Bounding extreme values on attractors using sum-of-squares optimization, with application to the Lorenz attractor

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Abstract

We describe methods for bounding extreme values of quantities on global attractors of differential dynamical systems. Such bounds apply, in particular, along every trajectory at sufficiently late times. The methods use Lyapunov functions to find absorbing sets that contain the global attractor, and the choice of Lyapunov function is optimized based on the quantity whose extreme value one aims to bound. When the governing equations and quantities of interest are polynomials, the optimization constraints require two polynomial expressions to be nonnegative. We enforce nonnegativity by requiring these polynomials to be representable as sums of squares, leading to a convex optimization problem that can be recast as a semidefinite program and solved computationally. This computer assistance makes it possible to construct complicated polynomial Lyapunov functions. We apply these methods to the chaotic Lorenz attractor, bounding extreme values of various moments of the coordinates \((x, y, z)\) using Lyapunov functions of polynomial degrees up to 8. In all cases we obtain bounds that are sharp to three or more significant figures, most of which are much sharper than prior results. Some of the absorbing sets constructed also give precise localizations of the attractor as a whole.

1 Introduction

In many complex systems it is desirable to predict the magnitudes of extreme events—for instance, the maximum height of a rogue wave, or the greatest instantaneous force applied by a turbulent fluid flow. The present work considers extreme events in eventual behavior, as opposed to transient behavior. In particular we consider systems governed by differential equations, especially those with chaotic or otherwise complicated attractors, and we bound the values that quantities of interest can assume on such attractors.

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When solutions of a differential equation cannot be characterized exactly, a common way to estimate their eventual behavior is to find absorbing sets—subsets of phase space that all solutions eventually remain in and which therefore contain the global attractor. These sets can be used to estimate properties of the attractor, including extreme values of various quantities. Absorbing sets can be found using Lyapunov functions, as described below, but generally there exist an infinite number of such functions. A typical approach is to first construct one or several of the simplest possible Lyapunov functions, such as quadratic forms, and then use them to estimate properties of the attractor. In the present work we combine these two steps. For each attractor property to be estimated, the construction of a corresponding Lyapunov function that implies the sharpest bound is posed as an optimization problem.

The construction of optimal Lyapunov functions is difficult in general. Here we restrict attention to ordinary differential equations (ODEs) with polynomial righthand sides because then we can use methods of polynomial optimization. In particular, we formulate sufficient conditions wherein certain polynomials must have sum-of-squares (SOS) representations. The optimization over Lyapunov functions subject to these SOS constraints can be carried out numerically after being recast as a semidefinite program (SDP)—a well studied type of convex optimization problem [5]. The use of SDPs to solve SOS optimization problems has become standard since being pointed out nearly two decades ago [20, 27, 29] and has found numerous applications in the study and control of ODEs. These applications include the construction of Lyapunov functions to show that a solution is attracting, or to approximate a basin of attraction [4, 7, 9, 15, 28, 29, 37, 40], as well as related methods for bounding infinite-time averages [6, 10, 12]. Some progress has been made applying SOS methods to nonlinear PDEs also [13, 14, 16]. These works are similar in spirit to our present method, which was suggested but not applied in [13], but they are not the same. As far as we know, the present study is the first to construct Lyapunov functions by optimizing the bounds that they imply.

Section 2 formulates a convex optimization framework for bounding extreme values on attractors, including an SOS-based version of this framework in cases where all quantities are polynomial. Section 3 reports computational results for the example of the Lorenz attractor. In particular, we bound extreme values of various moments—monomials of the coordinate variables \((x, y, z)\). The method appears to produce arbitrarily sharp bounds as the polynomial degree of Lyapunov functions is raised. For all moments considered here, our bounds on extreme values are sharp to three or more significant figures. All of these bounds are substantially sharper than previously reported estimates, aside from the well known lower bound \(0 \leq z\) which is sharp already. These results complement the similarly sharp bounds on infinite-time averages in the Lorenz equations that we obtained by SOS methods in [12].
2 Optimizing bounds over classes of Lyapunov functions

Consider an autonomous ODE system,

\[ \frac{d}{dt} x(t) = f(x(t)), \quad x(0) = x_0, \]  

(1)

that is well-posed for any initial condition \( x_0 \in \mathbb{R}^n \). Assume that all trajectories \( x(t) \) are continuously differentiable and eventually remain in a bounded subset of \( \mathbb{R}^n \). The latter can be proved by the Lyapunov function methods used in this work. The global attractor \( \mathcal{A} \) of (1) can be defined as the maximal subset of \( \mathbb{R}^n \) that is invariant under the dynamics, or equivalently as the minimal set that attracts all initial conditions in every bounded subset of \( \mathbb{R}^n \) [33].

Let \( \Phi : \mathbb{R}^n \to \mathbb{R} \) denote a quantity of interest in the model (1). Our present objective is to bound the maximum and minimum values of \( \Phi(x) \) over the global attractor \( \mathcal{A} \),

\[ \Phi^+_{\mathcal{A}} := \max_{\mathcal{A}} \Phi(x), \quad \Phi^-_{\mathcal{A}} := \min_{\mathcal{A}} \Phi(x). \]  

(2)

Our objective is to compute upper bounds on \( \Phi^+_{\mathcal{A}} \) and lower bounds on \( \Phi^-_{\mathcal{A}} \). Such results also bound values of \( \Phi \) along all trajectories \( x(t) \) at sufficiently late times; the forward-time limit points of the system are a subset of the global attractor, and therefore

\[ \Phi^-_{\mathcal{A}} \leq \inf_{x_0 \in \mathbb{R}^n} \liminf_{t \to \infty} \Phi(x(t)) \leq \sup_{x_0 \in \mathbb{R}^n} \limsup_{t \to \infty} \Phi(x(t)) \leq \Phi^+_{\mathcal{A}}. \]  

(3)

It suffices to discuss upper bounds since lower bounds on \( \Phi^-_{\mathcal{A}} \) are equivalent to upper bounds on \( (-\Phi)^+_{\infty} \).

We bound \( \Phi^+_{\mathcal{A}} \) above by constructing absorbing sets. Every absorbing set contains \( \mathcal{A} \), so the maximum of \( \Phi \) over any absorbing set is an upper bound on \( \Phi^+_{\mathcal{A}} \). Like many authors, we find absorbing sets using continuously differentiable Lyapunov functions, \( V : \mathbb{R}^n \to \mathbb{R} \). Recalling that \( \frac{d}{dt} V(x(t)) = \mathbf{f} \cdot \nabla V(x(t)) \) along all trajectories of (1), we seek \( V(x) \) satisfying

\[ \lambda \mathbf{f} \cdot \nabla V(x) \leq C - V(x) \]  

(4)

throughout \( \mathbb{R}^n \) for some \( C \in \mathbb{R} \) and \( \lambda > 0 \). Applying Gronwall’s lemma to (4) gives

\( V(x(t)) - C \leq e^{-t/\lambda} [V(x_0) - C] \),

which implies that the set

\[ \Omega^C_V := \{ x \in \mathbb{R}^n : V(x) \leq C \} \]  

(5)

is absorbing. This yields the upper bound

\[ \Phi^+_{\mathcal{A}} \leq \max_{x \in \Omega^C_V} \Phi(x). \]  

(6)

The righthand maximum can be prohibitively difficult to evaluate for complicated \( V \). We avoid this difficulty by adding a second constraint on \( V \): we require not only that (4)
hold but also that $\Phi(x) \leq V(x)$ on all of $\mathbb{R}^n$. Both inequalities together imply the upper bound $\Phi_A^+ \leq C$. Then it is natural to seek the best upper bound that can be proved using Lyapunov functions within some class $\mathcal{V}$:

$$\Phi_A^+ \leq \inf_{\lambda \in \mathbb{R}} \min_{V \in \mathcal{V}} C \quad s.t. \quad \begin{align*}
V(x) - \Phi(x) &\geq 0 \forall x \in \mathbb{R}^n, \\
C - V(x) - \lambda f \cdot \nabla V(x) &\geq 0 \forall x \in \mathbb{R}^n.
\end{align*}$$

(7)

The optimization (7) is convex in $V$ for each fixed value of $\lambda$, as long as $\mathcal{V}$ is a convex set of functions. This convexity makes it tractable to optimize bounds in certain cases, which is why we favor the inequalities in (7) over other sufficient conditions for $\Phi_A^+ \leq C$. Many previous authors have taken a different approach, choosing a particular function or simple ansatz for $V$ at the start of their analyses. With $V$ so fixed, one can use more complicated sufficient conditions that might give absorbing sets $\Omega_C^\mathcal{V}$ with smaller values of $C$ than can be obtained using (4).\footnote{One weaker sufficient condition is to let $C$ be the maximum of $V$ on the set where $f \cdot \nabla V$ vanishes [18]. This amounts to imposing (4) on that set instead of on $\mathbb{R}^n$; the value $C$ is attained at a stationary point of the Lagrangian $V + \lambda f \cdot \nabla V$, where here $\lambda$ is a Lagrange multiplier. Additionally, constraints on $V$ can be restricted to subsets of $\mathbb{R}^n$ already known to be absorbing, and various absorbing sets can be intersected to produce a smaller absorbing set.} Nonetheless, there are many cases in the literature where the best bounds on extreme values are not close to being sharp. We propose that better bounds can be obtained by considering larger classes of Lyapunov functions, even with suboptimal sufficient conditions. This is borne out by the bounds for the Lorenz attractor that we report in the next section.

Optimization over Lyapunov functions as in (7) can be carried out by methods of polynomial optimization if the ODE righthand side $f(x)$ and quantity of interest $\Phi(x)$ are both polynomials. Henceforth we assume this is the case, and we let the class of Lyapunov functions be the set of real polynomials in $n$ variables up to a specified degree $d$—that is, $\mathcal{V} = \mathbb{R}[x]_{n,d}$. The inequalities in (7) then require nonnegativity of two multivariable polynomials. Deciding whether a polynomial is nonnegative has NP-hard computational complexity unless $n$ or $d$ is small [26], and we want to optimize among higher-degree Lyapunov functions for which such computations would be intractable. Thus we employ a standard SOS relaxation, replacing nonnegativity of a polynomial with the generally stronger constraint that the polynomial can be represented as a sum of squares of other polynomials [30]. The resulting SOS optimization is

$$\Phi_A^+ \leq \inf_{\lambda \in \mathbb{R}} \min_{V \in \mathbb{R}[x]_{n,d}} C \quad s.t. \quad \begin{align*}
V(x) - \Phi(x) &\in \Sigma_n, \\
C - V(x) - \lambda f \cdot \nabla V(x) &\in \Sigma_n,
\end{align*}$$

(8)

where $\Sigma_n$ denotes the set of SOS polynomials in $n$ variables. The best bounds provable using this framework improve or remain unchanged as the degree $d$ of $V$ is raised. In the typical situation where $V$ has a higher polynomial degree than $\Phi$, the first constraint in (8) requires that $d$ is even. The second constraint requires that the degree of $f \cdot \nabla V$ is even also.
The inner minimization in (8) is equivalent to a semidefinite program (SDP) because the SOS constraints and optimization objective are linear in the tunable variables [30]. This linearity is why we do not optimize over \( \lambda \) simultaneously, instead tuning \( C \) and the coefficients of \( V \) with \( \lambda \) fixed. The outer minimization might be difficult in some cases since the dependence of the inner minimum on \( \lambda \) need not be convex or even continuous. It is only a one-dimensional search, however, and at least for the Lorenz equations we find simple dependence on \( \lambda \).

3 Bounds for the Lorenz attractor

To test the quality of bounds computed using (8) we consider the Lorenz equations [24], in which case the components of the generic ODE (1) are

\[
\mathbf{x} = (x, y, z), \quad \mathbf{f} = (-\sigma x + \sigma y, rx - y - xz, -\beta z + xy).
\]

We consider only the standard chaotic parameter values \((\beta, \sigma, r) = (8/3, 10, 28)\), at which there exists a strange attractor to which almost every trajectory tends [39]. Invariant structures embedded in this attractor include an equilibrium at the origin and an infinite number of periodic orbits, as well as their unstable manifolds [34]. The global attractor includes all such structures, as well as two equilibria at the points \( \mathbf{x}_\pm = (\pm 6\sqrt{2}, \pm 6\sqrt{2}, 27) \), and their unstable manifolds. Our bounds apply to extreme values over this global attractor.

We have computed bounds for various moments of the coordinates, meaning \( \Phi = x^l y^m z^n \) where the exponents are nonnegative integers. More general polynomial \( \Phi(x, y, z) \) can be bounded just as easily. Bounds were computed by solving (8) as described above—sweeping through \( \lambda \) and solving the inner minimization as an SDP— with polynomial \( V(x, y, z) \) of even degrees up to 8. The ansatz for \( V \) need not be fully general: the requirement that \( \mathbf{f} \cdot \nabla V \) be of even degree requires that all highest-degree terms of \( V \) take the form \( x^p (y^2 + z^2)^q \) [12, 36]. For \( \Phi \) that are invariant under the symmetry \((x, y) \mapsto (-x, -y)\) of the Lorenz equations, we further find that optimal \( V \) contain only symmetric monomials, as when bounding time averages by a related method [12, 13]. The software YALMIP [22, 23] was used to translate SOS formulations into SDPs, which were solved using MOSEK [25]. The ODE variables were rescale by \((x, y, z) \mapsto 25(x, y, z)\) to improve SDP conditioning as in [12], after which MOSEK converged with relative infeasibilities below \(5 \times 10^{-7}\) in all cases.

In order to judge the sharpness of our bounds we have sought extreme values of each \( \Phi \) among particular trajectories of the Lorenz equations. Such a search might be impossible in more complicated systems, which is one motivation for our bounding approach, but it is possible here. Trajectories we examined include numerical integrations beginning from random initial conditions (with initial transients removed), numerical integration approximating the one-dimensional unstable manifold of the origin, and the many periodic orbits computed by Viswanth [41, 42]. It is on the origin or its unstable manifold that
Figure 1: Upper bounds $C$ on the maximum of $x$ over the Lorenz global attractor at the standard parameters. The bounds are optima of the inner minimization in (8) for various $\lambda$ and polynomial $V$ of degree 2 (····), 4 (···), 6 (·--), and 8 (----).

we find the largest and smallest values of each $\Phi$, and the closeness of these values to our computed bounds suggests that they are indeed global extrema. Numerical integration from random initial conditions does not give very good approximations to these various extrema; integrating for $10^7$ times steps of size 0.005 gives values that share one or two significant figures with the true extrema, but no more.

Bounds produced by the inner minimization problem in (8) depend on $\lambda$ and the degree of $V$ in similar ways for all $\Phi$ bounded here. As a typical example, figure 1 shows this dependence for upper bounds on the maximum of $x$. For all $\Phi$, our computations give finite bounds with degree-$d$ Lyapunov functions when $\lambda \geq 1/d$, and the bounds are convex in $\lambda$ on these intervals. Thus it is not hard to optimize $\lambda$ over these intervals, which apparently suffices to give arbitrarily sharp bounds as the degree of $V$ is raised. However, this dependence of $C$ on $\lambda$ is particular to the Lorenz equations. As an example of the absorbing sets $\Omega_V^C$ that give the bounds on $x$ reported in figure 1, let us consider quadratic and quartic $V$ at the optimal values of $\lambda \approx 0.5659$ and $\lambda \approx 0.3743$, respectively. Figure 2 shows the quadratic and quartic absorbing sets $\Omega_V^C$, where $V$ and $C$ solve the inner minimization in (8) at the specified $\lambda$ values. Also shown in figure 2 is a numerical approximation to the unstable manifold of the origin, which is part of the global

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2For the Lorenz equations, terms in $V$ of the form $c_1 x^d$, $c_2 y^d$, and $c_3 z^d$ produce terms in $-(V + \lambda \mathbf{f} \cdot \nabla V)$ of the form $c_1(-1 + \sigma \lambda d)x^d$, $c_2(-1 + \lambda d)y^d$, and $c_3(-1 + \beta \lambda d)z^d$, respectively. The latter three coefficients must be nonnegative in order for the second constraint in (8) to hold. At the standard parameters this requires $\lambda \geq 1/d$ if $c_1, c_2, c_3 > 0$. In most cases we obtain finite bounds only when $c_1, c_2, c_3 > 0$, and thus only when $\lambda \geq 1/d$ also. An exception is the lower bound on $z$ with quadratic $V$, where finite bounds are possible with $c_2 = 0$ and $\lambda = 3/8 \notin [1/2, \infty)$. 

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Figure 2: Absorbing sets $\Omega^C_V$ that give our best bounds $x \leq C$ with Lyapunov functions $V$ of degree 2 (……) and 4 (---). Each $(V,C)$ pair solves the inner minimization in (8) with $\lambda = 0.5659$ and $\lambda = 0.3743$, respectively. The plotted curves are boundaries of the projections of $\Omega^C_V$ onto the $xz$-plane. Also shown are numerically integrated trajectories (——) starting along each half of the origin’s unstable manifold.

Figure 3: Absorbing set $\Omega^C_V$ for the degree-8 $V$ that minimizes the resulting upper bound on $z$ with the near-optimal value $\lambda = 3/8$. Also shown are numerically integrated trajectories starting along each half of the origin’s unstable manifold.
attractor. Evidently the quartic absorbing set implies a much sharper upper bound on \( x \) than the quadratic set does.

Absorbing sets constructed by solving (8) do not necessary localize the global attractor well since this is not the optimization objective. The quartic absorbing set in figure 2 provides a very good bound on \( x \) but a poor localization of the attractor as a whole. Surprisingly, some other absorbing sets constructed by solving (8) nonetheless localize the global attractor well. Figure 3 shows one such \( \Omega^C_V \), which was constructed by optimizing upper bounds on \( z \) using \( V \) of degree 8. This may be the smallest absorbing set that has been reported for the Lorenz attractor. It would be harder to minimize the volume of \( \Omega^C_V \) directly because this volume does not have convex dependence on the coefficients of \( V \).

For all moments \( x^l y^m z^n \) considered here, we have computed bounds on extreme values over the Lorenz attractor that are either exactly sharp or very close to being so. For the example of upper bounds on \( x \), this sharpness can be inferred from the quartic \( \Omega^C_V \) in figure 2. Our upper bounds on \( x \) and other moments up to cubic degree are given in table 1, alongside the apparently maximal values found on the unstable manifold of the origin. For convenience the tabulated values are normalized by each quantity’s magnitude at the nonzero fixed points \( x_{\pm} \). At the standard parameters these normalized moments are

\[
\Phi = \frac{x^l y^m z^n}{|x^l y^m z^n|_{x_{\pm}}} = \frac{x^l y^m z^n}{(6\sqrt{2})^{l+m}2^m n}.
\]

(10)

Quadratic Lyapunov functions, to which many past studies have been confined, do not produce particularly good bounds. On the other hand, \( V \) of degree 4 and 6 produce upper bounds for all 13 moments that are sharp to at least 2 and 4 significant figures, respectively.

As for lower bounds on minimum values over the Lorenz attractor, many can be anticipated without additional computation. Manifestly nonnegative moments such as \( x^2 \) attain their minima on the equilibrium at the origin. For moments that are antisymmetric under the symmetry \((x, y) \mapsto (-x, -y)\) of the Lorenz equations, the upper bound \( \Phi^+_A \leq C \) implies the lower bound \(-C \leq \Phi^-_A\). We thus compute lower bounds only for symmetric moments that are not obviously nonnegative. Table 2 reports our lower bounds on such moments up to cubic degree, computed by solving (8) for upper bounds on \( \Phi = -x^l y^m z^n \). In all cases, the bounds appear to become sharp as the degree of \( V \) is raised.

Complications arise with the lower bounds on \( z, x^2 z \), and \( y^2 z \) that do not arise in our other examples. These three quantities are minimized at the origin, whereas all other extrema we have bounded appear to occur elsewhere on the origin’s unstable manifold. The sharp lower bound \( 0 \leq z \) can be proved using the sufficient condition (4) with quadratic \( V \) only if \( \lambda = 3/8 \), but a naive search over \( \lambda \) may not find this result since other \( \lambda \) values smaller than 1/2 do not give finite bounds.\(^3\) Raising the degree of \( V \) to \( d \geq 4 \) removes this

\(^3\)With \( \lambda = 1/\beta, C = 0, \Phi = -z \), the quadratic Lyapunov function \( V = -z + \frac{1}{\beta} x^2 \) satisfies (4) and thus proves the known result \( z \geq \frac{1}{\beta x^2} \). In the past this has been proved by showing that a condition like (4) holds on a compact set already known to be absorbing [11, 34], but choosing \( \lambda = 3/8 \) makes (4) hold on all of phase space.
Table 1: Upper bounds on the maxima over the Lorenz global attractor of all normalized moments (10) up to cubic degree, computed by solving (8) with $V$ of degree 2, 4, and 6. Powers of $x, y, z$ are omitted since their extrema are determined by those of $x, y, z$. Also shown is each moment’s maximum known value, which occurs along the unstable manifold of the origin. Numerically computed bounds are rounded to the precision shown. Corresponding values of $\lambda$ are given by table 3 in Appendix A.

| Moment | Normalized upper bounds | Maximum |
|--------|-------------------------|---------|
|        | deg 2 | deg 4 | deg 6 | deg 6 |
| $x$    | 3.9317 | 2.3378 | 2.3365 | 2.3365 |
| $y$    | 3.4081 | 3.2630 | 3.2630 | 3.2630 |
| $z$    | 2.1081 | 1.7943 | 1.7912 | 1.7912 |
| $xy$   | 10.1143 | 6.8780 | 6.8699 | 6.8698 |
| $xz$   | 7.9238 | 3.9949 | 3.9872 | 3.9872 |
| $yz$   | 4.6415 | 4.0834 | 4.0832 | 4.0832 |
| $x^2y$ | 15.2385 | 15.2288 | 15.2288 | 15.2288 |
| $x^2z$ | 21.9543 | 21.9483 | 21.9483 | 21.9483 |
| $xy^2$ | 9.4056 | 9.3945 | 9.3944 | 9.3944 |
| $xyz$  | 7.0518 | 7.0276 | 7.0276 | 7.0276 |
| $x^2z$ | 12.2374 | 12.2258 | 12.2258 | 12.2258 |
| $yz^2$ | 6.1676 | 6.1668 | 6.1668 | 6.1668 |

Table 2: Lower bounds on the minima over the Lorenz global attractor of normalized symmetric moments (10) up to cubic degree, computed by solving (8) with $V$ of degree 2, 4, 6, and 8. Also shown is each moment’s minimum known value, which occurs along the unstable manifold of the origin. Corresponding values of $\lambda$ are given by table 4 in Appendix A.

| Moment | Normalized lower bounds | Minimum |
|--------|-------------------------|---------|
|        | deg 2 | deg 4 | deg 6 | deg 8 | deg 8 |
| $z$    | 0     | 0     | 0     | 0     | 0     |
| $xy$   | −10.1143 | −1.5644 | −0.9048 | −0.9042 | −0.9042 |
| $x^2z$ | −0.3484 | −0.0177 | −0.0013 | 0     | 0     |
| $xyz$  | −2.5369 | −1.3920 | −1.3914 | −1.3914 | 0     |
| $y^2z$ | −0.2898 | −0.0309 | −0.0061 | 0     | 0     |
difficulty since then the optimal value $\lambda = 3/8$ falls in the interval $[1/d, \infty)$ over which the lower bound on $z$ is convex in $\lambda$. The nonnegativity of $z$ on the Lorenz attractor implies that $x^2z$ and $y^2z$ are nonnegative also. However, as reflected in table 2, we have not been able to prove exact lower bounds on $x^2z$ and $y^2z$ using the framework (8) alone.

Various bounds on coordinates of the Lorenz equations have appeared in the literature, and bounds on other functions of $(x, y, z)$ can be inferred from known absorbing sets. The bounds reported in tables 1 and 2 are sharper than the best results in the literature, except for the already sharp lower bound $0 \leq z$. For the example of upper bounds on $y$ and $z$, the best prior results we know of are identical to the bounds we report in table 1 for quadratic $V$; both bounds follow from the fact that the cylinder $y^2 + (z - r)^2 \leq \frac{\beta^2 r^2}{4(\beta - 1)}$ is absorbing when $\beta \geq 2$ [8, 21]. These bounds exceed the true maxima of $y$ and $z$ by more than 4% and 17%, respectively, whereas the bounds we compute with quartic $V$ are much sharper. While most authors have considered only quadratic Lyapunov functions, a few have suggested particular quartic functions [18, 31, 35]. None of these quartic functions do as well as our optimized quartic $V$, although the quartic absorbing set of [35] implies bounds on $y$ and $z$ that are slightly better than our quadratic-$V$ results.

Some results in the literature use analyses more complicated than the sufficient condition (4). The best prior upper bound on $x$ seems to be that of [19], whose approach [17] is to first use a quadratic Lyapunov function to show that a certain ellipsoid is absorbing, and then use $V = |x|$ as a Lyapunov function on that ellipsoid. The resulting bound, normalized according to (10), is about 3.180. This is sharper than our quadratic-$V$ bound of 3.9317 but not our quartic-$V$ bound of 2.3378. Similarly, a large number of quadratic Lyapunov functions are constructed in [32] using computer algebra, and the implied bounds are stronger than those of a single quadratic $V$ but weaker than those of quartic $V$. These results reflect the fact that the sufficient condition (4) is not the strongest possible. However, they also suggest that inferring the best possible bound from a particular $V$ is not as important as having a computationally tractable way to optimize $V$ beyond the quadratic case.

4 Conclusions

We have illustrated a method for bounding extreme values of quantities on global attractors. It involves constructing Lyapunov functions by solving convex optimization problems. When all quantities are polynomial, the optimization problems can be cast as semidefinite programs. Applied to the Lorenz attractor at the standard chaotic parameters, our approach produces very sharp bounds on all quantities considered. In most cases they are far sharper than the best results in the literature. The bounds appear to become arbitrarily sharp as the polynomial degree of the Lyapunov function is raised. This is also true of preliminary results for the Kuramoto–Sivashinsky equation that will be reported elsewhere.
A fundamental theoretical question is: under what conditions does the present method produce sharp bounds? In a related optimization framework for bounding infinite-time averages, it has been proved that arbitrarily sharp bounds are possible for bounded trajectories of all well posed differential equations [38]. A similar theorem for the present method would ensure that our success with the Lorenz equations is typical.

The results reported here constitute yet another instance where methods based on polynomial optimization, when applicable, produce stronger results about dynamical systems than any other approach. Related methods have been similarly successful in demonstrating stability [4, 28, 29], bounding time averages [6, 10, 12], and estimating basins of attraction [4, 7, 9, 15, 37, 40]. Application to high-dimensional dynamical systems remains a practical challenge that calls for improving scalability, perhaps by replacing sum-of-squares constraints with stronger constraints that are more computationally tractable [1, 2, 3, 43, 44]. Nevertheless, the further development of polynomial optimization methods for ordinary differential equation is sure to remain fruitful, as is the extension of such methods to partial differential equations.

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A Supplementary results

Tables 3 and 4 give the values of $\lambda$ that appear to solve the outer minimization in (8). For these values, the inner minimization in (8) produces the upper and lower bounds reported in tables 1 and 2, respectively. We believe these $\lambda$ values are optimal but have not proved it. With the exception of the lower bound $0 \leq z$ computed using quadratic $V$, all $\lambda$ values fall in the intervals $[1/d, \infty)$ on which the bounds produced using degree-$d$ $V$ appear to have convex dependence on $\lambda$.

References

[1] A. A. Ahmadi and G. Hall. Sum of squares basis pursuit with linear and second order cone programming. In H. A. Harrington, M. Omar, and M. Wright, editors, Algebr. Geom. methods Discret. Math. American Mathematical Society, 2017.

[2] A. A. Ahmadi and A. Majumdar. DSOS and SDSOS optimization: more tractable alternatives to sum of squares and semidefinite optimization. arXiv:1706.02586v2, 2017.
Table 3: Values of $\lambda$ for which we find the minimum upper bounds in (8) when bounding various moments over the Lorenz global attractor using $V$ of degree 2, 4, and 6. The corresponding upper bounds appear in table 1.

| Moment | $\lambda$ |
|--------|-----------|
|        | deg 2    | deg 4    | deg 6    |
| $x$    | 0.5659   | 0.3743   | 0.3752   |
| $y$    | 0.5      | 0.3749   | 0.3750   |
| $z$    | 0.5808   | 0.3747   | 0.3753   |
| $xy$   | 0.5539   | 0.3778   | 0.3750   |
| $xz$   | 0.5948   | 0.3743   | 0.3750   |
| $yz$   | 0.5      | 0.3749   | 0.3750   |
| $x^2y$ |          | 0.3749   | 0.3750   |
| $x^2z$ |          | 0.3786   | 0.3747   |
| $xy^2$ |          | 0.3737   | 0.3750   |
| $xyz$  |          | 0.3785   | 0.3749   |
| $xz^2$ |          | 0.3750   | 0.3750   |
| $y^2z$ |          | 0.3796   | 0.3750   |
| $yz^2$ |          | 0.3747   | 0.3750   |

Table 4: Values of $\lambda$ for which we find the maximum lower bounds in (8) when bounding various moments over the Lorenz global attractor using $V$ of degree 2, 4, 6, and 8. The corresponding lower bounds appear in table 2.

| Moment | Lower bounds |
|--------|--------------|
|        | deg 2    | deg 4    | deg 6    | deg 8    |
| $z$    | 0.375     |          |          |          |
| $xy$   | 0.5539   | 0.4084   | 0.3753   | 0.3750   |
| $x^2z$ | 0.3879   | 0.2959   | 0.3236   |          |
| $xyz$  | 0.4248   | 0.3755   | 0.3753   |          |
| $y^2z$ | 0.3503   | 0.3118   | 0.2905   |          |
[3] A. A. Ahmadi, S. Dash, and G. Hall. Optimization over structured subsets of positive semidefinite matrices via column generation. *Discret. Optim.*, 24:129–151, 2017.

[4] J. Anderson and A. Papachristodoulou. Advances in computational Lyapunov analysis using sum-of-squares programming. *Discret. Contin. Dyn. Syst. B*, 20:2361–2381, 2015.

[5] S. Boyd and L. Vandenberghe. *Convex Optimization*. Cambridge University Press, 2004.

[6] S. I. Chernyshenko, P. Goulart, D. Huang, and A. Papachristodoulou. Polynomial sum of squares in fluid dynamics: a review with a look ahead. *Philos. Trans. R. Soc. A*, 372:20130350, 2014.

[7] G. Chesi. *Domain of Attraction Analysis and Control via SOS Programming*. Springer, 2011.

[8] C. R. Doering and J. D. Gibbon. On the shape and dimension of the Lorenz attractor. *Dyn. Stab. Syst.*, 10:255–268, 1995.

[9] R. Drummond, G. Valmorbida, and S. R. Duncan. Generalized absolute stability using Lyapunov functions with relaxed positivity conditions. *IEEE Control Syst. Lett.*, 2:207–212, 2018.

[10] G. Fantuzzi, D. Goluskin, D. Huang, and S. I. Chernyshenko. Bounds for deterministic and stochastic dynamical systems using sum-of-squares optimization. *SIAM J. Appl. Dyn. Syst.*, 15:1962–1988, 2016.

[11] H. Giacomini and S. Neukirch. Integrals of motion and the shape of the attractor for the Lorenz model. *Phys. Lett. A*, 227:309–318, 1997.

[12] D. Goluskin. Bounding averages rigorously using semidefinite programming: mean moments of the Lorenz system. *J. Nonlinear Sci.*, 28:621–651, 2018.

[13] D. Goluskin and G. Fantuzzi. Bounds on mean energy in the Kuramoto–Sivashinsky equation computed using semidefinite programming. *arXiv:1802.08240v2*, 2018.

[14] P. J. Goulart and S. Chernyshenko. Global stability analysis of fluid flows using sum-of-squares. *Physica D*, 241:692–704, 2012.

[15] D. Henrion and M. Korda. Convex computation of the region of attraction of polynomial control systems. *IEEE Trans. Automat. Contr.*, 59:297–312, 2014.

[16] D. Huang, S. Chernyshenko, P. Goulart, D. Lasagna, O. Tutty, and F. Fuentes. Sum-of-squares polynomials approach to nonlinear stability of fluid flows: an example of application. *Proc. R. Soc. A*, 471:20150622, 2015.

13
[17] A. P. Krishchenko. Estimations of domains with cycles. Comput. Math. with Appl., 34:325–332, 1997.

[18] A. P. Krishchenko. Localization of invariant compact sets of dynamical systems. Diff. EquaT., 41:1669–1676, 2005.

[19] A. P. Krishchenko and K. E. Starkov. Localization of compact invariant sets of the Lorenz system. Phys. Lett. A, 353:383–388, 2006.

[20] J. B. Lasserre. Global optimization with polynomials and the problem of moments. SIAM J. Optim., 11:796–817, 2001.

[21] G. A. Leonov, A. I. Bunin, and N. Koksch. Attraktorlokalisierung des Lorenz-Systems. ZAMM, 67:649–656, 1987.

[22] J. Löfberg. YALMIP: a toolbox for modeling and optimization in MATLAB. In Proceedings of the CACSD Conference, pages 284–289, Taipei, Taiwan, 2004.

[23] J. Löfberg. Pre- and post-processing sum-of-squares programs in practice. IEEE Trans. Automat. Contr., 54:1007–1011, 2009.

[24] E. N. Lorenz. Deterministic nonperiodic flow. J. Atmos. Sci., 20:130–141, 1963.

[25] MOSEK ApS. The MOSEK optimization toolbox for MATLAB manual. Version 7.1 (Revision 54), 2015.

[26] K. G. Murty and S. N. Kabadi. Some NP-complete problems in quadratic and non-linear programming. Math. Program., 39:117–129, 1987.

[27] Y. Nesterov. Squared functional systems and optimization problems. In H. Frenk, K. Roos, T. Terlaky, and S. Zhang, editors, High performance optimization, pages 405–440. Springer, 2000.

[28] A. Papachristodoulou and S. Prajna. On the construction of Lyapunov functions using the sum of squares decomposition. In Proceedings of the 41st IEEE Conference on Decision and Control, pages 3482–3487, 2002.

[29] P. A. Parrilo. Structured semidefinite programs and semialgebraic geometry methods in robustness and optimization. PhD thesis, California Institute of Technology, 2000.

[30] P. A. Parrilo. Polynomial optimization, sums of squares, and applications. In G. Blekherman, P. A. Parrilo, and R. R. Thomas, editors, Semidefinite optimization and convex algebraic geometry, chapter 3, pages 47–157. SIAM, 2013.

[31] A. Y. Pogromsky, G. Santoboni, and H. Nijmeijer. An ultimate bound on the trajectories of the Lorenz system and its applications. Nonlinearity, 16:1597–1605, 2003.
[32] K. Röbenack, R. Voßwinkel, and H. Richter. Automatic generation of bounds for polynomial systems with application to the Lorenz system. Chaos, Solitons and Fractals, 113:25–30, 2018.

[33] J. C. Robinson. Infinite-dimensional dynamical systems: an introduction to dissipative parabolic PDEs and the theory of global attractors. Cambridge University Press, 2001.

[34] C. Sparrow. The Lorenz equations: bifurcations, chaos, and strange attractors. Springer-Verlag, 1982.

[35] M. Suzuki, N. Sakamoto, and T. Yasukochi. A butterfly-shaped localization set for the Lorenz attractor. Phys. Lett. A, 372:2614–2617, 2008.

[36] P. Swinnerton-Dyer. Bounds for trajectories of the Lorenz equations: an illustration of how to choose Liapunov functions. Phys. Lett. A, 281:161–167, 2001.

[37] W. Tan and A. Packard. Stability region analysis using polynomial and composite polynomial Lyapunov functions and sum-of-squares programming. IEEE Trans. Automat. Contr., 53:565, 2008.

[38] I. Tobasco, D. Goluskin, and C. R. Doering. Optimal bounds and extremal trajectories for time averages in dynamical systems. Phys. Lett. A, 382:382–386, 2018.

[39] W. Tucker. The Lorenz attractor exists. Comptes Rendus l’Académie des Sci. Série I, 328:1197–1202, 1999.

[40] G. Valmorbida and J. Anderson. Region of attration estimation using invariant sets and rational Lyapunov functions. Automatica, 75:37–45, 2017.

[41] D. Viswanath. Symbolic dynamics and periodic orbits of the Lorenz attractor. Nonlinearity, 16:1035–1056, 2003.

[42] D. Viswanath. The fractal property of the Lorenz attractor. Physica D, 190:115–128, 2004.

[43] H. Waki, S. Kim, M. Kojima, and M. Muramatsu. Sums of squares and semidefinite program relaxations for polynomial optimization problems with structured sparsity. SIAM J. Optim., 17:218–242, 2006.

[44] Y. Zheng, G. Fantuzzi, and A. Papachristodoulou. Sparse sum-of-squares (SOS) optimization: A bridge between DSOS/SDSOS and SOS optimization for sparse polynomials. arXiv:1807.05463v1, 2018.