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# Optimal bounds and extremal trajectories for time averages in nonlinear dynamical systems

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ABSTRACT

For any quantity of interest in a system governed by ordinary differential equations, it is natural to seek the largest (or smallest) long-time average among solution trajectories, as well as the extremal trajectories themselves. Upper bounds on time averages can be proved *a priori* using auxiliary functions, the optimal choice of which is a convex optimization problem. We prove that the problems of finding maximal trajectories and minimal auxiliary functions are strongly dual. Thus, auxiliary functions provide arbitrarily sharp upper bounds on time averages. Moreover, any nearly minimal auxiliary function provides phase space volumes in which all nearly maximal trajectories are guaranteed to lie. For polynomial equations, auxiliary functions can be constructed by semidefinite programming, which we illustrate using the Lorenz system.



## 1. Introduction

For dynamical systems governed by ordinary differential equations (ODEs) whose solutions are complicated and perhaps chaotic, the primary interest is often in long-time averages of key quantities. Time averages can depend on initial conditions, so it is natural to seek the largest or smallest averages among all trajectories, as well as the extremal trajectories that realize them. For various purposes including the control of chaos [1], it is valuable to know extremal trajectories regardless of their stability. In other situations one is interested only in stable trajectories, but determining extrema only among these can be prohibitively difficult. The next best option is to determine extrema among all trajectories.

One common way to seek extremal time averages is to construct a large number of candidate trajectories. However, for many nonlinear systems it is challenging both to compute trajectories and to determine that the extremal ones have not been overlooked. In this Letter we study an alternative approach that is broadly applicable and often more tractable: constructing sharp *a priori* bounds on long-time averages. We focus on upper bounds; lower bounds are analogous.

The search for an upper bound on a long-time average can be posed as a convex optimization problem [2], as described in the next section. Its solution requires no knowledge of trajectories. What is optimized is an auxiliary function defined on phase space, similar to but distinct from Lyapunov functions in stability theory. We prove here that the best bound produced by solving this convex optimization problem coincides exactly with the extremal long-time average. That is, arbitrarily sharp bounds on time averages can be produced using increasingly optimal auxiliary functions. Moreover, nearly optimal auxiliary functions yield volumes in phase space where maximal and nearly maximal trajectories must reside. Whether such auxiliary functions can be computed in practice depends on the system being studied, but when the ODE and quantity of interest are polynomial, auxiliary functions can be constructed by solving semidefinite programs (SDPs) [2–4]. The resulting bounds can be arbitrarily sharp. We illustrate these methods using the Lorenz system [5].

Consider a well-posed autonomous ODE on $\mathbb{R}^d$,

$$\tfrac{d}{dt}\mathbf{x} = \mathbf{f}(\mathbf{x}), \tag{1}$$

whose solutions are continuously differentiable in their initial conditions. To guarantee this, we assume that $\mathbf{f}(\mathbf{x})$ is continuously differentiable. Given a continuous quantity of interest $\Phi(\mathbf{x})$, we

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define its *long-time average* along a trajectory $\mathbf{x}(t)$ with initial condition $\mathbf{x}(0) = \mathbf{x}_0$ by

$$\overline{\Phi}(\mathbf{x}_0) = \limsup_{T\to\infty} \frac{1}{T} \int_0^T \Phi(\mathbf{x}(t))\,dt. \tag{2}$$

Time averages could be defined using lim inf instead; our results hold *mutatis mutandis*.[1]

Let $B \subset \mathbb{R}^d$ be a closed bounded region such that trajectories beginning in $B$ remain there. In a dissipative system $B$ could be an absorbing set; in a conservative system $B$ could be defined by constraints on invariants. We are interested in the maximal long-time average among all trajectories eventually remaining in $B$:

$$\overline{\Phi}^* = \max_{\mathbf{x}_0 \in B} \overline{\Phi}(\mathbf{x}_0). \tag{3}$$

As shown below, there exist $\mathbf{x}_0$ attaining the maximum. The fundamental questions addressed here are: what is the value of $\overline{\Phi}^*$, and which trajectories attain it?

## 2. Bounds by convex optimization

Upper bounds on long-time averages can be deduced using the fact that time derivatives of bounded functions average to zero. Given any initial condition $\mathbf{x}_0$ in $B$ and any $V(\mathbf{x})$ in the class $C^1(B)$ of continuously differentiable functions on $B$,[2]

$$\overline{\tfrac{d}{dt}V} = \overline{\mathbf{f}\cdot\nabla V} = 0. \tag{4}$$

This generates an infinite family of functions with the same time average as $\Phi$ since for all such $V$

$$\overline{\Phi} = \overline{\Phi + \mathbf{f}\cdot\nabla V}. \tag{5}$$

Bounding the righthand side pointwise gives

$$\overline{\Phi}(\mathbf{x}_0) \le \max_{\mathbf{x}\in B} \{\Phi + \mathbf{f}\cdot\nabla V\} \tag{6}$$

for all initial conditions $\mathbf{x}_0 \in B$ and *auxiliary functions* $V \in C^1(B)$. Expression (6) is useful since no knowledge of trajectories is needed to evaluate the righthand side.

To obtain the optimal bound implied by (6), we minimize the righthand side over $V$ and maximize the lefthand side over $\mathbf{x}_0$:

$$\max_{\mathbf{x}_0\in B} \overline{\Phi} \le \inf_{V\in C^1(B)} \max_{\mathbf{x}\in B} \{\Phi + \mathbf{f}\cdot\nabla V\}. \tag{7}$$

The minimization over auxiliary functions $V$ in (7) is convex, although minimizers need not exist. The main mathematical result of this Letter is that the lefthand and righthand optimizations are dual variational problems, and moreover that strong duality holds, meaning that (7) can be improved to an equality:

$$\max_{\mathbf{x}_0\in B} \overline{\Phi} = \inf_{V\in C^1(B)} \max_{\mathbf{x}\in B} \{\Phi + \mathbf{f}\cdot\nabla V\}. \tag{8}$$

Thus, arbitrarily sharp bounds on the maximal time average $\overline{\Phi}^*$ can be obtained using increasingly optimal $V$. The result (8) can be considered part of the field of ergodic optimization [6,7], where an analogue for discrete dynamics has been proved.

The auxiliary function method is not the same as the various Lyapunov-type methods used to show stability or boundedness in ODE systems. However, in instances where $\Phi(\mathbf{x})$ approaches infinity as $|\mathbf{x}| \to \infty$, auxiliary functions that are bounded below and imply finite upper bounds $\overline{\Phi} \le U$ also imply the existence of trapping sets by the following argument. Suppose $V \in C^1(\mathbb{R}^d)$ is an auxiliary function for which the maximum of $\Phi + \mathbf{f}\cdot\nabla V$ over $\mathbb{R}^d$ is no larger than $U$. Then,

$$\tfrac{d}{dt}V = \mathbf{f}\cdot\nabla V \le U - \Phi \to -\infty \tag{9}$$

as $|\mathbf{x}| \to \infty$. Expression (9) is a typical Lyapunov-type condition implying that all sufficiently large sublevel sets of $\Phi$ must be trapping sets.

The remainder of this Letter is organized as follows. The next section describes how nearly optimal $V$ can also be used to locate maximal and nearly maximal trajectories in phase space. The section after illustrates these ideas using the Lorenz system, for which we have constructed nearly optimal $V$ by solving SDPs. The final section proves the strong duality (8) and establishes the existence of maximal trajectories.

## 3. Near optimizers

In light of the duality (8), an initial condition $\mathbf{x}_0^*$ and auxiliary function $V^*$ are optimal if and only if they satisfy

$$\overline{\Phi}(\mathbf{x}_0^*) = \max_{\mathbf{x}\in B} \{\Phi + \mathbf{f}\cdot\nabla V^*\}. \tag{10}$$

Even if the infimum over $V$ in (8) is not attained, there exist nearly optimal pairs. That is, for all $\epsilon > 0$ there exist $(\mathbf{x}_0, V)$ for which (6) is within $\epsilon$ of an equality:

$$0 \le \max_{\mathbf{x}\in B} \{\Phi + \mathbf{f}\cdot\nabla V\} - \overline{\Phi}(\mathbf{x}_0) \le \epsilon. \tag{11}$$

In such cases, $\max_{\mathbf{x}\in B}\{\Phi + \mathbf{f}\cdot\nabla V\}$ is within $\epsilon$ of being a sharp upper bound on $\overline{\Phi}^*$, while the trajectory starting at $\mathbf{x}_0$ achieves a time average $\overline{\Phi}$ within $\epsilon$ of $\overline{\Phi}^*$.

Nearly optimal $V$ can be used to locate all trajectories consistent with (11). Moving the constant term inside the time average and subtracting the identity (4) gives

$$0 \le \overline{\max_{\mathbf{x}\in B} \{\Phi + \mathbf{f}\cdot\nabla V\} - (\Phi + \mathbf{f}\cdot\nabla V)} \le \epsilon \tag{12}$$

for such trajectories. The integrand in (12) is nonnegative, and the fraction of time it exceeds $\epsilon$ can be estimated. Consider the set where the integrand is no larger than $M > \epsilon$,

$$\mathcal{S}_M = \left\{ \mathbf{x} \in B : \max_{\mathbf{x}\in B} \{\Phi + \mathbf{f}\cdot\nabla V\} - (\Phi + \mathbf{f}\cdot\nabla V)(\mathbf{x}) \le M \right\}. \tag{13}$$

Let $\mathcal{F}_M(T)$ denote the fraction of time $t \in [0, T]$ during which $\mathbf{x}(t) \in \mathcal{S}_M$. For any trajectory obeying (12), this time fraction is bounded below as

$$\liminf_{T\to\infty} \mathcal{F}_M(T) \ge 1 - \epsilon/M. \tag{14}$$

This follows from an application of Markov's inequality: as the integrand in (12) is nonnegative,

$$\epsilon \ge \overline{M \mathbb{1}_{\mathbf{x}\notin\mathcal{S}_M}} = M\left(1 - \liminf_{T\to\infty} \mathcal{F}_M(T)\right). \tag{15}$$

In practice, it may not be known if there exist trajectories satisfying (11) for a given $V$ and $\epsilon$. Still, the estimate (14) says that any such trajectories would lie in $\mathcal{S}_M$ for a fraction of time no smaller than $1 - \epsilon/M$. The conclusion is strongest when $\epsilon \ll M$, but if $M$ is too large the volume $\mathcal{S}_M$ is large and featureless, failing to distinguish nearly maximal trajectories. The result is most informative

[1] The lim sup and lim inf averages need not coincide on every trajectory, but their maxima over trajectories do.

[2] Here $C^1(B)$ denotes functions on $B$ admitting a continuously differentiable extension to a neighborhood of $B$.