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Peak Estimation and Recovery with Occupation Measures

Jared Miller^{*‡}; Didier Henrion[†]; Mario Sznaier^{*‡}

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Abstract

Peak Estimation aims to find the maximum value of a state function achieved by a dynamical system. This problem is non-convex when considering standard Barrier and Density methods for invariant sets, and has been treated heuristically by using auxiliary functions. A convex formulation based on occupation measures is proposed in this paper to solve peak estimation. This method is dual to the auxiliary function approach. Our method will converge to the optimal solution and can recover trajectories even from approximate solutions. This framework is extended to safety analysis by maximizing the minimum of a set of costs along trajectories.

1 Introduction

The behavior of dynamic systems may be analyzed by bounding state functions along trajectories. If the height of an aircraft along a trajectory falls below a threshold, then the craft will crash into the ground. Other such questions include the amplitude of a rogue wave [17] and the infection rate in an epidemic [21]. These questions may be posed as a peak estimation task. For a system with dynamics f , find the maximum value of a function $p(x)$ for trajectories starting from X_0 running until some maximum time $T \in [0, \infty)$:

$$\begin{aligned} p^* &= \max_{t, x(t)} p(x(t)) \\ \dot{x}(t) &= f(t, x), \quad t \in [0, T] \\ x(0) &\in X_0. \end{aligned} \tag{1}$$

The goal of peak estimation is to find the tight upper bound p^* . It is also desired to recover the optimal trajectories that achieve $p(x(t)) = p^*$ for some time $t \in [0, T]$. Arbitrary lower bounds to p^* are trivial to find: choose an initial point $x_0 \in X_0$ and find the maximum value of $p(x)$ along $x(t \mid x_0)$. Upper bounds of p^* are universal properties and are more

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difficult to compute. This paper focuses on generating a convergent sequence of upper bounds to p^* by translating Problem (1) into a hierarchy of Linear Matrix Inequalities (LMI) in moments of occupation measures [12, 7].

Use of Barrier [18] and Density [19] functions for peak estimation results in non-convex programs. Previous convex work in this area includes [5], which offers sum-of-squares (SOS) criteria for producing upper bounds. Results for safety analysis are presented in [3]. Specialized results for analyzing impulse responses of linear systems are in [4]. This paper introduces a convex program to solve peak estimation with the following advantages over competing approaches:

- The sequence of upper bounds will converge to the global optimum p^* as the relaxation degree tends towards infinity.
- Optimal trajectories (and their estimates) can be recovered from solutions of the LMI relaxations without requiring postprocessing.
- Safety of trajectories can be verified by a numerically robust maximin program of multiple cost functions.

A motivating example of a unit pendulum with friction is provided in Figure 1. Pendulum dynamics with angle θ and angular velocity $\dot{\theta} = \omega$ are $\dot{\omega} = -\sin \theta - 0.1\omega$. The initial set is $X_0 : \theta \in [-\frac{\pi}{2}, \frac{\pi}{2}]$, $\omega \in [-1, 1]$. The $d = 4$ LMI relaxation in Section 3 produces an upper bound on pendulum height of $h_4^* = 1 - \cos \theta^* \approx 1.4682$ over $t \in [0, \infty)$. The initial points generating the optimal trajectory are $x_0 = [\theta_0, \omega_0] = \pm[\frac{\pi}{2}, 1]$, and the peak is achieved at $x_p = \pm[2.058, 0]$ (swing angle of $\theta^* \approx 117.92^\circ$). Figure 1 displays the upper bound as a red plane. The two optimal trajectories are marked by thick blue curves, originating from x_0^* (circles) and reaching the maximum height x_p^* (stars). The black contour is an invariant set of trajectories starting X_0 from the dual LMI.

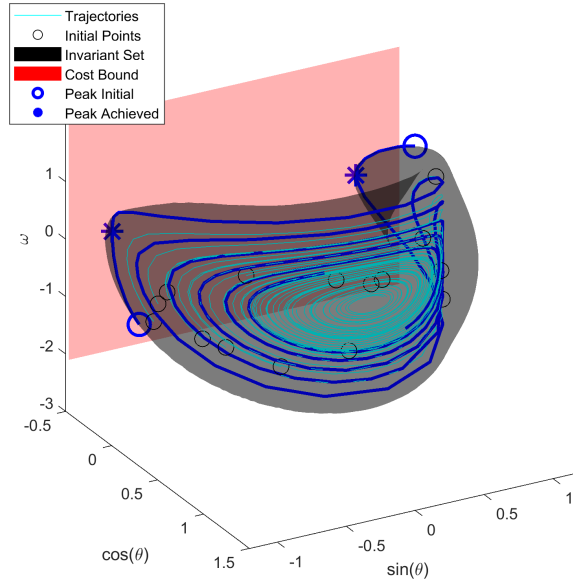


Figure 1: Maximize $h = 1 - \cos \theta$ along pendulum with friction

This paper is organized as follows: Section 2 defines notation and reviews preliminaries. Section 3 introduces the convergent and recoverable peak estimation framework based on occupation measures. Section 4 maximizes the minimum of multiple costs. Section 5 poses safety evaluation as a maximin problem. Section 6 concludes the paper. Appendix A provides proofs of convex duality.

2 Preliminaries

2.1 Notation

\mathbb{R} is the space of real numbers, and \mathbb{R}^n is an n -dimensional real vector space. Let $x = (x_1 \dots x_n)$ be a set of n indeterminate variables. For a set of nonnegative integers $\alpha \in \mathbb{N}_+^n$, the monomial $\prod_{i=1}^n x_i^{\alpha_i} = x^\alpha$ with degree $|\alpha| = \sum_i \alpha_i$. A polynomial $p(x) = \sum_{\alpha \in A} p_\alpha x^\alpha$ for a finite index set A , and the degree of p is the maximum $|\alpha|$ in A . $\mathbb{R}[x]$ is the ring of polynomials in x , and $\mathbb{R}[x]_{\leq d}$ is the subset of polynomials with total degree at most d . A basic semialgebraic set $\mathbb{K} = \{x \mid g_i(x) \geq 0 \ i = 1 \dots N_c\}$ for N_c inequality constraints g_i of bounded degree.

Assume for this paper that $X \subset \mathbb{R}^d$ for some dimension d . Let $C(X)$ be the set of continuous functions defined over X , and $C^1(X)$ has continuous first derivatives. The space of finite signed Borel measures over X is $\mathcal{M}(X)$, which is the topological dual of $C(X)$ with inner product $\langle f, \mu \rangle = \int_X f(x) d\mu$ for $f \in C(X)$ and $\mu \in \mathcal{M}(X)$ if X is compact. The nonnegative subcones of each set $C_+(X)$ and $\mathcal{M}_+(X)$ are dual cones with an induced inner product. If $B \subseteq X$ and $I_B(x)$ is the indicator function on B , then the ‘size’ of B with respect to μ is $\mu(B) = \int_X I_B(x) d\mu = \int_B dx$. The support $\text{supp}(\mu)$ is the smallest closed subset $S \subseteq X$ such that $\mu(X \setminus S) = 0$. $\mu_1 \otimes \mu_2$ denotes the product measure formed by μ_1 and μ_2 . μ is a probability measure on X if $\mu(X) = 1$. The Dirac delta is a probability measure $\delta_x \in \mathcal{M}_+(X)$ with $\text{supp}(\delta_x) = x$.

2.2 Moment-SOS Hierarchy

Convex optimization problems with polynomial objectives may be defined with respect to a nonnegative measure μ :

$$p^* = \max_{\mu \in \mathcal{M}_+(X)} \langle c, \mu \rangle, \quad \mathcal{A}(\mu) = b \quad (2)$$

where $c \in \mathbb{R}[x] \subset C(X)$ is a cost, and \mathcal{A}, b define a set of affine constraints. A measure μ may be parameterized by an infinite sequence of moments $y_\alpha = \langle x^\alpha, \mu \rangle$ such that $\langle p, \mu \rangle = \sum_\alpha p_\alpha y_\alpha$ for all polynomials p . Problem (2) may therefore be expressed as a semi-infinite linear program in terms of the moments y_α , which must be truncated into a problem with a finite number of variables. The moment-sum-of-squares (SOS) hierarchy uses the moment sequence y_α with degree $\alpha \leq d$ for some bound d as variables. Refer to [13] for more details on all material in this subsection.

If $X = \{x \mid g_k(x) \geq 0\}$ is a basic semialgebraic set, define $\mathbb{M}_d(y)$ as the Moment Matrix of degree d and $\mathbb{M}_{d-d_X}(g_X y)$ as the set of localizing matrices for each inequality constraint $g_k(x)$ with degree d_k . Precise definitions of $\mathbb{M}(y)$ and $\mathbb{M}(g_X y)$ are in [13]. The degree- d

relaxation of problem (2) is:

$$p_d^* = \max_y \sum_{\alpha} c_{\alpha} y_{\alpha}, \quad \mathcal{A}(y) = b \quad (3a)$$

$$\mathbb{M}_d(y), \mathbb{M}_{d-d_X}(g_X y) \succeq 0 \quad (3b)$$

The sequence $p_d^* \geq p_{d+1}^* \geq p_{d+2}^* \dots$ is a sequence of upper bounds to the true optimum p^* . For a polynomial optimization problem, the sequence of upper bounds will converge to p^* at a finite degree d if there exists a sufficiently large R such that $X \subset \{x \mid R - \|x\|_2^2 \geq 0\}$ (Archimedean condition). This is verified by a ‘flat extension’ of moment matrices, which is a condition that ensures the rank $\mathbb{M}_{\delta}(y)$ does not increase as the degree $\delta \leq d$ increases [13]. A moment sequence y has a representing measure μ supported at r points in X if $\mathbb{M}_d(y)$ has rank r and the flat extension holds. Each of the r support points are called ‘atoms’, and μ is therefore an rank- r atomic measure. The r atoms may be recovered by an Cholesky decomposition [9]. A rank-1 moment matrix always has a flat extension.

2.3 Occupation Measures

Occupation measures are a valuable tool in solving optimal control and reachable set problems. Resources on this topic include [12, 11]. This section follows the exposition of [10]. For a single initial point $x_0 \in X_0$, the occupation measure $\mu(A \times B \mid x_0)$ is the amount of time the trajectory $x(t \mid x_0)$ spends in the region $A \times B \subseteq [0, T] \times X$:

$$\mu(A \times B \mid x_0) = \int_0^T I_{A \times B}(t, x(t)) dt. \quad (4)$$

The average occupation measure μ yields the μ_0 -weighted time trajectories spend in $A \times B$ for some $\mu_0 \in \mathcal{M}_+(X_0)$:

$$\mu(A \times B) = \int_X \mu(A \times B \mid x_0) d\mu_0(x_0). \quad (5)$$

It holds that $\mu([0, T] \times X) = T$. The final occupation measure is the distribution of $x \in X$ that results after following trajectories in μ_0 for time T :

$$\mu_T(B) = \int_X I_B(x(T \mid x_0)) d\mu_0(x_0). \quad (6)$$

For a test first-order-differentiable function $v(t, x) \in C^1([0, T] \times X)$, the Lie derivative operator \mathcal{L}_f is defined:

$$\mathcal{L}_f v(t, x) = \partial_t v(t, x) + \nabla_x v(t, x)^T f(t, x). \quad (7)$$

The three measures μ_0, μ_T, μ are linked together by Liouville’s Equation which tracks trajectories evolving from μ_0 to μ_T along dynamics f . Liouville’s Equation can be written as a linear equation on measures with the help of test functions $v(t, x) \in C^1([0, T] \times X)$:

$$\delta_T \otimes \mu_T = \delta_0 \otimes \mu_0 + \mathcal{L}_f^{\dagger} \mu \quad (8a)$$

$$\langle v(T, x), \mu_T \rangle = \langle v(0, x), \mu_0 \rangle + \langle \mathcal{L}_f v(t, x), \mu \rangle \quad (8b)$$

where \mathcal{L}_f^{\dagger} is the adjoint of \mathcal{L}_f such that $\langle \mathcal{L}_f v, \mu \rangle = \langle v, \mathcal{L}_f^{\dagger} \mu \rangle$ for any measurable function $v : [0, T] \times X \rightarrow \mathbb{R}$. Moments of each measure can be computed by substituting in $v(t, x) = [t, x]^{\alpha}$ and evaluating the inner product.

2.4 Previous Approaches

A set \mathcal{S} is forward invariant for $t \in [0, T]$ if $x(t) \in \mathcal{S}$ implies that $x(t') \in \mathcal{S}$ for $\forall(t, t') : 0 \leq t \leq t' \leq T$. A value c is an upper bound on the peak p^* of a family of trajectories if the set $X_c = X \cap \{x \mid p(x) \leq c\}$ is forward invariant for trajectories with $x(0) \in X_0$. Barrier [18] and Density [19] functions may be used to prove invariance through SOS methods in case of polynomial dynamics. Computing p^* by infimizing c with Barrier and Density functions are non-convex programs, since the algebraic certificate and value c are multiplied together in constraints.

A bisection approach on c is convex for each fixed c . Infeasibility of an LMI with fixed c has two explanations. Either c is an invalid upper bound ($p^* > c$), or insufficient polynomial degree was used to generate the relaxation. Because the cause of infeasibility cannot be distinguished, bisection of Barrier and Density methods are not a reliable method for peak estimation.

Auxiliary functions have been recently used for convex peak estimation [5]. Sublevel sets of these functions are forward-invariant sets, and bounds to p^* may be computed through SOS methods. The auxiliary function approach is equivalent to the dual program in Section 3.2. The trajectories that achieve p^* cannot be exactly located or recovered from the solution of an auxiliary function program. Instead, the range of initial conditions that may contain the optimal trajectory is localized in a sublevel set of the solved auxiliary functions. Adjoint optimization is used in order to find the initial condition inside the sublevel set [6].

3 Peak Estimation with Occupation Measures

Peak estimation can be formalized as a measure program by defining a new peak measure $\mu_p \in \mathcal{M}_+([0, T] \times X)$, which is a generalization of $\delta_T \otimes \mu_T$ with free terminal time. This section proposes four programs to solve Peak Estimation. The Measure program is a convex infinite-dimensional linear program in measures. The Function program is the convex dual of the Measure program in terms of continuous functions. The LMI program is a finite-degree relaxation of the Measure program that can be solved by semidefinite programming, in contrast to the infinite Measure Program. The SOS program is a finite-degree relaxation of the Function program, and is dual to the LMI program.

3.1 Measure Program

Peak estimation may be posed as a Measure program:

Theorem 3.1. *The following convex program posed over measures has the same optimal value and mutually recoverable solutions as Problem (1):*

$$p^* = \max \langle p(x), \mu_p \rangle \tag{9a}$$

$$\mu_p = \delta_0 \otimes \mu_0 + \mathcal{L}_f^\dagger \mu \tag{9b}$$

$$\mu_0(X_0) = 1 \tag{9c}$$

$$\mu, \mu_p \in \mathcal{M}_+([0, T] \times X) \tag{9d}$$

$$\mu_0 \in \mathcal{M}_+(X_0) \tag{9e}$$

Proof. Let the solution of Problem (1) be $p_{(1)}^*$ and (9) be $p_{(9)}^*$. Theorem 3.1 is proven if $p_{(1)}^* = p_{(9)}^*$ and solutions are mutually recoverable. Each solution trajectory $x^r(t)$ to

Problem (1) that achieves $p_{(1)}^*$ may be encoded by a triple (x_0^r, t_p^r, x_p^r) such that $p_{(1)}^* = p(x_p^r) = p(x(t_p^r | x_0^r))$. A trajectory $x(t)$ in which $p(x)$ is reached multiple times is separated into triples for each attainment.

Let the triple (x_0, t_p, x_p) be a solution to Problem (1). Probability measures $\mu_0 \in \mathcal{M}_+(X_0)$ and $\mu_p \in \mathcal{M}_+([0, T] \times X)$ can be set to $\mu_0 = \delta_{x_0}$ and $\mu_p = \delta_{(t_p, x_p)}$ (rank-1 atomic measures). The occupation measure μ starting from x_0 is defined as in Equation (4) with an endpoint t_p instead of T . The measures (μ_0, μ, μ_p) satisfy constraints (9b)-(9e). The objective $\langle p(x), \mu_p \rangle = p(x_p) = p_{(1)}^*$. As $p_{(1)}^*$ is reached with valid constraints, $p_{(9)}^* \geq p_{(1)}^*$.

To prove the other side $p_{(9)}^* \leq p_{(1)}^*$, select any measures (μ_0, μ, μ_p) that obey constraints (9b)-(9e). The peak measure μ_p is a probability measure given that $\mu_0(X_0) = 1$:

$$\langle 1, \mu_p \rangle = \langle 1, \delta_0 \otimes \mu_0 \rangle + \langle \mathcal{L}_f(1), \mu \rangle = 1 + 0 = 1. \quad (10)$$

For any probability measure $\nu \in \mathcal{M}_+(\mathbb{K})$ for a set \mathbb{K} [13]:

$$\mathbb{E}_\nu[p(x)] = \langle p(x), \nu \rangle \leq \max_{x \in \mathbb{K}} p(x) \quad (11)$$

Solving problem (9) will therefore find a bound $p_{(9)}^* \leq p_{(1)}^*$. The measures reaching $p_{(9)}^*$ are $\mu_0 = \delta_{x_0}$, $\mu_p = \delta_{(t_p, x_p)}$, and μ in Equation (5) w.r.t. μ_0 . As both cost inequalities are satisfied, $p_{(9)}^* = p_{(1)}^*$. The optimal measures in case of $\{(x_0^j, t_p^j, x_p^j)\}_{j=1}^r$ are convex combinations of the admissible single atoms for each triple. For all weights $\alpha \in \mathbb{R}_+^R$ with $\mathbf{1}^T \alpha = 1$, $\mu_0 = \sum_{j=1}^r \alpha_j \delta_{x_0^j}$ and $\mu_p = \sum_{j=1}^r \alpha_j \delta_{(t_p^j, x_p^j)}$. \square

Remark 1. *The mass of the occupation measure $\mu([0, T] \times X) = \langle 1, \mu \rangle$ is equal to the expected time at which the optimal solution is reached:*

$$\langle t, \mu_p \rangle = \langle t, \delta_0 \otimes \mu_0 \rangle + \langle \mathcal{L}_f(t), \mu \rangle = 0 + \langle 1, \mu \rangle + \mathbf{0}^T f. \quad (12)$$

This is distinct from Relation (8a) in which $\langle 1, \mu \rangle = T$. The terminal measure μ_T can be reconstructed by propagating μ_0 along f by Equation (6).

Remark 2. *Two instances in which Problem (1) is solved by an uncountable number of trajectories are if (p, f) admits a continuous symmetry, and if p is a potential function of f ($\exists \lambda \neq 0 \mid \nabla_x p = \lambda f$). Problem (9) then may be solved by non-atomic measures μ_0, μ_p .*

3.2 Function Program

Peak estimation may be dualized into a function program:

Theorem 3.2. *The following program is the dual of Problem (9) (proof of duality in Appendix A.1):*

$$d^* = \min_{\gamma \in \mathbb{R}} \gamma \quad (13a)$$

$$v(0, x) + \gamma \geq 0 \quad \forall x \in X_0 \quad (13b)$$

$$\mathcal{L}_f v(t, x) \geq 0 \quad \forall (t, x) \in [0, T] \times X \quad (13c)$$

$$v(t, x) + p(x) \leq 0 \quad \forall (t, x) \in [0, T] \times X \quad (13d)$$

$$v \in C^1([0, T] \times X) \quad (13e)$$

The function $v(t, x)$ is the dual variable of constraint (9b), and the scalar γ is the dual variable of constraint (9c). $p^* = d^*$ as there is no duality gap between Problems (9) and (13) [16]. The region $v(t, x) \geq -\gamma$ is an invariant set for all trajectories starting in X_0 : $v(t, x)$ starts at a value $\geq -\gamma$ at time $t = 0$ (13b) and increases monotonically along trajectories (13c). Constraint (13d) is an equality at (t_p^*, x_p^*) .

3.3 LMI Program

Assume that the regions X and X_0 are compact basic semialgebraic sets. The measures μ_0, μ, μ_p have moment sequences of y^0, y, y^p up to degree d . μ is supported over entire trajectories and is non-atomic at optimality, so $\mathbb{M}_d(y)$ will have full rank. If $\mathbb{M}_d(y^0)$ has a flat extension, then the atoms of μ_0 are a discrete set of initial points $\{x_0^j\}_{j=1}^r$. Likewise, a flat extension of $\mathbb{M}_d(y^p)$ yields atoms $\{x_p^j\}_{j=1}^{r_p}$ such that $p(x_p^j) = p_d^*$. Numerically evaluating $p^j = \max_{t \in [0, T]} p(x(t | x_0^j))$ yields a lower bound of p^* for each atom j . If the LMI solution at degree d returns an upper bound p_d^* and $|p_d^* - \max_j p^j| \leq \epsilon$ for a sufficiently small $\epsilon > 0$, then p_d^* is approximately global optimal up to the tolerance of the ODE solver. If $\text{Liou}(y^0, y, y^p) = b$ are affine constraints in moments such that Liouville's equation is satisfied, then the degree- d LMI relaxation of Problem (9) is:

$$p_d^* = \max \sum_{\alpha} p_{\alpha} y_{\alpha}^p. \quad (14a)$$

$$\text{Liou}(y^0, y, y^p) = b \quad (14b)$$

$$y_0^0 = 1 \quad (14c)$$

$$\mathbb{M}_d(y^0), \mathbb{M}_d(y), \mathbb{M}_d(y^p) \geq 0 \quad (14d)$$

$$\mathbb{M}_{d-d_{X_0}}(g_{X_0} y^0) \geq 0 \quad (14e)$$

$$\mathbb{M}_{d-d_X}(g_X y), \mathbb{M}_{d-d_X}(g_X y^p) \geq 0 \quad (14f)$$

$$\mathbb{M}_{d-2}(t(T-t)y), \mathbb{M}_{d-2}(t(T-t)y^p) \geq 0. \quad (14g)$$

By relation (10) and (14d), $y_0^p = 1$. When $\mathbb{M}_d(y^0)$ and $\mathbb{M}_d(y^p)$ have a flat extension up to numerical accuracy, estimates for x_0^* , x_p^* and t_p^* can be extracted by methods in [9]. If $\mathbb{M}_d(y^0)$ and $\mathbb{M}_d(y^p)$ are nearly rank-1 (second largest eigenvalue of \mathbb{M}_d is small compared to largest eigenvalue), then x_0^* , x_p^* and t_p^* can be read from the moment sequences y^0 and y^p . Constraints (14b) are of the form $\text{Liou}_{\alpha}(y^0, y, y^p)$ for each monomial α with dual variables v_{α} . At SDP optimality, the degree d SOS problem (13) is solved by $v(t, x) = \sum_{\alpha} v_{\alpha} [t, x]^{\alpha}$ and $\gamma = p_d^*$.

Remark 3. A flat extension of $\mathbb{M}_d(y^0)$ and $\mathbb{M}_d(y^p)$ is insufficient to determine global optimality of (14). It is additionally required that there exists a measure μ supported on the trajectories between $\{x_0^j \rightarrow x_p^j\}_{j=1}^r$ where the first $2d$ moments of μ agree with the truncated moment sequence y . Attempting to prove a ‘flat extension on curves’ to verify global optimality at finite degree is out of scope for this paper, and instead a numerical test is used.

Remark 4. Problem (9) solves (1) even with $T = \infty$. Convergence of (14) to (9) is not guaranteed, as $[0, \infty) \times X$ is non-Archimedean. If $f(t, x) = f(x)$, excluding t from (9) yields an infinite-horizon problem with convergence for compact X . An atomic solution will return x_0^* and x_p^* , but not the time t_p^* for which $x(t_p^* | x_0^*) = x_p^*$.

3.4 SOS Program

Problem (13) is infinite dimensional, as it optimizes over a continuous function $v(t, x)$. Problem (13) may be truncated into a finite dimensional semidefinite program by restricting $v(t, x)$ to polynomials of bounded degree $\mathbb{R}[t, x]_{\leq d}$, and replacing all nonnegativity constraints with Sum of Squares (SOS) constraints. A polynomial $q(x) \in \mathbb{R}[x]$ is SOS ($q(x) \in \Sigma[x]$) if there exists a finite set of polynomials $\{q_i(x)\}_{i=1}^{N_q}$ with bounded degree such that $q(x) = \sum_{i=1}^{N_q} q_i(x)^2$. The SOS reformulation of Problem (13) by the Putinar Positivstellensatz [12] is:

$$d_d^* = \min_{\gamma \in \mathbb{R}} \gamma \quad (15a)$$

$$\sigma_0(x) = v(0, x) + \gamma - \sum_{i=1}^{N_{X_0}} g_{X_0}^i(x) \sigma_{X_0}^i(x) \quad (15b)$$

$$\sigma(t, x) = \mathcal{L}_f v(t, x) - t(T-t)\sigma_{t,f}(t, x) - \sum_{i'=1}^{N_X} g_X^{i'}(x) \sigma_{X,f}^{i'}(t, x) \quad (15c)$$

$$\sigma_p(t, x) = -v(t, x) - p(x) - t(T-t)\sigma_{t,p}(t, x) - \sum_{i=1}^{N_X} g_X^i(x) \sigma_{X,p}^i(t, x) \quad (15d)$$

$$v(t, x) \in \mathbb{R}[t, x]_{\leq d} \quad (15e)$$

$$\sigma_0, \sigma_{X_0}^{i'} \in \Sigma[x] \quad (15f)$$

$$\sigma, \sigma_p, \sigma_{t,f}, \sigma_{X,f}^i, \sigma_{t,p}, \sigma_{X,p}^i \in \Sigma[t, x] \quad (15g)$$

The SOS multipliers $\sigma_0, \sigma, \sigma_p$ are dual to the measures μ_0, μ, μ_p . The polynomials $\sigma_{X_0}^{i'}, \sigma_{t,\cdot}^i, \sigma_{X,\cdot}^i$ ensure that the nonnegativity in constraints (13b)-(13d) hold over their regions of validity. The degrees of the multipliers in (15f)-(15g) must be compatible with degrees of $v(t, x)$, f , g_X , and g_{X_0} .

Remark 5. *Function program (13) is equivalent to the approach in [5], and SOS program (15) is likewise equivalent for continuous bounded degree polynomials $v(t, x)$. The YALMIP [14] SOS preprocessing used in [5] reformulates the SDP into a different set of variables, and the new SDP is no longer dual to the LMI in (14). Approximate moments therefore cannot be recovered by [5].*

3.5 Numerical example

Code in this paper is publicly available at <https://github.com/jarmill/peak/> and was written in MATLAB 2020a. SDPs were formulated in YALMIP [14] and Gloptipoly 3 [8], and solved with Mosek 9.2 [1].

Example 4.1 from [5] is the following system:

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \begin{bmatrix} 0.2x_1 + x_2 - x_2(x_1^2 + x_2^2) \\ -0.4x_1 + x_1(x_1^2 + x_2^2) \end{bmatrix} \quad (16)$$

System (16) features a symmetry $f(-x) = -f(x)$ and has a saddle point at $(0, 0)$ spiraling off into two attractors at $\pm[0.362, 0.971]$. For the infinite-horizon problem of maximizing

$\|x\|_2^2$ while starting at X_0 with $X_0 : \|x\|_2^2 = 0.5$, $X = [-2, 2]^2$, the first six upper bounds are:

$$p_{1:6}^* = [8.000, 2.184, 1.930, 1.922, 1.909, 1.093]$$

Figure 2a plots the optimal trajectories for the $d = 7$ problem with the bound $p_7^* = 1.90318$. Moment matrices obtained by solving Problem (14) are block diagonal due to the central symmetry of the set X_0 and equivariance of $f : f(-x) = -f(x)$ [20]. The optimal $\mathbb{M}_7(y_0), \mathbb{M}_7(y_p)$ are nearly rank-2, but the approximate orbits of $\pm x_0^*$ and $\pm x_p^*$ can be extracted from the nearly rank-1 (second singular value $\leq 1e-4$) matrix of second-order moments. The black dotted curve wrapping around trajectories is the contour $v(x) + \gamma = 0$. Figure 2b compares the extracted x_0^* and x_p^* against a sublevel-set approximation to locations of optimal trajectories and their initial conditions ([5] Sec. 3: $\{x \mid 0 \leq v(x) + p_7^* \leq 0.002, 0 \leq \mathcal{L}_f v(x) \leq 0.004\}$). [5] requires a postprocessing step to locate x_0^* inside the sublevel set.

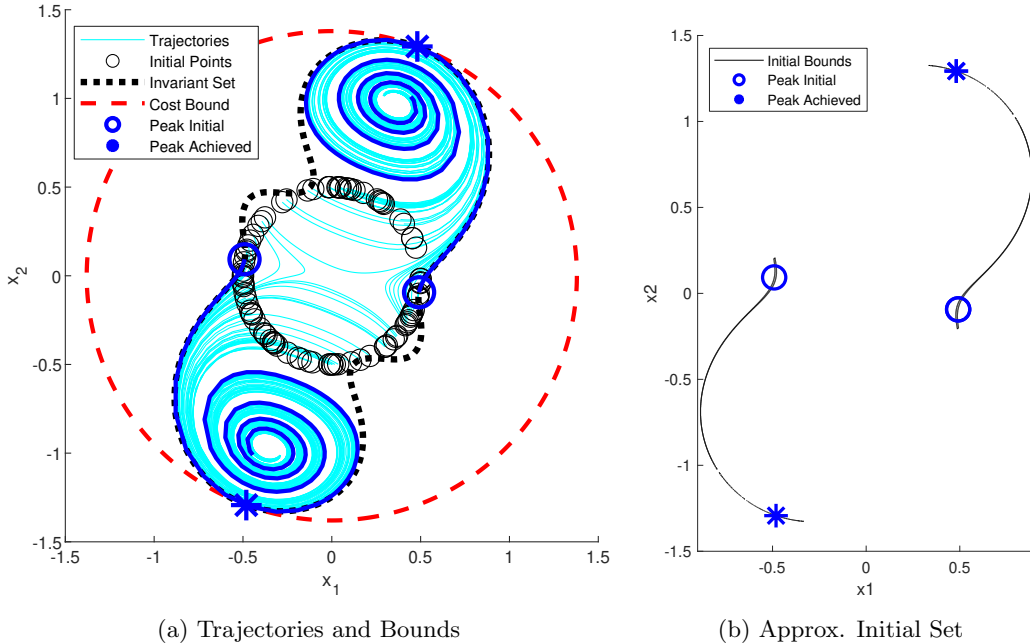


Figure 2: Maximize $\|x\|_2^2$ along (16)

Care must be taken to ensure that the numerical solution to Problem (14) is strictly feasible [15]. Constraint (13c) must be an equality for trajectories along a limit cycle of an autonomous system. Results of these LMIs are typically ‘marginally feasible’ and invalid as polynomials cannot generally match limit cycle trajectories. Examples of this degeneracy are shown in [5] with the Van der Pol oscillator.

4 Maximin Objective

The peak estimation framework presented in section 3 may be used to maximize the minimum (Maximin) of costs for use in safety analysis of trajectories.

4.1 Maximin Formulation

Let $\{p_i(x)\}$ be a finite number of polynomial objectives for $i = 1 \dots N_p$. The new objective aims to maximize the minimum value of all $p_i(x)$ along trajectories. The peak estimation of trajectories (1) can be extended to maximin penalties by adding a new variable q :

$$\begin{aligned}
p^* &= \max_{x(t), t, q} q \\
q &\leq p_i(x(t)) \quad \forall i = 1 \dots N_p \\
x(0) &\in X_0 \\
\dot{x}(t) &= f(x, t) \\
t &\in [0, T] \\
q &\in \mathbb{R}
\end{aligned} \tag{17}$$

Theorem 4.1. *The maximin peak estimation problem may be expressed by the measure program:*

$$p^* = \max_{q \in \mathbb{R}} q \tag{18a}$$

$$\mu_p = \delta_0 \otimes \mu_0 + \mathcal{L}_f^\dagger \mu \tag{18b}$$

$$\mu_0(X_0) = 1 \tag{18c}$$

$$q \leq \langle p_i(x), \mu_p \rangle \quad \forall i = 1 \dots N_p \tag{18d}$$

$$\mu, \mu_p \in \mathcal{M}_+([0, T] \times X) \tag{18e}$$

$$\mu_0 \in \mathcal{M}_+(X_0) \tag{18f}$$

At optimality, q^* is the maximal value of the minimum of all $p_i(x)$ along trajectories. Degree- d LMI relaxations provide a decreasing sequence of upper bounds to p^* . The dual problem may be considered by treating $p(x)$ as the vectorization of $p_i(x)$, and introducing new dual variables β .

$$d^* = \min_{\gamma \in \mathbb{R}} \gamma \tag{19a}$$

$$v(0, x) + \gamma \geq 0 \quad \forall x \in X_0 \tag{19b}$$

$$\mathcal{L}_f v(t, x) \geq 0 \quad \forall (t, x) \in [0, T] \times X \tag{19c}$$

$$v(t, x) + \beta^T p(x) \leq 0 \quad \forall (t, x) \in [0, T] \times X \tag{19d}$$

$$v \in C^1([0, T] \times X) \tag{19e}$$

$$\beta \in \mathbb{R}_{\geq 0}^{N_p} \quad \mathbf{1}^T \beta = 1 \tag{19f}$$

$$\tag{19g}$$

A proof of this duality is in Appendix A.2. At optimality, nonzero β_i indicates that the cost $p_i(x)$ is minimal among all $p_i(x^*)$. An example is the following non-autonomous ODE (Example 2.1 from [5]):

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \begin{bmatrix} x_2 t - 0.1 x_1 - x_1 x_2 \\ x_1 t - x_2 + x_1^2 \end{bmatrix} \tag{20}$$

Figure 3 plots trajectories from equation (20) on the initial set $X_0 : (x_1 + 0.75)^2 + x_2^2 = 1$ and total set $X = [-3, 2] \times [-2, 2]$. Fig. 3a maximizes $p(x) = x_1$ over the time range $[0, 5]$

by a $d = 3$ relaxation, which certifies the bound $p^* \leq p_3^{a*} = 0.4931373$. The second-largest eigenvalue of $M_1(y) = 2.943 \times 10^{-6}$, so the moment matrix is nearly rank-1 and approximate optimal trajectories can be recovered. The nearly optimal trajectory is plotted in blue, and the points $x_0^* = [-1.674, -0.383]$ and $x_p^* = [0.493, 0.029]$ are displayed. The first five bounds are:

$$p_{1:5}^{*a} = [1.5473, 0.4981, 0.4931, 0.4931, 0.4931]$$

Fig. 3b solves the maximin program with $p(x) = [x_1, x_2]$ on system (20). The $d = 3$ bound for times $[0, T]$ is $p_3^{*b} = 0.389115$, which is the value of each coordinate of x_p^* . Optimality is reached at $t_p^* = 1.801$. The optimal $\beta = [0.647, 0.353]$ has both elements nonzero, as $p_1(x_p^*) = p_2(x_p^*) = p_3^{*b}$. The first five maximin bounds are:

$$p_{1:5}^{*b} = [1.0765, 0.3905, 0.3891, 0.3891, 0.3891]$$

Fig. 4 displays the maximin objective $\min(x_1, x_2)$ along trajectories in Fig. 3. Fig. 5 plots the nonnegative (SOS) functions in the dual Program (19) along sampled and optimal trajectories. x_p^* is reached at time $t_p^* = 2.19$, which is indicated by the blue stars on Figs. 4 and 5.

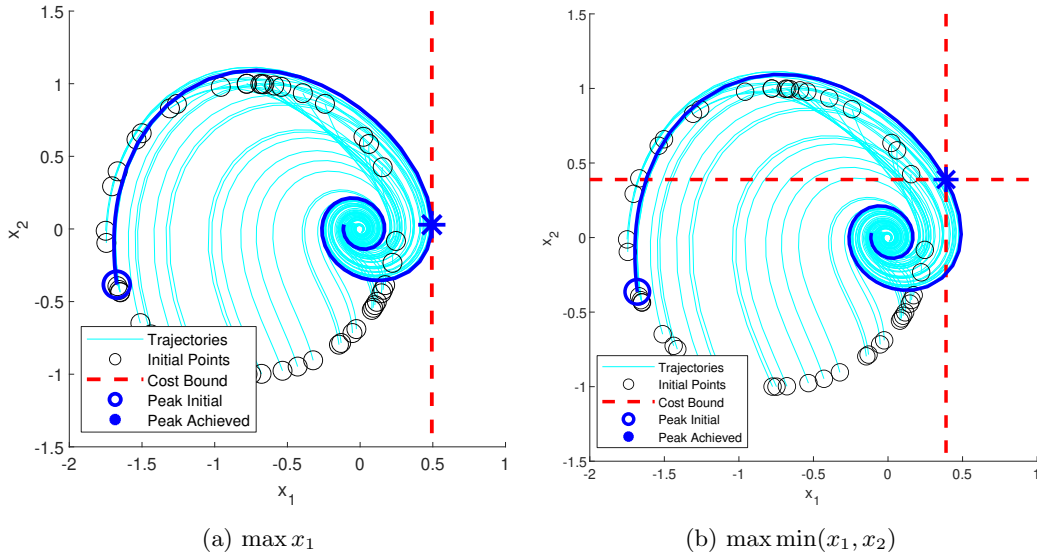


Figure 3: Peak analysis of system (20) at $d = 3$

5 Safety Margins

Assume that X_0 and the unsafe set X_u are basic semialgebraic sets where $X_u = \{x \mid g_i(x) \geq 0 \forall i = 1 \dots N_u\}$. If the maximum value of $\min_i g_i(x)$ is negative for all trajectories starting from X_0 , then X_u is never entered.

Let p_d^* be the optimal value of the degree- d relaxation to Problem (18). A value of $p_d^* < 0$ for any degree d certifies that no trajectory enters X_u , and the magnitude of p_d^* serves as a safety margin. At least one trajectory touches or passes through X_u if the global optimum $p^* \geq 0$.

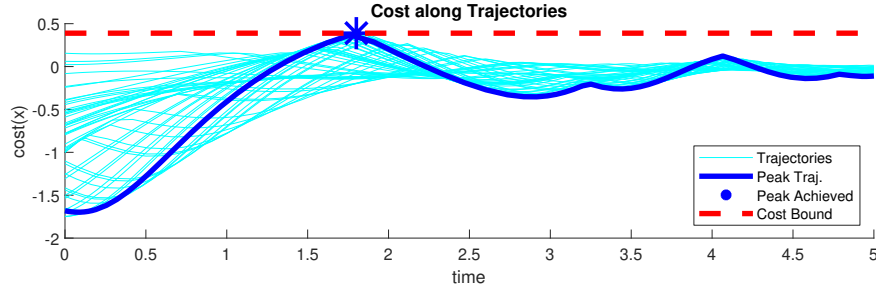


Figure 4: The value of $\min(x_1, x_2)$ along trajectories (20)

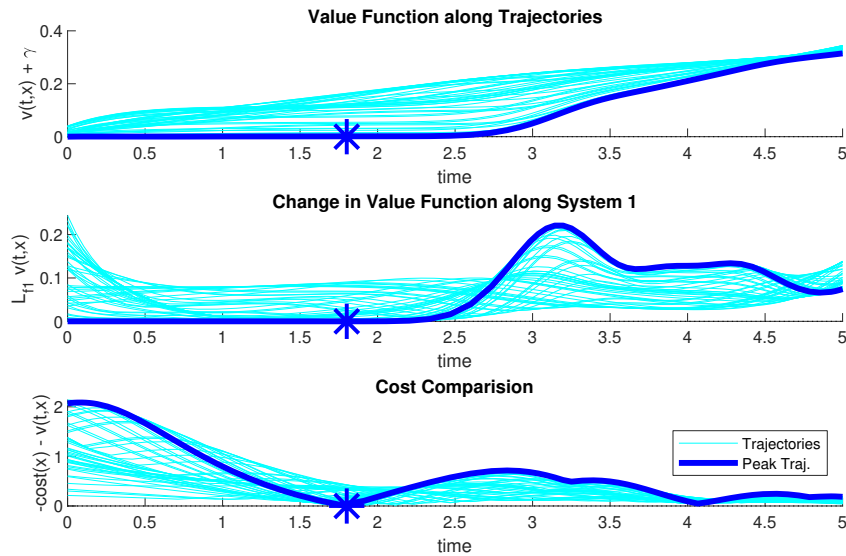


Figure 5: Nonnegativity of Program (19)

Figure 6 demonstrates safety margins on the following system $f(x) = [x_2, -x_1 - x_2 + x_1^3/3]$ from [18] with an infinite-horizon. Trajectories originate from $X_0 : (x_1 - 1.5)^2 + x_2^2 \leq 0.4^2$. The unsafe set is a half-circle formed by a circle with radius $R_u = 0.5$ centered at $C_u = [0, -0.5]$ cut by a half-space $[\cos \theta, \sin \theta]'[x - C_u] \geq 0$ for some angle θ . With $\theta = 5\pi/4$ in Fig. 6a, $p_{3,5}^* = [0.1178, -0.1326, -0.1417]$. All trajectories are safe because $p_4^* < 0$. The flow in Fig. 6b with $\theta = 3\pi/4$ is unsafe, as some trajectory (the approximate optimal trajectory with $d = 5$) passes through X_u . [18] offers a binary determination of safety, and does not indicate how close trajectories approach X_u (measured by p^*). As mentioned in Sec. 2.4, [18] cannot distinguish between unsafety and insufficient degree for $\theta = 3\pi/4$.

Safety verification by occupation measures has been presented in [3] by solving a measure program to find the expected amount of time trajectories spend in X_u . Trajectories never enter X_u if $\mathbb{E}_u[t] = \mathbb{E}[t \mid x(t) \in X_u] = 0$ for any LMI relaxation. Due to numerical inaccuracies, 0 will never be reached even for safe trajectories. The system in Fig. 6a with $\theta = 5\pi/4$ has $\mathbb{E}_u[t] = 2.38 \times 10^{-3} > 0$ with $d = 10$, $T = 5$ even though it is verifiably safe with $p_4^* < 0$. The safety-time criterion is insufficient to prove avoidance, and the safety

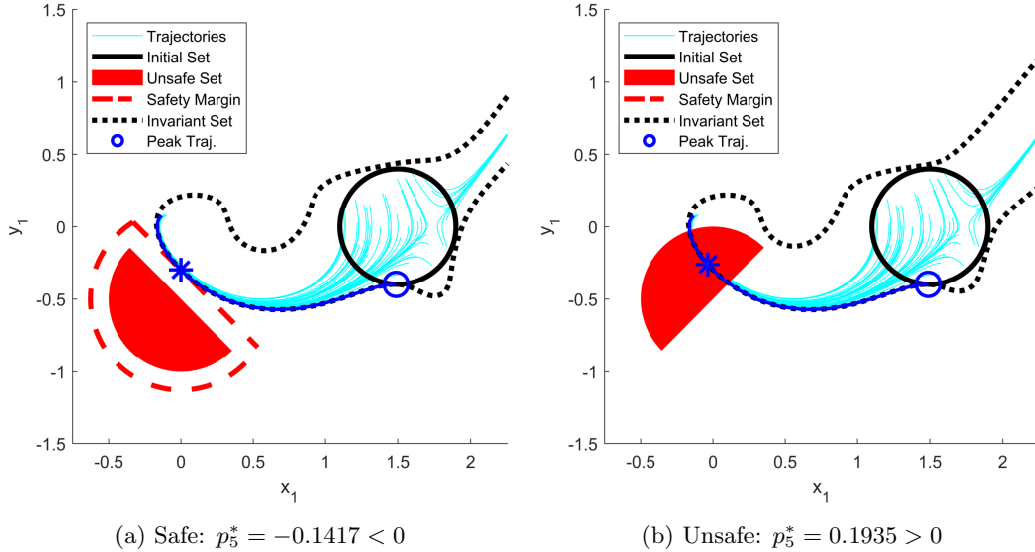


Figure 6: Safety margins for half-circle sets

margin p^* is comparatively a robust metric for safety.

6 Conclusion

This paper presented an occupation measure-based technique to perform peak estimation and obtain a converging and certifiable sequence of upper bounds to the global optimum. Near-optimal trajectories can be immediately recovered from approximate solutions to LMIs. Peak estimation is extended to maximin problems with multiple costs for safety analysis. Future work includes peak estimates for uncertain systems.

A Proofs of Convex Duality

This section proves equivalence between Measure and Function programs, based on methods in [11, 3]. Let \mathcal{K} be a cone with dual cone \mathcal{K}^* , where $\mathcal{K}^* = \{v \mid \langle v, x \rangle \geq 0, \forall x \in \mathcal{K}\}$ for linear functionals v [2]. Further let $c \in \mathcal{K}^*$ be an objective, and $\mathcal{A} : \mathcal{K} \rightarrow \mathcal{R}$ be a linear operator with domain \mathcal{R} , and $b \in \mathcal{R}$ be constraint values. A generic primal-form convex program is:

$$p^* = \sup_{x \in \mathcal{K}} \langle c, x \rangle, \quad \mathcal{A}(x) = b \quad (21)$$

Let the adjoint of \mathcal{A} be $\mathcal{A}^\dagger : \mathcal{R}' \rightarrow \mathcal{K}^*$ where \mathcal{R}' is an affine translation of \mathcal{R}^* (in KKT optimality conditions, $\langle y, \mathcal{A}(x) - b \rangle = \langle y, \mathcal{A}(x) \rangle - \langle b, y \rangle = \langle \mathcal{A}^\dagger(y), x \rangle - \langle b, y \rangle$ [2]). The corresponding dual-form program is:

$$d^* = \inf_{y \in \mathcal{R}'} \langle b, y \rangle, \quad \mathcal{A}^*(y) - c \in \mathcal{K}^* \quad (22)$$

Strong duality holds if $p^* = d^*$. All suprema/infima are attained for peak estimation if X is compact.

A.1 Duality of Programs in Section 3

Program (9) is a primal-form (21) program with quantities:

$$\mathcal{K} = \mathcal{M}_+(X_0) \times \mathcal{M}_+([0, T] \times X)^2 \quad (23a)$$

$$x = [\mu_0, \mu, \mu_p] \quad (23b)$$

$$\mathcal{A}(x) = [\delta_0 \otimes \mu_0 + \mathcal{L}_f^\dagger \mu - \mu_p, \mu_0(X_0)] \quad (23c)$$

$$\mathcal{R} = C^1([0, T] \times X)^* \times \mathbb{R} \quad (23d)$$

The constraints and objective are:

$$c = [0, 0, p(x)], \quad b = [0, 1] \quad (24)$$

The dual problem (22) has:

$$\mathcal{R}' = C^1([0, T] \times X) \times \mathbb{R} \quad (25a)$$

$$y = [v(t, x), \gamma] \quad (25b)$$

$$\mathcal{A}^\dagger(y) = [v(0, x) + \gamma, \mathcal{L}_f v(t, x), -v(t, x)] \quad (25c)$$

$$\mathcal{K}^* = C_+(X_0) \times C_+([0, T] \times X)^2 \quad (25d)$$

Substituting (24) and (25) into (22) yields Problem (13).

A.2 Duality of Programs in Section 4

This section proves the convex duality of Programs (18) and (19). The costs $p(x)$ are a vector of length N_p . New variables q (cost) and α (slack) are added.

$$\mathcal{K} = \mathcal{M}_+(X_0) \times \mathcal{M}_+([0, T] \times X)^2 \times \mathbb{R} \times \mathbb{R}_+^{N_p} \quad (26a)$$

$$x = [\mu_0, \mu, \mu_p, q, \alpha] \quad (26b)$$

$$\mathcal{A}(x) = [\delta_0 \otimes \mu_0 + \mathcal{L}_f^\dagger \mu - \mu_p, \mu_0(X_0), -p(x) + \mathbf{1}q + \alpha] \quad (26c)$$

$$\mathcal{R} = C^1([0, T] \times X)^* \times \mathbb{R} \times \mathbb{R}^{N_p} \quad (26d)$$

The constraints and objective are:

$$c = [0, 0, 0, 1, \mathbf{0}], \quad b = [0, 1, \mathbf{0}] \quad (27)$$

The dual problem (22) has:

$$\mathcal{R}' = C^1([0, T] \times X) \times \mathbb{R} \times \mathbb{R}^{N_p} \quad (28a)$$

$$y = [v(t, x), \gamma, \beta] \quad (28b)$$

$$\mathcal{A}^\dagger(y) = [v(0, x) + \gamma, \mathcal{L}_f v(t, x), -v(t, x) - \beta^T p(x), \mathbf{1}^T \beta, \beta] \quad (28c)$$

$$\mathcal{K}^* = C_+(X_0) \times C_+([0, T] \times X)^2 \times 0 \times \mathbb{R}_+^{N_p} \quad (28d)$$

The last entries of $\mathcal{A}^\dagger(y)$ in (28c) (with c in (25)) are the same as constraint (19d), which proves program equivalence.

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