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

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

$$\frac{d}{dt} \mathbf{x} = \mathbf{f}(\mathbf{x})$$

with solutions continuously differentiable in the initial conditions (e.g., continuously differentiable $\mathbf{f}(\mathbf{x})$).

In dynamical systems governed by DEs whose solutions are complicated the primary interest is often in long-time averages of key quantities.

Time averages can depend on initial conditions and it is natural to seek the largest or smallest average among all trajectories, as well as extremal trajectories themselves.
Consider well-posed autonomous ODE on \( \mathbb{R}^d \)

\[
\frac{d}{dt} \mathbf{x} = \mathbf{f}(\mathbf{x})
\]

with solutions continuously differentiable in the initial conditions (e.g., continuously differentiable \( \mathbf{f}(\mathbf{x}) \)).

Given a continuous quantity of interest \( \Phi(\mathbf{x}) \), define its \textit{long-time average} along a trajectory \( \mathbf{x}(t) \) with initial condition \( \mathbf{x}(0) = \mathbf{x}_0 \) by

\[
\overline{\Phi}(\mathbf{x}_0) = \limsup_{T \to \infty} \frac{1}{T} \int_0^T \Phi(\mathbf{x}(t)) \, dt
\]

This can be \( +\infty \) ... so consider “bounded” systems.
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, or 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 $B$:

$$
\Phi^* = \max_{x_0 \in B} \Phi(x_0).
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The fundamental questions we address:

- what is the value of $\Phi^*$, and

- which trajectories attain it?
Upper bounds on time averages follow from the fact that time derivatives of bounded functions average to zero.

Given $x_0$ in $B$ and $V(x) \in C^1(B)$ consider $f(x) \cdot \nabla V(x)$

$$\bar{f} \cdot \nabla V = \frac{d}{dt} V = \lim_{T \to \infty} \frac{1}{T} \int_0^T \frac{dV(x(t))}{dt} dt = \lim_{T \to \infty} \frac{V(x(T)) - V(x(0))}{T} = 0$$

Thus for all such $V$

$$\bar{\Phi} = \Phi + f \cdot \nabla V$$

Bounding the righthand side pointwise gives

$$\bar{\Phi}(x_0) \leq \max_{x \in B} \{ \Phi(x) + f(x) \cdot \nabla V(x) \}$$

This generalizes the “background” method!
We are interested in the maximal long-time average among all trajectories eventually remaining in a closed bounded region such that trajectories beginning in it stay there: in a dissipative or conservative system.

Let $B$ be a closed bounded region such that trajectories beginning in it stay there. Let $\Phi(x)$ be a continuous quantity of interest to compute trajectories and to determine that none have a maximal long-time average.

The fundamental questions we address: What is the value of $\Phi(x)$ on long-time averages. We focus on upper bounds; lower bounds have been overlooked. In this Letter we study an alternative approach to compute trajectories and to determine that none have a maximal long-time average.

Given a continuous quantity of interest $\Phi(x)$, we consider the function $\Phi(x_0) \leq \max_{x \in B} \{ \Phi(x) + f(x) \cdot \nabla V(x) \}$

"Auxiliary function"

To obtain the optimal bound minimize the righthand side over $V$ and maximize the lefthand side over $x_0$:

$$\Phi^* = \max_{x_0 \in B} \Phi \leq \inf_{V \in C^1(B)} \max_{x \in B} \{ \Phi + f \cdot \nabla V \}$$

The minimization over auxiliary functions $V$ is convex although minimizers need not exist.
\[
\Phi(x_0) \leq \max_{x \in B} \{ \Phi(x) + f(x) \cdot \nabla V(x) \}
\]

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\]

The main result is that these optimizations are dual variational problems, and moreover that \textit{strong} duality holds, meaning that it can be improved to an \textit{equality}:

\[
\max_{x_0 \in B} \Phi \equiv \inf_{V \in C^1(B)} \max_{x \in B} \{ \Phi + f \cdot \nabla V \}
\]

\textit{cf. “ergodic optimization”}

Thus arbitrarily sharp bounds on the maximal time average \( \Phi^* \) can be obtained using increasingly optimal \( V \).
\( \overline{\Phi}(x_0) \leq \max_{x \in B} \{ \Phi(x) + f(x) \cdot \nabla V(x) \} \)

To obtain the optimal bound minimize the righthand side over \( V \) and maximize the lefthand side over \( x_0 \):

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The main result is that these optimizations are dual variational problems, and moreover that strong duality holds, meaning that it can be improved to an equality:

\[
\max_{x_0 \in B} \overline{\Phi} = \inf_{V \in C^1(B)} \max_{x \in B} \{ \Phi + f \cdot \nabla V \}
\]

Moreover, nearly optimal \( V \) can be used to locate maximal and nearly maximal trajectories in phase space.
Outline of proof:

\[
\max_{x_0 \in B} \Phi(x_0) = \max_{\mu \in Pr(B)} \int \Phi d\mu \quad \mu \text{ is invariant}
\]

\[
= \sup_{\mu \in Pr(B)} \inf_{V \in C^1(B)} \int (\Phi + f \cdot \nabla V) d\mu
\]

\[
= \inf_{V \in C^1(B)} \sup_{\mu \in Pr(B)} \int (\Phi + f \cdot \nabla V) d\mu
\]

\[
= \inf_{V \in C^1(B)} \max_{x \in B} \{\Phi(x) + f(x) \cdot \nabla V(x)\}
\]
Optimizers, near optimizers & optimal trajectories –

An initial condition $\mathbf{x}_0^*$ and auxiliary function $V^*$ are optimal if and only if they satisfy

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

In that case for the trajectory starting at $\mathbf{x}_0^*$

$$
\Phi(\mathbf{x}(t)) + \mathbf{f}(\mathbf{x}(t)) \cdot \nabla V^*(\mathbf{x}(t)) \overset{\text{almost}}{=} \max_{\mathbf{x} \in B} \{ \Phi + \mathbf{f} \cdot \nabla V^* \}
$$

$$
\overset{\text{always}}{=} \text{constant}
$$

$\Rightarrow$ extremal trajectories $\subset$ max set of $\Phi + \mathbf{f} \cdot \nabla V^*$

... simple example
\[ \dot{x} = x - x^3 = f(x) \]

\[ \Phi(x) = x^2 \]

\[ \Phi(x) + f(x)V'(x) = x^2 + (x - x^3) \cdot x \]

\[ = 2x^2 - x^4 \]

\[ = 1 - (1 - x^2)^2 \]

\[ \leq 1 \quad \forall x \in \mathbb{R} \]
Optimizers, near optimizers & optimal trajectories –

Even if the infimum over $V$ is not attained there are nearly optimal pairs $(x_0, V)$: $\forall \epsilon > 0 \exists (x_0, V)$ for which

$$0 \leq \max_{x \in B} \{ \Phi(x) + f(x) \cdot \nabla V(x) \} - \Phi(x_0) \leq \epsilon$$

with

$$\Phi + f \cdot \nabla V(x_0) \leq \Phi^* \leq \max_{x \in B} \{ \Phi + f \cdot \nabla V \}$$
Optimizers, near optimizers & optimal trajectories –

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\[
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\]

Choose \( M > \epsilon \) and consider the set \( S_M = \)

\[
\left\{ x \in B : \max_{\xi \in B} \{ \Phi(\xi) + f(\xi) \cdot \nabla V(\xi) \} - (\Phi + f \cdot \nabla V)(x) \leq M \right\}
\]

Let \( \mathcal{F}_M(T) = \) the fraction of time \( t \in [0, T] \) during which any nearly optimal \( x(t) \in S_M \). Then

\[
\liminf_{T \to \infty} \mathcal{F}_M(T) \geq 1 - \epsilon/M.
\]
\[ \dot{x} = x - x^3 = f(x) \]

\[ \Phi(x) = x^2 \]

\[ V(x) \neq \frac{1}{2} x^2 \]
How to operationally compute bounds?

Consider polynomial problems

\[ \overline{\Phi}^* \leq U \]

\[ \Phi(x) + f(x) \cdot \nabla V(x) \leq U \]

\[ U - \Phi(x) - f(x) \cdot \nabla V(x) \geq 0 \]

\[ U - \Phi(x) - f(x) \cdot \nabla V(x) \in \text{Pos Poly } (x) \]

\[ U - \Phi(x) - f(x) \cdot \nabla V(x) \in \text{Sum of Squares Poly } (x) \]

Minimizing \( U \) over polynomial \( V(x) \) may be performed via **semidefinite programming**!
Nearly optimal bounds & orbits in Lorenz’s system –

Bounding Averages Rigorously Using Semidefinite Programming: Mean Moments of the Lorenz System

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https://doi.org/10.1007/s00332-017-9421-2
Nearly optimal bounds & orbits in Lorenz’s system – standard chaotic parameters \((b, \sigma, r) = (8/3, 10, 28)\)

\[
\begin{align*}
\dot{x} &= \sigma y - \sigma x \\
\dot{y} &= rx - y - xz \\
\dot{z} &= xy - bz,
\end{align*}
\]

Invariant sets = chaotic attractor plus fixed points (3 of them, all unstable)
Nearly optimal bounds & orbits in Lorenz’s system –
standard chaotic parameters \((b, \sigma, r) = (8/3, 10, 28)\)

... plus periodic orbits \((\infty \# \text{ of them, all unstable})\)
Semidefinite programming produces sharp bounds on 

\[ \Phi(x, y, z) = z, z^2, z^3, x^2, xy, xyz, xyz^2 \]

Each of these \( \Phi \) is maximized on the nonzero equilibria.

\[ z_{eq} = r - 1 \]
Claim: \((r - 1)z^3 \leq (r - 1)^4\)

Proof: use \(\Phi(x, y, z) = (r - 1)z^3\)

\[
V = \frac{1}{4\beta} \left[ \frac{1}{\sigma} x^4 + (y^2 + z^2 - 2rz + 2z)^2 + 8(r - 1)^2 (y^2 + z^2 - 2rz + 2z) + \frac{6}{\sigma} (r - 1)^2 x^2 \right] \\
- \frac{\sigma}{2(1+\sigma)} (r - 1) \left( \frac{1}{\sigma} x + y \right)^2
\]

Then \(\Phi + \mathbf{f} \cdot \nabla V = (r - 1)^4 - \text{Sum of Squares}\)
Level set of
\[ \Phi + f \cdot \nabla V = (r - 1)^4 \]
\[
\max_{x_0} z^4 > (r - 1)^4
\]
Nearly optimal bounds & orbits in Lorenz’s system – standard chaotic parameters $(b, \sigma, r) = (8/3, 10, 28)$

$$\Phi(x, y, z) = z^4 \mid_{\text{fixed points}} = (28 - 1)^4 = 531441$$

TABLE I. Upper bounds on $z^4$ in the Lorenz system computed using polynomial $V(x, y, z)$ of various degrees.

| Degree of $V$ | Upper bound     |
|--------------|-----------------|
| 4            | 635908.         |
| 6            | 595152.         |
| 8            | 592935.         |
| 10           | 592827.568      |
| 12           | 592827.344      |
Any trajectory where $z^4$ is at least $592827 - 1000$ lies in the red region at least 99.97% of the time...
Nearly optimal bounds & orbits in Lorenz’s system –
standard chaotic parameters \((b, \sigma, r) = (8/3, 10, 28)\)

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Underlined digits agree with the value \(\bar{z}^4 \approx 592827.338\) attained on the shortest periodic orbit.
$S_{1000}$ for degree-10 $V(x)$

Any trajectory where $z^4$ is at least $592827 - 1000$ lies in the red region at least 99.97% of the time ...
Summary –

- Optimal extrema exist ...
- Optimal extrema are accessible ...
- Optimal trajectories can be localized ...

Frontiers –

- Partial differential equations ...