function \( w_i \), we impose the following set of \( N \) constraints:

\[
\left\{ v'_y = \frac{\sum_{j=1}^N w_i (y - f(u_j)) (f_u v'_{u_j} + f_s)}{\sum_{j=1}^N w_i (y - f(u_j))} \right\}, \quad \text{for all } y \in \{u_1, \cdots, u_N\}
\]

(4.8)
where \( \{v'_y, y \in \{u_1, \ldots, u_N\}\} \) is a set of approximate shadowing directions. In what follows, we will show that as \( N \to \infty \) and \( \epsilon \to 0 \), the approximate shadowing directions computed by LSSR respect (4.7). The convergence is proved in two steps. First, we have a Monte Carlo estimation:

\[
\frac{\sum_{j=1}^{N} w_{\epsilon}(y - f(u_j))(f_{u}v'_{u_j} + f_{s})}{\sum_{j=1}^{N} w_{\epsilon}(y - f(u_j))} \xrightarrow{N \to \infty} \frac{\int_{A} w_{\epsilon}(y - f(x))(f_{u}v'_{u_j} + f_{s})d\rho}{\int_{A} w_{\epsilon}(y - x)d\rho}. \tag{4.9}
\]

The second step is:

\[
\int_{A} w_{\epsilon}(y - f(x))(f_{u}v'_{u_j} + f_{s})d\rho \xrightarrow{\epsilon \to 0} \sum_{i=1, \ldots, m} \frac{\rho(x_i)}{\rho(y)} f_{u}(y_{x_i} + f_{s}). \tag{4.10}
\]

as the weight function converges to a Dirac distribution.

### 4.3.1 Convergence of the first term

The convergence of the first term is straightforward because the quantity on the left is a Monte Carlo estimator of the quantity on the right of equation (4.9). If the samples \( \{u_1, \ldots, u_N\} \) are sequential points of a real trajectory, then our sampling method is equivalent to a Markov Chain Monte Carlo method. Reducing the correlation between samples can increase the speed of convergence of the method.

### 4.3.2 Convergence of the second term

Next, we have that:

\[
v'_y = \frac{\int_{A} w_{\epsilon}(y - f(x))(f_{u}v'_{u_j} + f_{s})d\rho}{\int_{A} w_{\epsilon}(y - x)d\rho}, \tag{4.11}
\]

\[
= \frac{1}{\int_{A} w_{\epsilon}(y - x)d\rho} \left( \sum_{i=1, \ldots, m} \int_{B(x_i, \delta) \cap A} w_{\epsilon}(y - f(x))(f_{u}v'_{x} + f_{s})d\rho \right) \tag{4.12}
\]

\[
+ \int_{f_{u}}(y - f(x))(f_{u}v'_{x} + f_{s})d\rho \tag{4.13}
\]
where \( \bar{I} = \Lambda \setminus \cup_{i=1,...,m} B(x_i, \delta) \). Based on property (4.3) of the weight function \( w_\epsilon \), we can eliminate the latter integral for \( \delta > 0 \) arbitrarily small:

\[
\frac{\int_{\bar{I}} w_\epsilon(y - f(x))(f_u v'_x + f_s) \, dp}{\int_{\Lambda} w_\epsilon(y - x) \, dp} \leq \sup_{x \in \Lambda} ((f_u v'_x + f_s)) \frac{\int_{\bar{I}} w_\epsilon(y - f(x)) \, dp}{\int_{\Lambda} w_\epsilon(y - x) \, dp},
\]

(4.14)

\[
\leq M \frac{\int_{\bar{I}} w_\epsilon(y - f(x)) \, dp}{\int_{\Lambda} w_\epsilon(y - x) \, dp},
\]

(4.15)

\[
\lim_{\epsilon \to 0} \frac{\int_{\bar{I}} w_\epsilon(y - f(x))(f_u v'_x + f_s) \, dp}{\int_{\Lambda} w_\epsilon(y - x) \, dp} = 0,
\]

(4.16)

where \( M = \sup_{x \in \Lambda} ((f_u v'_x + f_s)) < \infty \) because the shadowing direction is bounded, \( f_u \) and \( f_s \) are continuous on \( \Lambda \), which is a compact set of \( \mathbb{R}^n \).

Furthermore, \( f \) is a measurable function (with respect to \( \rho \)), which maps \( B(x_i, \delta) \) to \( f(B(x_i, \delta)) \). We can make the following change of variable:

\[
u = f(x)|_{B(x_i, \delta)},
\]

(4.17)

and obtain:

\[
\int_{B(x_i, \delta)} w_\epsilon(y - f(x))(f_u v'_x + f_s) \, dp = \int_{f(B(x_i, \delta))} w_\epsilon(y - u)(f_u v'_{f^{-1}(u)} + f_s) \, d\rho, \quad (4.18)
\]

\[
\int_{B(x_i, \delta)} w_\epsilon(y - f(x))(f_u v'_x + f_s) \, dp = \lim_{\epsilon \to 0} \int_{f(B(x_i, \delta))} w_\epsilon(y - u)(f_u v'_{f^{-1}(u)} + f_s) \, d\rho, \quad (4.19)
\]

where \( f_* \rho \) is the pushforward measure of \( \rho \) under \( f \) given by \( f_* \rho(\Gamma) = \rho(f^{-1}(\Gamma)) \) for any Borel set \( \Gamma \) of \( f(B(x_i, \delta)) \). Assuming that \( f \) is \( C^1 \) and that \( f_u|_{x_i} \neq 0 \), the inverse function theorem states that we can find a ball \( B(x_i, \alpha) \) containing \( x_i \) on which \( f \) is a diffeomorphism. Consequently, \( f(B(x_i, \delta)) \) contains a ball \( B(y, \alpha') \) and as \( \epsilon \) decreases:

\[
\lim_{\epsilon \to 0} \int_{B(x_i, \delta)} w_\epsilon(y - f(x))(f_u v'_x + f_s) \, dp = \lim_{\epsilon \to 0} \int_{f(B(x_i, \delta))} w_\epsilon(y - u)(f_u v'_{f^{-1}(u)} + f_s) \, d\rho, \quad (4.20)
\]

\[
= (f_u v'_x + f_s) \lim_{\epsilon \to 0} \int_{B(y, \alpha)} w_\epsilon(y - u) \, d\rho, \quad (4.21)
\]

\[
= (f_u v'_x + f_s) f_* \rho(y), \quad (4.22)
\]
thanks to property (4.3). Finally, based on the invariance of the measure $\rho$, we have that:

$$\rho(y) = \sum_{i=1,...,m} \frac{\rho(x_i)}{|f_{u_i}|_{x_i}}$$  \hspace{1cm} (4.23)

so $f_* \rho(y) = \frac{\rho(x_i)}{|f_{u_i}|_{x_i}}$ (proportion of $\rho(y)$ that comes from $x_i$). We conclude that:

$$\lim_{\varepsilon \to 0} \int_{B(x,\varepsilon)} w_i(y - f(x))(f_{u_i} v'_{x_i} + f_s) d\rho = \frac{\rho(x_i)}{|f_{u_i}|_{x_i}}(f_{u_i} v'_{x_i} + f_s).$$  \hspace{1cm} (4.24)

As for the denominator, using property (4.3) again:

$$\lim_{\varepsilon \to 0} \int w_i(y - x) d\rho(x) = \rho(y).$$  \hspace{1cm} (4.25)

Combining (4.24) and (4.25) we get:

$$\frac{\int w_i(y - f(x))(f_{u_i} v'_{x_i} + f_s) d\rho}{\int w_i(y - x) d\rho} \xrightarrow{\varepsilon \to 0} \sum_{i=1,...,m} \frac{\rho(x_i)}{|\rho(y)|_{f_{u_i}}}(f_{u_i} v'_{x_i} + f_s),$$  \hspace{1cm} (4.26)

which concludes the proof.

### 4.4 Relaxing the constraints

Based on some LSSR numerical results (presented in the next section), we notice that the KKT matrix used to solve the minimization problem can be ill conditioned. We can address this problem by relaxing the constraints (4.8) and giving more flexibility to the $v_{u_i}$ terms. We introduce new variables $\alpha_{ij}$, where $i, j$ belong to $\{1, \ldots, N\}$ and $i < j$ (total of $N(N+1)/2$ new variables) and formulate a new set of constraints:

$$\left\{v_{u_i} + \sum_{j > i} \delta_{ij} \alpha_{ij} |u_i - u_j| - \sum_{j < i} \delta_{ij} \alpha_{ji} |u_i - u_j| = \frac{\sum_{j=1}^{N} w_i(u_i - f(u_j))(f_{u_i} v_{u_j} + f_s)}{\sum_{j=1}^{N} w_i(u_i - f(u_j))}, \text{ for all } i \in \{1, \ldots, N\}\right\}$$  \hspace{1cm} (4.27)
The cost function of the optimization problem becomes:

$$\sum_i \frac{1}{2} v_i^2 + p \sum_i \sum_{j>i} \frac{1}{2} \alpha_{ij}^2,$$

where $p > 0$ is the penalty for violating the standard LSSR constraints. The terms $|u_i - u_j|$ appear as normalization constants and are intuitive: if $u_i$ and $u_j$ are very close to each other then we expect $|v_{ui} - v_{uj}|$ to be small because the shadowing direction is assumed to be smooth. Thus, a big gap $|v_{ui} - v_{uj}|$ should be severely penalized. Indeed, for a constant difference in norm between $v_{ui}$ and $v_{uj}$, $\alpha_{ij}$ increases when $|u_i - u_j|$ decreases.

### 4.5 Applying LSSR to the sawtooth map

We will now run the different LSSR variations to a 1-D map known as the sawtooth map (Figure 4-2):

$$x_{i+1} = f(x_i, s) = 2x_i + s \sin(2\pi x_i) \mod[1],$$

where $x_i \in [0, 1]$ and $s$ is the design parameter. The objective function is $J(x) = \cos(2\pi x_i)$ and does not depend on $s$. For $s = 0.055$, it is known that $\frac{d<\frac{d_J}{ds}}{ds} = 0.44$. First of all, standard LSS does not give us a good estimation of the derivative (for an integration length of 500, the computed value is 1.42).

In the following simulations we have tried out the three weight functions: cut-off, Cauchy, and Gaussian. For each weight, we have run the non-relaxed and relaxed LSSR with a penalty $p = 50$ for the relaxed version.

In Figure 4-4, we computed the condition number of the KKT matrix obtained by applying relaxed and non-relaxed LSSR with the three different weight functions over a large spectrum of $\epsilon$. We clearly notice that the relaxed version of LSSR leads to a much better conditioned KKT matrix, irrespective of the choice of the weight function. In addition to that, as $\epsilon$ decreases, the condition number increases. This is due to the
fact that, for a fixed number of samples $N = 500$ (or integration length), as $\epsilon$ goes to 0 the points are less "connected", making the matrix closer to being singular. All weights seem to have similar performances with a slight advantage for the heavy-tailed Cauchy function. The relative difference between the real $\frac{d<\mathcal{J}>}{ds}$ and the computed one (Figure 4-3), confirms our previous analysis of the condition numbers: relaxed LSSR provides better results than the original version and the Cauchy weight performs well in a slightly broader range of $\epsilon$ compared with the other two weights. Finally, Figure 4-5 shows the root-mean-square (RMS) error of each variant of the algorithm when changing the parameter $\epsilon$ and the integration length $N$. The two-dimensional parameter space has been discretized to a $20 \times 20$ logarithmic grid and, for each point in this grid, we have launched 20 simulations with different initial conditions for the trajectories. The RMS error has been computed as follows:

$$RMS = \sqrt{\frac{1}{20} \sum_{i=1}^{20} \left( \frac{d<\mathcal{J}>}{ds}|_{i} - 0.44 \right)^{2}},$$

(4.30)

where $\frac{d<\mathcal{J}>}{ds}|_{i}$ is the result of the simulation for the $i^{th}$ sample. As expected, the relaxed version of LSSR gives much better results than the non-relaxed version. Choosing a heavy-tailed weight can also improve the performance of the algorithm. Above all, we notice that as $N$ increases, the range of $\epsilon$ for which we obtain acceptable results becomes larger. Then, for a large enough $N$, decreasing $\epsilon$ improves the algorithm (till a certain limit for $\epsilon$). This result confirms what we have found in the convergence analysis of LSSR.

This numerical example has shown us that relaxing LSSR may improve the quality of the results. Nevertheless, the relaxed version is more expensive in terms of computation time and memory because the Schur complement of the KKT matrix becomes dense. Even though all weight functions seem to work well for the relaxed version, choosing a heavy tailed one such as the Cauchy function may give more stability to the algorithm. We are encouraged to do so because this operation is practically costless.
Figure 4-2: Sawtooth map for $s = 0.055$

Figure 4-3: Relative error for the computed $\frac{d<\Delta>}{ds}$ for each variant of LSSR, integration length $N = 500$
Figure 4-4: Condition number of the system for each variant of LSSR, integration length $N = 500$
Figure 4-5: RMS error for each variant of LSSR: Three different weights/non-relaxed and relaxed versions with penalty $= 50$
Chapter 5

Conclusion

Throughout this thesis, we have presented the Least Squares Shadowing algorithm and how it allows us to compute the derivative of ergodic quantities for chaotic dynamical systems. In simplified LSS, the time dilation factors have been removed by introducing a windowing function that mitigates the linear growth of the shadowing direction. This leads us to a much simpler system of equations to solve, especially in high-dimensional spaces. In terms of improvements to the robustness of the algorithm, we have introduced LSSR in both its relaxed and non-relaxed versions. This algorithm is based on the properties of the steady-state density distribution and imposes a new set of constraints on the shadowing direction. In fact, despite being very similar to the original LSS through its formulation as a minimization problem, it shares the same foundations as the density adjoint algorithm. While still in a relatively empirical formulation, especially the relaxed version, LSSR is very promising.

The potential of LSS and its variants is far from being fully explored and future work can go in different directions. First, LSSR should be better understood and adapted to high-dimensional ODEs and PDEs. Then, high-scale, industrial simulations should be conducted with LSS to test its performance and compare it with currently available tools. For this purpose, it is essential to reduce even more the computational cost of the algorithm. NI-LSS, which stands for Non-Intrusive LSS, is currently under development and has shown some spectacular results in this aspect. 73
In fact, the computation time has been reduced by orders of magnitude thanks to the reduction of the minimization problem. We can reduce our search of a minimizing shadowing direction to a search of a minimizing perturbation in the unstable subspace. Because the unstable subspace usually has a much lower dimension than the whole phase space, this new algorithm reduces the computational costs drastically.
Appendix A

Convergence of LSS

A.1 Appendix 1

In our case, we have an explicit expression for \( \{v_i^{h,\infty}, \eta_i^{h,\infty}\} \):

\[
v_i^{h,\infty} = \sum_{j=0}^{\infty} (D\varphi_0(u_i^0, jh)) \partial_s \varphi_0(u_i^{0, j}, h)^- - \sum_{j=1}^{\infty} (D\varphi_0(u_i^0, -jh)) \partial_s \varphi_0(u_i^{0, j}, h)^+, \quad (A.1)
\]

\[
\eta_i^{h,\infty} = \frac{1}{h} \frac{(\partial_s \varphi_0(u_i^0, h)^0; \partial_h \varphi_0(u_i^0, h))}{(\partial_h \varphi_0(u_i^0, h); \partial_h \varphi_0(u_i^0, h))}. \quad (A.2)
\]

As we did previously:

\[
\|v_i^{h,\infty}\| \leq \sum_{j=0}^{\infty} \|(D\varphi_0^{(j)}(u_i^{0, j}, h)) \partial_s \varphi_0(u_i^{0, j}, h)^-\| + \sum_{j=1}^{\infty} \|(D\varphi_0^{(-j)}(u_i^{0, j}, h)) \partial_s \varphi_0(u_i^{0, j}, h)^+\|, \quad (A.3)
\]

\[
\leq \sum_{j=0}^{\infty} C\lambda^j h \|\partial_s \varphi_0(u_i^{0, j}, h)^-\| + \sum_{j=1}^{\infty} C\lambda^j h \|\partial_s \varphi_0(u_i^{0, j}, h)^+\|, \quad (A.4)
\]

\[
\leq 2C \sup_{u\in\Lambda} (\|\partial_s \varphi_0(u, h)\|) \frac{1 - \lambda h}{\beta}. \quad (A.5)
\]
so:

\[
\|v_i^{\{h,\infty\}}\| \leq \frac{2C}{1 - \lambda^h} \sup_{u \in \Lambda} (\|\partial_s \varphi_0(u, h)\|) \leq \frac{2C}{\beta \ln(\varepsilon)} \sup_{u \in \Lambda} (\|\partial_s \varphi_0(u, h)\|),
\]

(A.6)

\[
\leq \frac{2C}{\beta \ln(\varepsilon)} \sup_{u \in \Lambda} \left(\frac{\|\partial_s \varphi_0(u, h) - \partial_s \varphi_0(u, 0)\|}{h}\right),
\]

(A.7)

\[
\leq \frac{2C}{\beta \ln(\varepsilon)} \sup_{(u, h) \in \Lambda \times H} \left(\|\partial_h \partial_s \varphi_0(u, h)\|\right) = \|v^{\{\infty\}}\|,
\]

(A.8)

where \( H \) is a compact set of \( \mathbb{R}^+ \) (for example \([0, 1]\)) and \( \partial_s \varphi_0(u, 0) = 0 \). We have also used the Taylor expansion of \( 1 - \lambda^h \) for \( h \to 0 \) and assumed that \( \partial_h \partial_s \) is well defined and continuous on the compact set \( \Lambda \times H \).

Following similar steps, we obtain:

\[
\eta_i^{\{h,\infty\}} \leq \frac{\sup_{u \in \Lambda} (\|\partial_s \varphi_0(u, h)\|)}{\beta h m},
\]

(A.9)

\[
\leq \frac{\sup_{(u, h) \in \Lambda \times H} (\|\partial_h \partial_s \varphi_0(u, h)\|)}{\beta m} = \|\eta^{\{\infty\}}\|.
\]

(A.10)

### A.2 Appendix 2

Let \( C \in \mathbb{R}^+ \) be an arbitrary bound and we will assume that \( \alpha = 1 \) for simplicity (without loss of generality). If \( n_e \) is the number of elements that are bigger or equal to \( C \), we have:

\[
n_e \leq \frac{T(\|v^{\{\infty\}}\|_B^2 + \|\eta^{\{\infty\}}\|^2)}{h C^2},
\]

(A.11)

with the equality being verified in the worst case scenario where all the unbounded terms are equal to \( C \), all the bounded terms are equal to 0 and \( n_e C^2 \) is exactly equal to \( \frac{T}{h} (\|v^{\{\infty\}}\|_B^2 + \|\eta^{\{\infty\}}\|^2) \). Then, let us compute the contribution of the terms that are unbounded. For that purpose, we introduce an indicator function \( \delta \) that is equal to 0 when both \( e_i^{\{h,T\}^0} \) and \( e_i^{\{h,T\}} \) are below \( C \) and equal to 1 when at least one of
them is bigger (or equal) than $C$. We have:

\[
\lim_{h \to 0} \lim_{T \to \infty} \left( \frac{h}{T} \sum_{i=1}^{[\frac{T}{h}]} \delta(i) \left[ (DJ(u_i, s))_i^{(h,T)} + (\epsilon_i^{(h,T)}(J(u_i, s) - \langle J(s) \rangle)) \right] \right), \tag{A.12}
\]

\[
\leq \lim_{h \to 0} \lim_{T \to \infty} \left( \frac{h}{T} \sum_{i=1}^{[\frac{T}{h}]} \delta(i) \left[ \|DJ\|_\infty A_i^{(h,T)} + \left( 2\|\epsilon_i^{(h,T)}\|_\infty \right) \right] \right), \tag{A.13}
\]

\[
\leq \lim_{h \to 0} \lim_{T \to \infty} \left( \frac{h}{T} \max \left( \|DJ\|_\infty A, 2\|J\|_\infty A \right) \sum_{i=1}^{[\frac{T}{h}]} \delta(i) \left( \|\epsilon_i^{(h,T)}\|_\infty + \|\epsilon_i^{(h,T)}\|_\infty \right) \right), \tag{A.14}
\]

\[
\leq \lim_{h \to 0} \lim_{T \to \infty} \left( \frac{h}{T} \max \left( \|DJ\|_\infty A, 2\|J\|_\infty A \right) \times n_e C \right), \tag{A.15}
\]

\[
\leq \lim_{h \to 0} \lim_{T \to \infty} \left( \frac{h}{T} \max \left( \|DJ\|_\infty A, 2\|J\|_\infty A \right) \times \frac{T(\|v\|_B^2 + \|\eta\|^2) C}{hC^2} \right), \tag{A.16}
\]

\[
\leq \frac{\max \left( \|DJ\|_\infty A, 2\|J\|_\infty A \right)(\|v\|_B^2 + \|\eta\|^2)}{C} \tag{A.17}
\]

We have used the fact that $\sum_{i=1}^{[\frac{T}{h}]} \delta(i) \left( \|\epsilon_i^{(h,T)}\|_\infty + \|\epsilon_i^{(h,T)}\|_\infty \right)$ is maximized when we have the maximum number of unbounded elements and when all of them have the same value. The worst case scenario is again the one where we have $n_e$ unbounded elements all equal to $C$. Because $C$ is arbitrarily large, the contribution of the unbounded terms
is as small as we want. Then, the limits can be permuted in the expression:

\[
\lim_{h \to 0} \lim_{T \to \infty} \left( \frac{h}{T} \sum_{i=1}^{\left\lfloor \frac{T}{h} \right\rfloor} (1 - \delta(i)) \left[ (DJ(u_i, s)) e_{i}^{(h,T)} + \left( \varepsilon_{i}^{(h,T)} (J(u_i, s) - \langle J(s) \rangle) \right) \right] \right), \quad (A.18)
\]

\[
= \lim_{h \to 0} \lim_{T \to \infty} \lim_{s \to 0} \left( (1 - \delta(i)) \frac{h}{T} \sum_{i=0}^{\left\lfloor \frac{h}{T} \right\rfloor} \frac{(J(u_i^s, s) - J(u_i^s, s))}{s} \right), \quad (A.19)
\]

\[
+ \lim_{h \to 0} \lim_{T \to \infty} \lim_{s \to 0} \left( (1 - \delta(i)) \frac{h\varepsilon_{i}^{(h,T)}}{T} \left( J(u_i^s, s) - \frac{1}{T} \sum_j hJ(u_i^s, s) \right) \right), \quad (A.20)
\]

\[
= \lim_{h \to 0} \lim_{T \to \infty} \lim_{s \to 0} \left( (1 - \delta(i)) \frac{1}{s} \sum_{i=0}^{\left\lfloor \frac{h}{T} \right\rfloor} \frac{h(\tau_i^s + s\varepsilon_{i}^{(h,T)}))J(u_i^s, s)}{h \sum_j (\tau_j^s + s\varepsilon_{j}^{(h,T)})} - \frac{h\tau_i^s J(u_i^s, s)}{h \sum_j \tau_j^s} \right) + O(s), \quad (A.21)
\]

\[
= \lim_{s \to 0} \lim_{h \to 0} \lim_{T \to \infty} \left( (1 - \delta(i)) \frac{1}{s} \sum_{i=0}^{\left\lfloor \frac{h}{T} \right\rfloor} \frac{h(\tau_i^s + s\varepsilon_{i}^{(h,T)}))J(u_i^s, s)}{h \sum_j (\tau_j^s + s\varepsilon_{j}^{(h,T)})} - \frac{h\tau_i^s J(u_i^s, s)}{h \sum_j \tau_j^s} \right) + O(s), \quad (A.22)
\]

\[
= \lim_{s \to 0} \frac{(J)(s) - \langle J(s) \rangle}{s} + O(s) = 0. \quad (A.23)
\]

The last equality comes from property (2.15) we had on Riemann sums.
Appendix B

Simplified Least Squares
Shadowing

B.1 Lemma 2

Given any $w \in C[0, 1]$, $w \geq 0$, and bounded function $x(t)$ such that $\langle x \rangle = \lim_{T \to \infty} \frac{1}{T} \int_0^T x(t)dt$ exists, there is the relation:

$$\lim_{T \to \infty} \frac{1}{T} \int_0^T w\left(\frac{t}{T}\right)x(t)dt = w \cdot \langle x \rangle. \quad (B.1)$$

Proof Given any $\epsilon > 0$, let $\epsilon_1 = \epsilon/2B_x$, here $B_x$ is the bound for $x(t)$. $w$ is continuous on a compact set, hence its range is also bounded, say, by $B_w$. Moreover, $w$ is uniformly continuous, hence $\exists K$, s.t. $\forall \tau_1, \tau_2 \in [0, 1], |\tau_1 - \tau_2| \leq 1/K$, we have $|w(\tau_1) - w(\tau_2)| \leq \epsilon_1$. Construct the partition $P = \{0, \frac{1}{K}, \frac{2}{K}, ..., 1\}$. Now $\forall i \in \{1, 2, ..., K\}$, let $w_i = K \cdot \int_{(i-1)/K}^{i/K} w(\tau)d\tau$, then $\bar{w} = \frac{1}{K} \sum_{i=1}^{K} w_i$. Let $\xi_i(\tau) = w(\tau) - w_i$, $\tau \in I_i = [(i-1)/K, i/K]$.

$\forall i$, $w$ is continuous on the segment $I_i$, which is a compact set, hence $w$ achieves its maximum and minimum values on this segment. Denote its maximum and minimum values on this segment by $w_{i,\text{max}}$ and $w_{i,\text{min}}$, respectively. By selection of $K$, $w_{i,\text{max}} - w_{i,\text{min}} \leq \epsilon_1$. By definition of $w_i$, $w_{i,\text{min}} \leq w_i \leq w_{i,\text{max}}$. Hence we have $\xi_i(\tau) \leq \epsilon_1, \tau \in I_i$. 

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With the above $K$, let $\epsilon_2 = \epsilon/2KB_w$. Because $\lim_{T \to \infty} \frac{1}{T} \int_0^T x(t)dt$ exists, $\exists T_0$, such that $\forall M \geq T_0$ , $\langle x \rangle - \frac{1}{M} \int_0^M x(t)dt \leq \epsilon_2$. Hence we have:

$$\left| \langle x \rangle - \frac{1}{iM} \int_0^{iM} x(t)dt \right| \leq \epsilon_2, \quad i = 1, 2, 3, ...$$

the i-th inequality is equivalent to:

$$-i\epsilon_2 \leq \langle x \rangle - \frac{1}{M} \int_0^M x(t)dt - \frac{1}{M} \int_{(i-1)M}^{iM} x(t)dt \leq i\epsilon_2, \quad i = 1, 2, 3, ...$$

the (i+1)-th inequality is equivalent to:

$$-(i+1)\epsilon_2 \leq -(i+1)\langle x \rangle + \frac{1}{M} \int_0^M x(t)dt + \frac{1}{M} \int_{(i-1)M}^{(i+1)M} x(t)dt \leq (i+1)\epsilon_2, \quad i = 0, 1, 2, ...$$

Adding the above two inequalities together,

$$-(2i + 1)\epsilon_2 \leq \langle x \rangle - \frac{1}{M} \int_{(i-1)M}^{(i+1)M} x(t)dt \leq (2i + 1)\epsilon_2, \quad i = 0, 1, 2, ...$$

Now $\forall T \geq K T_0$, let $M = T/K$, then $M \geq T_0$, and the difference between the two sides in B.1, when $T$ is finite, can be represented by:

$$\mathbf{w} \cdot \langle x \rangle - \frac{1}{T} \int_0^T \mathbf{w}(\frac{t}{T})x(t)dt,$$

$$= \frac{1}{K} \sum_{i=1}^K \left[ \mathbf{w}_i \cdot \langle x \rangle - \frac{1}{M} \int_{(i-1)M}^{iM} (\mathbf{w}_i + \xi_i(\frac{t}{T}))x(t)dt \right],$$

$$= \frac{1}{K} \sum_{i=1}^K \left[ -\frac{1}{M} \int_{(i-1)M}^{iM} \xi_i(\frac{t}{T})x(t)dt + \mathbf{w}_i \cdot \left( \langle x \rangle - \frac{1}{M} \int_{(i-1)M}^{iM} x(t)dt \right) \right],$$

the first term is confined by:

$$\left| \frac{1}{M} \int_{(i-1)M}^{iM} \xi_i(\frac{t}{T})x(t)dt \right| \leq \epsilon_1 \cdot \frac{1}{M} \int_{(i-1)M}^{iM} |x(t)| dt,$$

the second term is confined by:

$$\left| \mathbf{w}_i \cdot \left( \langle x \rangle - \frac{1}{M} \int_{(i-1)M}^{iM} x(t)dt \right) \right| \leq \mathbf{w}_i \cdot (2i - 1)\epsilon_2,$$
As a result,

\[
\left| w \cdot \langle x \rangle - \frac{1}{T} \int_0^T w(\frac{t}{T}) x(t) dt \right|
\leq \frac{1}{K} \sum_{i=1}^{K} \left[ \varepsilon_1 \cdot \frac{1}{M} \int_{(i-1)M}^{iM} |x(t)| dt + w_i \cdot (2i - 1) \varepsilon_2 \right],
\]

\[
\leq \varepsilon_1 \cdot B_x + \varepsilon_2 \cdot B_w K \leq \varepsilon.
\]

Now we find \( T^* = K T_0 \), s.t. \( \forall T \geq T^* \), \( \frac{1}{T} \int_0^T w(\frac{t}{T}) x(t) dt - w \cdot \langle x \rangle \leq \varepsilon \).

### B.2 Lemma 3.2.3

If \( \eta \) is bounded and \( \langle \eta \rangle \) exists, then

\[
\lim_{T \to \infty} \left( \sup_{\hat{T}, t \in [0, T]} \left( \frac{1}{\hat{T}} \left( \int_{\frac{\hat{T}}{T}}^t \eta(\tau) d\tau \right) - \langle \eta \rangle \frac{t - \hat{T}}{T} \right) \right) = 0.
\]

**Proof** By assumption, we know that \( t, \hat{T} \in [0, T] \) and \( \eta \leq \|\eta\|_\infty < \infty \) so:

\[
\frac{1}{T} \left( \int_{\frac{T}{T}}^{t} \eta(\tau) d\tau \right) - \langle \eta \rangle \frac{t - \hat{T}}{T} = \frac{t - \hat{T}}{T} \left( \frac{1}{t - \hat{T}} \left( \int_{\frac{T}{T}}^{t} \eta(\tau) d\tau \right) - \langle \eta \rangle \right),
\]

and we have the following bounds on the two terms of the product:

\[
\left| \frac{t - \hat{T}}{T} \right| \leq 1 \quad \text{as well as} \quad \left| \frac{1}{t - \hat{T}} \left( \int_{\frac{T}{T}}^{t} \eta(\tau) d\tau \right) - \langle \eta \rangle \right| \leq 2\|\eta\|_\infty.
\]

Let us define \( c = \max \left( 1, 2\|\eta\|_\infty \right) \). We also know that for any \( \varepsilon > 0 \) there is a constant \( M > 0 \) such that for all \( t_0 \) and \( T \geq M \):

\[
\left| \frac{1}{T} \int_{\tau = t_0}^{t_0 + T} \eta(\tau) d\tau - \langle \eta \rangle \right| < \varepsilon.
\]

Consequently, for all \( \varepsilon > 0 \) and for all \( T > \frac{cM}{\varepsilon} \), we have:
• if \(|t - \hat{\tau}| < M\), then \(\frac{t-\hat{\tau}}{T} \leq \frac{\xi}{\varepsilon}\), which means that:

\[
\left| \frac{t-\hat{\tau}}{T} \left( \frac{1}{t-\hat{\tau}} \left( \int_{\hat{\tau}}^{t} \eta(\tau) d\tau \right) - \langle \eta \rangle \right) \right| \leq \frac{\varepsilon}{\xi} \left| \frac{1}{t-\hat{\tau}} \left( \int_{\hat{\tau}}^{t} \eta(\tau) d\tau \right) - \langle \eta \rangle \right| \leq \varepsilon. \tag{B.5}
\]

• if \(|t - \hat{\tau}| \geq M\), thanks to relation (B.4):

\[
\left| \frac{1}{t-\hat{\tau}} \left( \int_{\hat{\tau}}^{t} \eta(\tau) d\tau \right) - \langle \eta \rangle \right| \leq \varepsilon, \tag{B.6}
\]

which again implies:

\[
\left| \frac{t-\hat{\tau}}{T} \left( \frac{1}{t-\hat{\tau}} \left( \int_{\hat{\tau}}^{t} \eta(\tau) d\tau \right) - \langle \eta \rangle \right) \right| \leq \varepsilon. \tag{B.7}
\]

That concludes the proof.

### B.3 Proof of convergence of \(\lim_{T \to \infty} \frac{\hat{\tau}}{T}\)

When minimizing the cost function \(\int_{0}^{T} \| \ddot{\varphi}(t) \|^2 dt\), the choice of \(\hat{\tau}\) is arbitrary, thus:

\[
\frac{d}{d\hat{\tau}} \left( \int_{0}^{T} \| \ddot{\varphi}(t) \|^2 dt \right) = 0 \tag{B.8}
\]

at the global minimum. We have:

\[
\int_{0}^{T} \| \ddot{\varphi}(t) \|^2 dt = \int_{0}^{T} \left( \| \nu(t) \|^2 + \| f(t) \|^2 \left( \int_{\hat{\tau}}^{t} \eta(\tau) d\tau \right)^2 - 2 \nu(t)^T \eta(t) \int_{\hat{\tau}}^{t} f(t) \right) dt. \tag{B.9}
\]

Thus:

\[
\frac{d}{d\hat{\tau}} \left( \int_{0}^{T} \| \ddot{\varphi}(t) \|^2 dt \right) = -2 \int_{0}^{T} \| f(t) \|^2 \eta(\hat{\tau}) \left( \int_{\hat{\tau}}^{t} \eta(\tau) d\tau \right) dt + 2 \int_{0}^{T} \nu(t)^T f(t) \eta(\hat{\tau}) dt,
\]

\[
= 2\eta(\hat{\tau}) \left( \int_{0}^{T} \nu(t)^T f(t) dt \right) - \int_{\hat{\tau}}^{T} \| f(t) \|^2 \left( \int_{\hat{\tau}}^{t} \eta(\tau) d\tau \right) dt. \tag{B.10}
\]
It can be shown that the $\tilde{\tau}$ such that $\eta(\tilde{\tau}) = 0$ if any, do not correspond to a global minimum. We consequently should have:

$$\int_0^T v(t)^T f(t) dt - \int_0^T \|f(t)\|^2 \left( \int_{\tilde{\tau}}^t \eta(\tau) d\tau \right) dt = 0,$$  \hspace{1cm} (B.12)

for the global minimum (and it exists). On one side:

$$\left| \int_0^T v(t)^T f(t) dt \right| \leq \int_0^T \|v\|^{\infty} \|f\|^{\infty} dt,$$

$$\leq T \|v\|^{\infty} \|f\|^{\infty}.$$  \hspace{1cm} (B.13) (B.14)

On the other, $\int_{\tilde{\tau}}^t \eta(\tau) d\tau \sim (t - \tilde{\tau}) \langle \eta \rangle$, which implies:

$$\left| \int_0^T \|f(t)\|^2 \left( \int_{\tilde{\tau}}^t \eta(\tau) d\tau \right) dt \right| \sim \left| \int_0^T \|f(t)\|^2 (t - \tilde{\tau}) \langle \eta \rangle dt \right|.$$  \hspace{1cm} (B.15)

After integrating by parts:

$$\left| \int_0^T \|f(t)\|^2 (t - \tilde{\tau}) \langle \eta \rangle dt \right| = |\langle \eta \rangle| \left| (T - \tilde{\tau}) \int_0^T \|f(s)\|^2 ds - \int_0^T \int_0^t \|f(s)\|^2 ds dt \right|,$$

$$\sim |\langle \eta \rangle| T(T - \tilde{\tau}) \langle \|f\|^2 \rangle - \frac{T^2}{2} \langle \|f\|^2 \rangle,$$

$$\sim \langle \eta \rangle \langle \|f\|^2 \rangle T^2 \left( \frac{1}{2} - \frac{\tilde{\tau}}{T} \right).$$  \hspace{1cm} (B.16) (B.17) (B.18)

which means that:

$$\left| \int_0^T \|f(t)\|^2 \left( \int_{\tilde{\tau}}^t \eta(\tau) d\tau \right) dt \right| \sim |\langle \eta \rangle| \langle \|f\|^2 \rangle | \times T^2 \left( \frac{1}{2} - \frac{\tilde{\tau}}{T} \right).$$  \hspace{1cm} (B.19)

This relation shows that if $\frac{\tilde{\tau}}{T} \not\to \frac{1}{2}$ as $T \to \infty$, the second term grows as $T^2$ while the first term grows as $T$. This contradicts equation (B.12) and concludes the proof.
Bibliography


