Data-driven optimal control of nonlinear dynamics under safety constraints

Hongzhe Yu, Joseph Moyalan, Umesh Vaidya, and Yongxin Chen

***Abstract*—This paper considers the optimal control problem of nonlinear systems under safety constraints with unknown dynamics. Departing from the standard optimal control framework based on dynamic programming, we study its dual formulation over the space of occupancy measures. For control-affine dynamics, with proper reparametrization, the problem can be formulated as an infinite-dimensional convex optimization over occupancy measures. Moreover, the safety constraints can be naturally captured by linear constraints in this formulation. Furthermore, this dual formulation can still be approximately obtained by utilizing the Koopman theory when the underlying dynamics are unknown. Finally, to develop a practical method to solve the resulting convex optimization, we choose a polynomial basis and then relax the problem into a semi-definite program (SDP) using sum-of-square (SOS) techniques. Simulation results are presented to demonstrate the efficacy of the developed framework.**

***Index Terms*—Optimal control, Data-driven control, Nonlinear control, Sum-of-square**

I. Introduction

In many real-world applications, one seeks to drive a dynamical system from an initial set to a target region while avoiding certain unsafe regions along the trajectory. This type of reach-safe problem appears in many scenarios in the control and robotics community, such as obstacle avoidance for quadrotors [1] as well as a safe control in human-robot interaction [2], [3]. Furthermore, in real applications, one often encounters a situation where the dynamical model of the plant is hard to obtain. At the same time, a collection of data is relatively easy to be sampled. To overcome this difficulty, data-driven path planning and obstacle avoidance are extensively studied in the literature. In [4], the authors consider the problem of designing finite-horizon safe controllers for a system without an analytical model while only limited data along a single system trajectory are available. In [5], the authors make use of control barrier functions and discrete-time Koopman operators to guarantee the safety of the autonomous systems. However, in most of the above works, the optimality of the control is not investigated.

Lyapunov theory [6] is considered as the most fundamental analytical tool in proving the stability of a given dynamical system. However, in the control synthesis problem, the joint-search of Lyapunov function and a controller is, in general, a non-convex problem. The authors of [7] leverage the notion of Lyapunov density [8] for control affine dynamics and provide a convex formulation by introducing a combined variable in the original bilinear non-convex problem.

In this paper, we formulate the optimal-safety problem into an optimal control problem with safety constraints. We adopt the Lyapunov density and the convex formulation introduced in [7], [8] and combine them with linear operator theory involving Koopman and Perron-Frobenius operator from [9]–[11] for optimal control. With the introduction of the occupancy measure, we incorporate the safety guarantee as a constraint to the obtained convex optimization problem. Towards unknown dynamics, a data-driven approach for optimal control from [11] is adopted in this paper to formulate the optimal control with safety constraints as infinite-dimensional optimization problem. The infinite-dimensional optimization problem is solved by parameterizing it using polynomials and deploying the Sum-of-squares (SOS) techniques [12] along with relaxation approach based on the results of penalty functions [13].

Methods towards solving optimal control problems widely exist in the literature [14], [15]. Dynamic programming numerically solves the Hamilton-Jacobi-Bellman equation. Indirect methods transform the problem into a boundary value problem. Direct methods, on the other hand, first discretize then solve it using nonlinear programming tools. Compared with the existing works, our method provides a convex formulation in a data-driven setting which can be solved efficiently without explicit discretization. The resulted closed-loop dynamics preserves optimality and also satisfies the safety constraints. Our work is closely related to the works in [16]–[19], and is a direct extension of the works in [20] from model-based settings to a data-driven approach. The results of [18] regarding optimal navigation using navigation measures are extended from discrete-time settings to continuous time settings in this paper.

The rest of the paper is structured as follows. In Section II, we provide a brief introduction to our framework's necessary fundamentals. Section III consists of problem formulation and the main theoretical results. In Section IV, we develop the algorithm details based on the SOS techniques. Numerical simulations follow this in Section V and a brief conclusion in Section VI.

II. Background and Notations

In this section we briefly introduce Koopman theory and the sum-of-squares techniques, on which our method relies.

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H. Yu and Y. Chen are with the School of Aerospace Engineering, Georgia Institute of Technology, Atlanta, GA; {hyu419,yongchen}@gatech.edu

J. Moyalan and U. Vaidya are with the Department of Mechanical Engineering, Clemson University, Clemson, SC; {josephraphelm,uvaidya}@clemson.edu

A. Koopman and Perron-Frobenius Operator

Consider the dynamical system

$$\dot{\mathbf{x}}(t) = \mathbf{f}(\mathbf{x}(t)), \;\; \mathbf{x}(t) \in \mathbf{X}, \;\; \mathbf{x}(0) = \mathbf{x}_0, \tag{1}$$

where $\mathbf{X} \subseteq \mathbb{R}^n$ denotes the domain of consideration. We use $\mathbf{s}_t(\mathbf{x}_0)$ and $\mathbf{x}(t)$ interchangeably to denote the non-singular map from initial state $\mathbf{x}_0$ to the solution of dynamical system (1) at time t. We often use $\mathbf{x}$ to denote arbitrary variable in the state space. The operator $\mathbf{s}_{-t}(\mathbf{x})$ represents the initial state of state $\mathbf{x}$ at time t, i.e., $\mathbf{s}_{-t}(\mathbf{x}) = \{\mathbf{y} : \mathbf{s}_t(\mathbf{y}) = \mathbf{x}\}$. Let $\mathcal{B}(\mathbf{X})$ be the Borel σ-algebra of sets on $\mathbf{X}$. For any set $A \in \mathcal{B}(\mathbf{X})$, denote by $\mathbb{1}_A(\mathbf{x})$ the indicator function of A, and $\mathbf{s}_{-t}(A) \triangleq \{\mathbf{x} : \mathbf{s}_t(\mathbf{x}) \in A\}$. Denote by $\mathcal{L}_\infty(\mathbf{X})$, $\mathcal{L}_1(\mathbf{X})$, and $\mathcal{C}^k(\mathbf{X})$ the space of essentially bounded, integrable, and k times continuously differentiable functions on $\mathbf{X}$ respectively. Koopman and Perron-Frobenius operators are two powerful tools to study the system behavior in the lifted function spaces [21].

Definition II.1 (Koopman Operator)**.** $\mathbb{K}_t$ *for dynamical system* (1) *is defined as*

$$[\mathbb{K}_t \varphi](\mathbf{x}) = \varphi(\mathbf{s}_t(\mathbf{x})), \tag{2}$$

where φ is called a test function in the lifted function space $\mathcal{L}_\infty(\mathbf{X}) \bigcap \mathcal{C}^1(\mathbf{X})$. The infinitesimal generator for Koopman operator is defined as

$$\lim_{t\to 0} \frac{[\mathbb{K}_t\varphi](\mathbf{x}) - \varphi(\mathbf{x})}{t} = \mathbf{f}(\mathbf{x}) \cdot \nabla\varphi(\mathbf{x}) =: \mathcal{K}_{\mathbf{f}}\varphi. \tag{3}$$

Definition II.2 (Perron-Frobenius Operator)**.** $\mathbb{P}_t : \mathcal{L}_1(\mathbf{X}) \to \mathcal{L}_1(\mathbf{X})$ *for dynamical system* (1) *is defined as*

$$\int_{\mathbf{s}_{-t}(A)} \psi(\mathbf{x}) d\mathbf{x} = \int_A \mathbb{P}_t[\psi](\mathbf{x}) d\mathbf{x}, \;\; \forall A \subset \mathbf{X}. \tag{4}$$

The infinitesimal generator for the P-F operator is given by

$$\lim_{t\to 0} \frac{[\mathbb{P}_t\psi] - \psi}{t} = -\nabla \cdot (\mathbf{f}(\mathbf{x})\psi(\mathbf{x})) =: \mathcal{P}_{\mathbf{f}}\psi \tag{5}$$

These two operators are dual to each other as

$$\int_{\mathbf{X}} [\mathbb{K}_t\varphi](\mathbf{x})\psi(\mathbf{x}) d\mathbf{x} = \int_{\mathbf{X}} [\mathbb{P}_t\psi](\mathbf{x})\varphi(\mathbf{x}) d\mathbf{x}. \tag{6}$$

Many methods [22]–[24] have been proposed to approximate the Koopman operator $\mathbb{K}_t$. In this paper, we adopt the gEDMD [24] method which approximates the infinitesimal generator $\mathcal{K}_{\mathbf{f}}$ (3) of the Koopman operator. In this method, the data is in pair form as $(\mathbf{x}_k, \dot{\mathbf{x}}_k), k = 1, 2, \ldots, M$. For a given basis $\mathbf{\Psi} = [\psi_1, \ldots, \psi_N]^T$, the gEDMD seeks a matrix $\mathbf{L}$, a matrix representation of the Koopman generator with respect to the basis Ψ, that minimizes

$$\sum_{k=1}^{M} \left\| \dot{\mathbf{\Psi}}(\mathbf{x}_k, \dot{\mathbf{x}}_k) - \mathbf{L}\mathbf{\Psi}(\mathbf{x}_k) \right\|_2^2, \tag{7}$$

where $\dot{\mathbf{\Psi}}(\mathbf{x}_k, \dot{\mathbf{x}}_k) = [\nabla\psi_1(\mathbf{x}_k) \cdot \dot{\mathbf{x}}_k, \ldots, \nabla\psi_N(\mathbf{x}_k) \cdot \dot{\mathbf{x}}_k]^T$. The minimizer is $\mathbf{L}^\star = \mathbf{B}\mathbf{A}^\dagger$ where

$$\mathbf{B} \;=\; \frac{1}{M} \sum_{k=1}^{M} \dot{\mathbf{\Psi}}(\mathbf{x}_k, \dot{\mathbf{x}}_k) \mathbf{\Psi}(\mathbf{x}_k)^T \tag{8a}$$

$$\mathbf{A} \;=\; \frac{1}{M} \sum_{k=1}^{M} \mathbf{\Psi}(\mathbf{x}_k) \mathbf{\Psi}(\mathbf{x}_k)^T. \tag{8b}$$

B. Positive polynomials and Sum-of-squares

We first define the monomial basis

$$\mathbf{\Psi}_d = [1, x_1, \ldots, x_n, x_1^2, x_1x_2, \ldots, x_n^2, \ldots, x_n^d]^T \tag{9}$$

as the concatenation of all the monomials of degree less or equal to d, which has dimension $\binom{n+d}{d}$. Any polynomial $p(\mathbf{x})$ of degree d can be expressed in $\mathbf{\Psi}_d$ with coefficients $C_p \in \mathbb{R}^{\binom{n+d}{d}}$ such that $p(\mathbf{x}) = C_p^T \mathbf{\Psi}_d$. Consider now the problem of verifying the global nonnegativity of a given polynomial with even degree $2d$, i.e., $p(\mathbf{x}) \geq 0, \forall \mathbf{x} = [x_1, \ldots, x_n]^T \in \mathbb{R}^n$. This problem is NP-hard when the degree of polynomial p is greater than 4 [12]. However, when $p(\mathbf{x})$ is of the form $p(\mathbf{x}) = \mathbf{\Psi}_d(\mathbf{x})^T \mathbf{Q} \mathbf{\Psi}_d(\mathbf{x})$ with $\mathbf{Q} \in \mathbb{R}^{\binom{n+d}{d} \times \binom{n+d}{d}}$, this problem is relatively easy to solve as it is equivalent to verifying the semidefinite positiveness of the matrix $\mathbf{Q}$. SOS technique reformulates the positive polynomial problem into a semidefinite program. More specifically, for monomials $\mathbf{\Psi}_{2d}$ and $\mathbf{\Psi}_d$, a polynomial $p(\mathbf{x})$ of degree $2d, p(\mathbf{x}) = C_p^T \mathbf{\Psi}_{2d}$ is globally positive if $\exists \mathbf{Q} \in \mathbb{R}^{\binom{n+d}{d} \times \binom{n+d}{d}}, \mathbf{Q} \succeq 0$ s.t. $p(\mathbf{x}) = \mathbf{\Psi}_d^T \mathbf{Q} \mathbf{\Psi}_d$. There are many available software toolboxes such as SOSTOOLS [25] and SOSOPT [26] which internally conduct the transformation from the problem of positive polynomial to SDP and call the underlying SDP solvers such as SEDUMI [27]. We define the existence of SOS decomposition of a given polynomial $p(\mathbf{x})$ as "$p(\mathbf{x}) \in SOS$".

III. Optimal-safety control problem

We consider hereafter the control system

$$\dot{\mathbf{x}}(t) = \mathbf{F}(\mathbf{x}(t), \mathbf{u}(\mathbf{x}(t))), \mathbf{x}(t) \in \mathbf{X} \subseteq \mathbb{R}^n, \mathbf{x}(0) = \mathbf{x}_0, \tag{10}$$

where $\mathbf{u} \in \mathbb{R}^m$ is the control input and $\mathbf{u}(\mathbf{x})$ is assumed to be a feedback control policy in this paper. For a fixed policy, denote $\mathbf{s}_t(\mathbf{x}_0)$ or $\mathbf{x}(t)$ the solution to (10) at time t. We seek an optimal policy $\mathbf{u}(\mathbf{x})$ that drives the system from an initial set $\mathbf{X}_0$ to a destination set $\mathbf{X}_r$ while avoiding pre-defined (unsafe) sets $\mathbf{X}_u$. The sets have the inclusion relations $\mathbf{X}_0, \mathbf{X}_u, \mathbf{X}_r \subseteq \mathbf{X}$.

Let $l(\mathbf{x}, \mathbf{u})$ be the running cost, and $h_0(\mathbf{x}_0)$ be an initial density supported on $\mathbf{X}_0$, then the problem is formulated as

$$\inf_{\mathbf{u}(\cdot)} \;\; \int_{\mathbf{X}} \int_0^\infty l(\mathbf{s}_t(\mathbf{x}_0), \mathbf{u}(\mathbf{s}_t(\mathbf{x}_0))) dt h_0(\mathbf{x}_0) d\mathbf{x}_0 \tag{11a}$$

$$\text{s.t.} \quad \int_0^\infty \mathbb{1}_{\mathbf{X}_u}(\mathbf{s}_t(\mathbf{x}_0)) dt = 0, \; \forall \mathbf{x}_0 \in \mathbf{X}_0. \tag{11b}$$

We consider the problem hereafter as function of arbitrary initial state variable $\mathbf{x}$ instead of $\mathbf{x}_0$. For each trajectory starting from $\mathbf{x}$, the individual cost is the infinite-horizon summation of the cost $l(\mathbf{x}(t), \mathbf{u}(\mathbf{x}(t)))$. The objective is thus the expectation of individual costs given the initial distribution h_0. The constraint (11b) ensures that any trajectory starts in $\mathbf{X}_0$ doesn't run into the unsafe set $\mathbf{X}_u$.

A. Dual formulation

By the definition of the Koopman operator (2), the objective function of problem (11) reads

$$J(h_0) = \int_{\mathbf{X}} \int_0^\infty [\mathbb{K}_t l(\mathbf{x}, u(\mathbf{x}))](\mathbf{x}) dt h_0(\mathbf{x}) d\mathbf{x}. \tag{12}$$

In view of the duality (6), it becomes

$$J(h_0) = \int_{\mathbf{X}} l(\mathbf{x}, \mathbf{u}(\mathbf{x})) \int_0^\infty [\mathbb{P}_t h_0](\mathbf{x}) dt d\mathbf{x}. \tag{13}$$

Now define

$$\rho(\mathbf{x}) \triangleq \int_0^\infty [\mathbb{P}_t h_0](\mathbf{x}) dt, \tag{14}$$

then this objective function can be rewritten as

$$J(h_0) = \int_{\mathbf{X}} l(\mathbf{x}, \mathbf{u}(\mathbf{x})) \rho(\mathbf{x}) d\mathbf{x}. \tag{15}$$

We next show that, when the controller drives all the trajectories from $\mathbf{X}_0$ to $\mathbf{X}_r$, the occupancy measure $\rho(\mathbf{x})$ defined in equation (14) satisfies

$$\nabla \cdot (\mathbf{F}(\mathbf{x}, \mathbf{u}(\mathbf{x}))\rho) = h_0. \tag{16}$$

It follows directly from

$$\begin{aligned}\nabla \cdot (\mathbf{F}\rho) &= \int_0^\infty \nabla \cdot ([\mathbb{P}_t h_0](\mathbf{x}) \mathbf{F}(\mathbf{x}, \mathbf{u}(\mathbf{x}))) dt \\ &= \int_0^\infty -\frac{\partial [\mathbb{P}_t h_0](\mathbf{x})}{\partial t} dt = h_0(\mathbf{x}).\end{aligned}$$

Since

$$\begin{aligned}\int_{\mathbf{X}_u} \rho(\mathbf{x}) d\mathbf{x} &= \int_{\mathbf{X}} \mathbb{1}_{X_u}(\mathbf{x}) \int_0^\infty [\mathbb{P}_t h_0](\mathbf{x}) dt d\mathbf{x} \\ &= \int_0^\infty \int_{\mathbf{X}} [\mathbb{K}_t \mathbb{1}_{\mathbf{X}_u}](\mathbf{x}) h_0(\mathbf{x}) d\mathbf{x} dt \\ &= \int_{\mathbf{X}} \int_0^\infty \mathbb{1}_{\mathbf{X}_u}(\mathbf{s}_t(\mathbf{x})) dt h_0(\mathbf{x}) d\mathbf{x},\end{aligned} \tag{17}$$

$\int_{\mathbf{X}_u} \rho(\mathbf{x}) d\mathbf{x} = 0$ implies $\int_0^\infty \mathbb{1}_{\mathbf{X}_u}(\mathbf{x}(t)) dt = 0$ for almost every $\mathbf{x}$ with respect to initial density h_0. Thus the constraint (11b) can be rewritten as $\int_{\mathbf{X}_u} \rho(\mathbf{x}) d\mathbf{x} = 0$.

Combining equations (15), (16) and (17), we arrive at the equivalent formulation

$$\inf_{\rho, \mathbf{u}} \int_{\mathbf{X}} l(\mathbf{x}, \mathbf{u}(\mathbf{x})) \rho(\mathbf{x}) d\mathbf{x} \tag{18a}$$

$$\text{s.t.} \quad \nabla \cdot (\mathbf{F}(\mathbf{x}, \mathbf{u}(\mathbf{x})) \rho(\mathbf{x})) = h_0(\mathbf{x}) \tag{18b}$$

$$\int_{\mathbf{X}} \mathbb{1}_{\mathbf{X}_u}(\mathbf{x}) \rho(\mathbf{x}) d\mathbf{x} = 0 \tag{18c}$$

of the optimal control problem (11) with a measurable $\mathbf{X}_u$. We call this formulation (18) the dual form of the optimal safety problem. It is not difficult to see that (18) is the Lagrangian dual to (11) where $\rho(\mathbf{x})$ is nothing but the Lagrange multiplier associated with the constraint (11b).

Remark. *The definition of ρ in* (14) *has a physical interpretation of occupancy [18]. Specifically, $\rho(A) := \int_A \rho(\mathbf{x})\ d\mathbf{x}$ for any given $A \in \mathcal{B}(\mathbf{X})$ signifies the time spent by system trajectory in A. Compared with the system evolution point of view with Koopman operator in (12), the occupancy defined by the P-F operator provides an alternative view of the objective function as the time occupancy of the system penalized by a predefined penalty field, $l(\mathbf{x}, \mathbf{u}(\mathbf{x}))$ in (15). This duality arises from the duality between the two operators. With the physical interpretation of ρ, the safety constraints are directly interpreted by the zero occupancy.*

B. Penalty function method for safety constraints

One approach to solve the constrained optimization problem of the form (18) is to introduce Lagrange multiplier with respect to the linear equality constraint (18c). Towards this, the optimization problem (18) can be equivalently written as

$$\begin{aligned}\inf_{\rho, \mathbf{u}} \sup_{\lambda \in \mathbb{R}} \quad & \int_{\mathbf{X}} (l(\mathbf{x}, \mathbf{u}(\mathbf{x})) + \lambda \mathbb{1}_{\mathbf{X}_u}(\mathbf{x})) \rho(\mathbf{x})\ d\mathbf{x} \\ \text{s.t.} \quad & \nabla \cdot (\mathbf{F}(\mathbf{x}, \mathbf{u}(\mathbf{x})) \rho(\mathbf{x})) = h_0(\mathbf{x}),\end{aligned} \tag{19}$$

where $\mathbb{1}_{\mathbf{X}_u}(\mathbf{x})$ is the indicator function of set $\mathbf{X}_u$ and $\lambda \in \mathbb{R}$ is the Lagrangian multiplier. The multiplier λ can be restricted to nonnegative values due to the nonnegativity of ρ. The standard primal-dual type algorithms [28] can be devised to solve the saddle point optimization problem (19), where one alternates between minimization step (gradient descent for primal variable) and maximization step (gradient ascent for dual variable). However, in general these problems are difficult to solve.

Alternatively, the Lagrangian multiplier term can be regarded as a penalty which penalizes the behavior of entering the obstacle set $\mathbf{X}_u$. Results from the penalty function methods show that a near-optimal solution of problem (18) can be obtained with a fixed large value of λ in (19), denoted as the penalty constant $\bar{\lambda}$. Problem (18) is thus transformed into

$$\begin{aligned}\inf_{\rho, \mathbf{u}} \quad & \int_{\mathbf{X}} \left(l(\mathbf{x}, \mathbf{u}(\mathbf{x})) + \bar{\lambda} \mathbb{1}_{\mathbf{X}_u}(\mathbf{x})\right) \rho(\mathbf{x})\ d\mathbf{x} \\ \text{s.t.} \quad & \nabla \cdot (\mathbf{F}(\mathbf{x}, \mathbf{u}(\mathbf{x})) \rho) = h_0(\mathbf{x}).\end{aligned} \tag{20}$$

A geometric interpretation for the penalty function method is provided in [13] in attacking equality-constrained problems. For a fixed $\bar{\lambda}$, solving the unconstrained problem with penalties on the equality constraints determines a supporting hyperplane and a dual functional for the original constrained problem. With the increase of the penalty term, the dual functional will approach the boundary point of the original problem's region of definition. In practice, the choice of $\bar{\lambda}$ is the result of a trade-off between maximizing the penalty to better approximate the constrained problem and minimizing the penalty to keep the original objectives.

C. Convex formulation for control-affine dynamical systems

We focus hereafter on the control-affine dynamical system from which a convex formulation will be established.

Assumption 1 (Control-affine system with state cost and input regularization)**.** *The dynamics is control-affine*[1]*, i.e.,*

$$\mathbf{F}(\mathbf{x}, \mathbf{u}) = \mathbf{f}(\mathbf{x}) + \mathbf{g}(\mathbf{x})\mathbf{u}. \tag{21}$$

The cost is of the form $l(\mathbf{x}, \mathbf{u}) = q(\mathbf{x}) + r(\mathbf{u})$ *with a state cost* $q(\mathbf{x})$ *and a regularization term* $r(\mathbf{u})$ *on the control.*

Under Assumption 1, the constraint in (20) can be written as $\nabla \cdot (\mathbf{f}\rho + \mathbf{g}\mathbf{u}\rho) = h_0$. The bi-linearity of the constraint renders the joint search for $\rho(\mathbf{x})$ and $\mathbf{u}(\mathbf{x})$ a non-convex problem. To overcome this, we define [7] $\rho\mathbf{u} \triangleq \bar{\boldsymbol{\rho}} = [\bar{\boldsymbol{\rho}}_1, \dots, \bar{\boldsymbol{\rho}}_m] \in \mathbb{R}^m$, and reformulate the problem into

$$\inf_{\rho(\mathbf{x}), \bar{\boldsymbol{\rho}}(\mathbf{x})} \int_{\mathbf{X}} (q(\mathbf{x}) + r(\frac{\bar{\boldsymbol{\rho}}(\mathbf{x})}{\rho(\mathbf{x})}) + \bar{\lambda}\mathbb{1}_{\mathbf{X}_u}(\mathbf{x}))\rho(\mathbf{x})\, d\mathbf{x} \tag{22a}$$
$$\text{s.t.} \quad \nabla \cdot (\mathbf{f}(\mathbf{x})\rho(\mathbf{x}) + \mathbf{g}(\mathbf{x})\bar{\boldsymbol{\rho}}(\mathbf{x})) = h_0(\mathbf{x}), \tag{22b}$$

which is a convex problem. The optimal policy can be recovered from the solution by $\mathbf{u}(\mathbf{x}) = \bar{\boldsymbol{\rho}}(\mathbf{x})/\rho(\mathbf{x})$.

Considering the actuation limits of dynamical systems, quadratic costs and absolute costs on the input are considered in this paper. The problem (22) with quadratic control cost is defined as $r(\frac{\bar{\boldsymbol{\rho}}}{\rho}) = \frac{\bar{\boldsymbol{\rho}}^T \mathbf{R} \bar{\boldsymbol{\rho}}}{\rho^2} = \mathbf{u}^T\mathbf{R}\mathbf{u}$ in (22a)

$$\begin{aligned} &\inf_{\rho, \bar{\boldsymbol{\rho}}} \int_{\mathbf{X}} (q + \bar{\lambda}\mathbb{1}_{\mathbf{X}_u})\rho + \frac{\bar{\boldsymbol{\rho}}^T\mathbf{R}\bar{\boldsymbol{\rho}}}{\rho}\, d\mathbf{x} \\ &\text{s.t.} \quad \nabla \cdot (\mathbf{f}\rho + \mathbf{g}\bar{\boldsymbol{\rho}}) = h_0, \end{aligned} \tag{23}$$

where $\mathbf{R} \succeq 0$ is a penalty constant. For absolute control cost, $r(\frac{\bar{\boldsymbol{\rho}}}{\rho}) = \frac{\beta}{\rho}\sum_{i=1}^m |\bar{\boldsymbol{\rho}}_i| = \beta \sum_{i=1}^m |\mathbf{u}_i|$ in equation (22a), and the problem (22) with absolute control cost reads

$$\begin{aligned} &\inf_{\rho, \bar{\boldsymbol{\rho}}} \int_{\mathbf{X}} (q + \bar{\lambda}\mathbb{1}_{\mathbf{X}_u})\rho + \beta\sum_{i=1}^m |\bar{\boldsymbol{\rho}}_i|\, d\mathbf{x} \\ &\text{s.t.} \quad \nabla \cdot (\mathbf{f}\rho + \mathbf{g}\bar{\boldsymbol{\rho}}) = h_0. \end{aligned} \tag{24}$$

Problem (23) and (24) are difficult to solve directly. In the following sections we relax the two problems into standard finite dimensional convex optimization problems.

IV. Polynomial parametrization, data approximation, and SDP relaxation

In this section we parameterize problem (22) using polynomials. A convex optimization problem with polynomial non-negativity constraints is obtained using SOS. We also approximate Koopman operator in a data-driven fashion.

A. Polynomial parametrization

We assume the rational parameterization [19] of ρ and $\bar{\boldsymbol{\rho}}$

$$\rho = \frac{a(\mathbf{x})}{b(\mathbf{x})^\alpha}, \quad \bar{\boldsymbol{\rho}} = \frac{\mathbf{c}(\mathbf{x})}{b(\mathbf{x})^\alpha} \tag{25}$$

where $a(\mathbf{x})$ and $b(\mathbf{x})$ are positive polynomials and $\mathbf{c}(\mathbf{x}) \triangleq [c_1(\mathbf{x}), \dots c_m(\mathbf{x})]^T$ is a vector of polynomials. We choose b and α such that $\deg(b^\alpha) > \max\{\deg(a), \deg(\mathbf{c})\}$, where $\deg(\mathbf{c})$ denotes the maximum degree among all the polynomials in $\mathbf{c}(\mathbf{x})$. We use the monomial basis $\boldsymbol{\Psi}_d$ defined in (9), where $d \geq \max\{\deg(a), \deg(\mathbf{c}), \deg(b^\alpha), \deg(ab), \deg(b\mathbf{c})\}$. All these polynomials and variable $\mathbf{x}$ can be expressed in $\boldsymbol{\Psi}_d$ as

$$\begin{aligned} a = C_a^T\boldsymbol{\Psi}_d, b = C_b^T\boldsymbol{\Psi}_d, \mathbf{c} = \mathbf{C}_{\mathbf{c}}^T\boldsymbol{\Psi}_d, \\ ab = C_{ab}^T\boldsymbol{\Psi}_d, b\mathbf{c} = \mathbf{C}_{b\mathbf{c}}^T\boldsymbol{\Psi}_d, \mathbf{x} = \mathbf{C}_{\mathbf{x}}^T\boldsymbol{\Psi}_d, \end{aligned} \tag{26}$$

where $\mathbf{C}_{\mathbf{c}}$ is the concatenation of the coefficients of polynomials in $\mathbf{c}(\mathbf{x})$, and $\mathbf{C}_{b\mathbf{c}}$ is the concatenation of the coefficients of polynomials in $b\mathbf{c}(\mathbf{x})$.

We now write the left hand side of (22b) as

$$\begin{aligned} &\nabla \cdot [\frac{1}{b^\alpha}(\mathbf{f}a + \mathbf{g}\mathbf{c})] \\ &= \frac{1}{b^{\alpha+1}}[(1+\alpha)b\nabla \cdot (\mathbf{f}a + \mathbf{g}\mathbf{c}) - \alpha\nabla \cdot (b\mathbf{f}a + b\mathbf{g}\mathbf{c})]. \end{aligned} \tag{27}$$

Since $b(\mathbf{x}) \geq 0$ and $h_0(\mathbf{x}) > 0$, we relax this constraint to

$$(1+\alpha)b\nabla \cdot (\mathbf{f}a + \mathbf{g}\mathbf{c}) - \alpha\nabla \cdot (b\mathbf{f}a + b\mathbf{g}\mathbf{c}) \geq 0. \tag{28}$$

B. Approximation of the constraints from data

Consider the dynamics as in Assumption 1 where $\mathbf{g} = [\mathbf{g}_1, \dots, \mathbf{g}_m] \in \mathbb{R}^{n \times m}$ and $\mathbf{u} = [\mathbf{u}^1, \dots, \mathbf{u}^m]^T \in \mathbb{R}^m$. Within the gEDMD framework introduced in Section II-A, we choose the monomial basis defined in (9), i.e., $\boldsymbol{\Psi} \triangleq \boldsymbol{\Psi}_d$. We collect experiment data of the form $(\mathbf{x}_k, \mathbf{u}_k, \dot{\mathbf{x}}_k)$ where $\mathbf{u}_k \triangleq [\mathbf{u}_k^1, \dots, \mathbf{u}_k^m]$ are arbitrary inputs for $k = 1, \dots, M$. Let $\dot{\boldsymbol{\Psi}}_d(\mathbf{x}_k, \dot{\mathbf{x}}_k) = [\nabla\psi_1(\mathbf{x}_k) \cdot \dot{\mathbf{x}}_k, \dots, \nabla\psi_N(\mathbf{x}_k) \cdot \dot{\mathbf{x}}_k]^T$. We then approximate the infinitesimal generators $\mathcal{K}_{\mathbf{f}}$ and $\mathcal{K}_{\mathbf{g_i}}, i = 1, \dots, m$ (with matrix representation $\mathbf{L}_0$ and $\mathbf{L}_i, i = 1, \dots, m$ respectively) by solving [19] [29]

$$\min_{\mathbf{L}_0, \dots, \mathbf{L}_m} \sum_{k=1}^M \left\| \dot{\boldsymbol{\Psi}}_d(\mathbf{x}_k, \dot{\mathbf{x}}_k) - [\mathbf{L}_0, \dots, \mathbf{L}_m] \begin{bmatrix} \boldsymbol{\Psi}_d(\mathbf{x}_k) \\ \boldsymbol{\Psi}_d(\mathbf{x}_k)\mathbf{u}_k^1 \\ \dots \\ \boldsymbol{\Psi}_d(\mathbf{x}_k)\mathbf{u}_k^m \end{bmatrix} \right\|_2^2 \tag{29}$$

Denote matrices in equation (29) as $\hat{\mathbf{L}} \triangleq [\mathbf{L}_0, \dots, \mathbf{L}_m]$ and $\boldsymbol{\Psi}_{\mathbf{x}}^{\mathbf{u}_k} \triangleq [\boldsymbol{\Psi}_d(\mathbf{x}_k), \boldsymbol{\Psi}_d(\mathbf{x}_k)\mathbf{u}_k^1, \dots, \boldsymbol{\Psi}_d(\mathbf{x}_k)\mathbf{u}_k^m]^T$, then the solution is given by

$$\hat{\mathbf{L}}^\star = (\frac{1}{M}\sum_{k=1}^M \dot{\boldsymbol{\Psi}}_d(\mathbf{x}_k, \dot{\mathbf{x}}_k)(\boldsymbol{\Psi}_{\mathbf{x}}^{\mathbf{u}_k})^T)(\frac{1}{M}\sum_{k=1}^M \boldsymbol{\Psi}_{\mathbf{x}}^{\mathbf{u}_k}(\boldsymbol{\Psi}_{\mathbf{x}}^{\mathbf{u}_k})^T)^\dagger. \tag{30}$$

By the definition of the infinitesimal generator of the Koopman operator (3), we can approximate the term $\nabla \cdot \mathbf{f}$ and $\nabla \cdot \mathbf{g}_i$

$$\nabla \cdot \mathbf{f} = \nabla \cdot [\mathcal{K}_{\mathbf{f}}\mathbf{x}_1, \dots, \mathcal{K}_{\mathbf{f}}\mathbf{x}_n] \approx \nabla \cdot (C_{\mathbf{x}}^T\mathbf{L}_0\boldsymbol{\Psi}_d), \tag{31a}$$
$$\nabla \cdot \mathbf{g}_i = \nabla \cdot [\mathcal{K}_{\mathbf{g}_i}\mathbf{x}_1, \dots, \mathcal{K}_{\mathbf{g}_i}\mathbf{x}_n] \approx \nabla \cdot (C_{\mathbf{x}}^T\mathbf{L}_i\boldsymbol{\Psi}_d). \tag{31b}$$

Without knowing the dynamics, the first term in constraint (28) can be approximated [19] using (31a) and (31b) as

$$\begin{aligned} \nabla \cdot (\mathbf{f}a + \mathbf{g}\mathbf{c}) &= \nabla \cdot \mathbf{f}a + \mathbf{f}^T\nabla a + \sum_{i=1}^m (\nabla \cdot \mathbf{g}_i c_i + \mathbf{g}_i^T\nabla c_i) \\ &\approx \nabla \cdot (C_{\mathbf{x}}^T\mathbf{L}_0\boldsymbol{\Psi}_d)a + C_a^T\mathbf{L}_0\boldsymbol{\Psi}_d \\ &\quad + \sum_{i=1}^m [\nabla \cdot (C_{\mathbf{x}}^T\mathbf{L}_i\boldsymbol{\Psi}_d)c_i + C_{c_i}^T\mathbf{L}_i\boldsymbol{\Psi}_d]. \end{aligned} \tag{32}$$

[1]This control-affine dynamics is widely used in robotics and can be used to model most mechanical systems. Moreover, any nonlinear dynamics can be converted into this form with a state augmentation trick.

Similarly, the second term can be approximated by

$$\nabla\cdot(\mathbf{f}ab+b\mathbf{g}\mathbf{c})\approx\nabla\cdot(C_{\mathbf{x}}^T\mathbf{L}_0\mathbf{\Psi}_d)ab+C_{ab}^T\mathbf{L}_0\mathbf{\Psi}_d + \sum_{i=1}^{m}[\nabla\cdot(C_{\mathbf{x}}^T\mathbf{L}_i\mathbf{\Psi}_d)bc_i+C_{bc_i}^T\mathbf{L}_i\mathbf{\Psi}_d]. \quad (33)$$

C. SOS techniques

With parametrization (25), problem (23) can be written as

$$\begin{aligned}\inf_{a,\mathbf{c}}\ & \int_{\mathbf{X}_1}\frac{q(\mathbf{x})a(\mathbf{x})}{b(\mathbf{x})^\alpha}+\frac{\mathbf{c}(\mathbf{x})^T\mathbf{R}\mathbf{c}(\mathbf{x})}{a(\mathbf{x})b(\mathbf{x})^\alpha}\,d\mathbf{x}+\bar{\lambda}\int_{\mathbf{X}_u}\frac{a(\mathbf{x})}{b(\mathbf{x})^\alpha}\,d\mathbf{x}\\ \text{s.t.}\ & a(\mathbf{x})\geq 0,(28)\geq 0.\end{aligned} \quad (34)$$

To avoid singularity, the integration is performed on $\mathbf{X}_1\triangleq\mathbf{X}\setminus\mathbf{X}_{excld}$ which is the whole set $\mathbf{X}$ minus a small region $\mathbf{X}_{excld}$ around origin. The term $\int_{\mathbf{X}_1}\frac{\mathbf{c}(\mathbf{x})^T\mathbf{R}\mathbf{c}(\mathbf{x})}{a(\mathbf{x})b(\mathbf{x})^\alpha}\,d\mathbf{x}$ contains $a(\mathbf{x})$ in the denominator and is hard to be expressed as SOS. We seek thus an upper bound polynomial $w(\mathbf{x})$ of this term.

Definition IV.1 ([30] PSD polynomial matrix**).** *Polynomial matrix* $\mathbf{H}(\mathbf{x})\in\mathbb{R}[\mathbf{x}]^{P\times P}$ *(*$\mathbf{H}_{ij}$ *is polynomial,* $\forall i,j\in\{1,\dots,P\}$*) is PSD w.r.t. monomial basis* $\mathbf{\Psi}_{N_\Psi}(\mathbf{x})=[\mathbf{\Psi}_{N_\Psi}^1(\mathbf{x}),\dots\mathbf{\Psi}_{N_\Psi}^{N_\Psi}(\mathbf{x})]^T$*, denoted as* $\mathbf{H}\succeq 0$*, if* $\exists\mathbf{D}$*, s.t.* $\mathbf{H}=(\mathbf{\Psi}_{N_\Psi}\otimes\mathbf{I}_P)^T\mathbf{D}(\mathbf{\Psi}_{N_\Psi}\otimes\mathbf{I}_P)$ *and* $\mathbf{D}\succeq 0$*.*

The PSD matrix SOS feasibility program is thus a SDP feasibility problem with $(P\times N_\Psi)^2$ linear constraints. We define in our problem $\hat{\mathbf{H}}\triangleq\begin{bmatrix}w(\mathbf{x}) & \mathbf{c}(\mathbf{x})^T\\ \mathbf{c}(\mathbf{x}) & a(\mathbf{x})\mathbf{R}^{-1}\end{bmatrix}$, then from Schur complement we know $\hat{\mathbf{H}}\succeq 0\Leftrightarrow w(\mathbf{x})\geq\frac{\mathbf{c}(\mathbf{x})^T\mathbf{R}\mathbf{c}(\mathbf{x})}{a(\mathbf{x})}$. The problem (34) reads

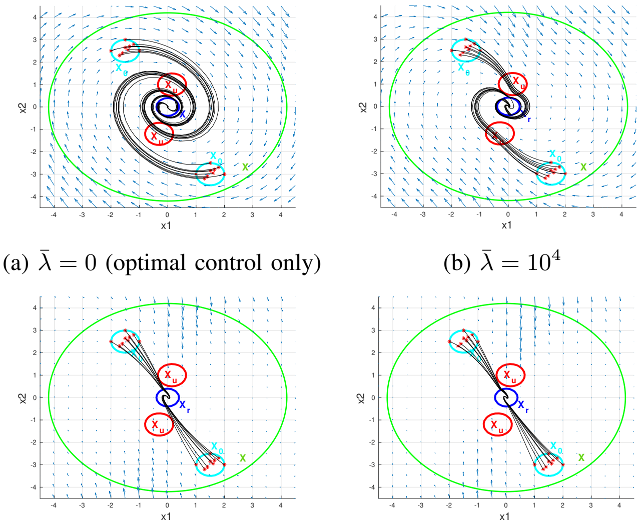
$$\begin{aligned}\inf_{C_a,C_{\mathbf{c}},C_w}\ & \int_{\mathbf{X}_1}\frac{q(\mathbf{x})a(\mathbf{x})}{b(\mathbf{x})^\alpha}+\frac{w(\mathbf{x})}{b(\mathbf{x})^\alpha}\,d\mathbf{x}+\bar{\lambda}\int_{\mathbf{X}_u}\frac{a(\mathbf{x})}{b(\mathbf{x})^\alpha}\,d\mathbf{x}\\ \text{s.t.}\ & a(\mathbf{x})\geq 0,(28)\geq 0\\ & \begin{bmatrix}w(\mathbf{x}) & \mathbf{c}(\mathbf{x})^T\\ \mathbf{c}(\mathbf{x}) & a(\mathbf{x})\mathbf{R}^{-1}\end{bmatrix}\succeq 0.\end{aligned} \quad (35)$$

Furthermore, $\int_{\mathbf{X}_1}\frac{q(\mathbf{x})a(\mathbf{x})}{b(\mathbf{x})^\alpha}\,d\mathbf{x}=C_a^T\mathbf{d}_1$, $\int_{\mathbf{X}_1}\frac{w(\mathbf{x})}{b(\mathbf{x})^\alpha}\,d\mathbf{x}=C_w^T\mathbf{d}_2$, and $\int_{\mathbf{X}_u}\frac{a(\mathbf{x})}{b(\mathbf{x})^\alpha}\,d\mathbf{x}=C_a^T\mathbf{d}_3$, with constants $\mathbf{d}_1\triangleq\int_{\mathbf{X}_1}\frac{q(\mathbf{x})\mathbf{\Phi}(\mathbf{x})}{b(\mathbf{x})^\alpha}\,d\mathbf{x}$, $\mathbf{d}_2\triangleq\int_{\mathbf{X}_1}\frac{\mathbf{\Phi}(\mathbf{x})}{b(\mathbf{x})^\alpha}\,d\mathbf{x}$, and $\mathbf{d}_3\triangleq\int_{\mathbf{X}_u}\frac{\mathbf{\Phi}(\mathbf{x})}{b(\mathbf{x})^\alpha}\,d\mathbf{x}$. Problem (35) reads

$$\begin{aligned}\inf_{C_a,C_{\mathbf{c}},C_w}\ & C_a^T(\mathbf{d}_1+\bar{\lambda}\mathbf{d}_3)+C_w^T\mathbf{d}_2\\ \text{s.t.}\ & (1+\alpha)b\nabla\cdot(\mathbf{f}a+\mathbf{g}\mathbf{c})-\alpha\nabla\cdot(b\mathbf{f}a+b\mathbf{g}\mathbf{c})\in SOS\\ & a(\mathbf{x})\in SOS\\ & \begin{bmatrix}w(\mathbf{x}) & \mathbf{c}(\mathbf{x})^T\\ \mathbf{c}(\mathbf{x}) & a(\mathbf{x})\mathbf{R}^{-1}\end{bmatrix}\succeq 0.\end{aligned} \quad (36)$$

Similarly, using the definition of $\mathbf{d}_1,\mathbf{d}_2$ and $\mathbf{d}_3$, the problem with absolute control cost (24) reads

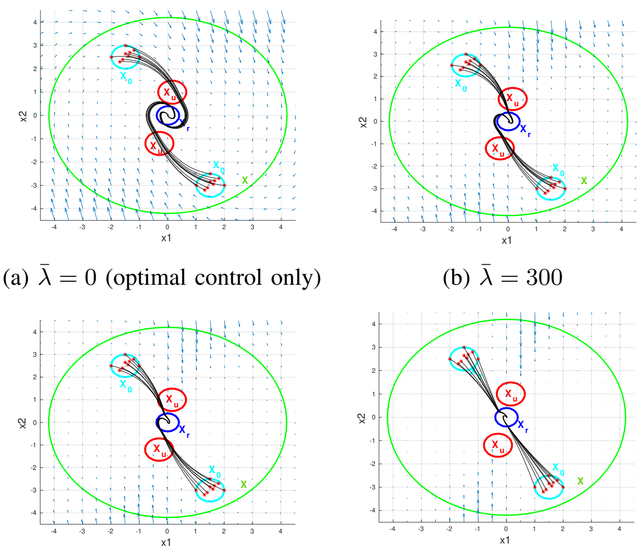
$$\begin{aligned}\inf_{C_a,C_{\mathbf{c}},C_{s_i}}\ & C_a^T(\mathbf{d}_1+\bar{\lambda}\mathbf{d}_3)+\beta\sum_{i=1}^{m}C_{s_i}^T\mathbf{d}_2\\ \text{s.t.}\ & (1+\alpha)b\nabla\cdot(\mathbf{f}a+\mathbf{g}\mathbf{c})-\alpha\nabla\cdot(b\mathbf{f}a+b\mathbf{g}\mathbf{c})\in SOS\\ & a(\mathbf{x})\in SOS, s_i\in SOS, i=1,\dots,m\\ & s_i(x)-\bar{\boldsymbol{\rho}}_i(x)\in SOS, i=1,\dots,m\\ & s_i(x)+\bar{\boldsymbol{\rho}}_i(x)\in SOS, i=1,\dots,m.\end{aligned} \quad (37)$$



(a) $\bar{\lambda}=0$ (optimal control only) (b) $\bar{\lambda}=10^4$

(c) $\bar{\lambda}=10^6$ (d) $\bar{\lambda}=5\times 10^7$

Fig. 1: System trajectories with increasing value of penalty constant $\bar{\lambda}$ in (36), with quadratic control cost.



(a) $\bar{\lambda}=0$ (optimal control only) (b) $\bar{\lambda}=300$

(c) $\bar{\lambda}=1000$ (d) $\bar{\lambda}=10^4$

Fig. 2: System trajectories with increasing value of penalty constant $\bar{\lambda}$ in (37), with absolute control cost.

By introducing SOS techniques, problems (23) and (24) are transformed into 2 SDPs which can be solved efficiently.

V. Experiments

Simulations are conducted in this section to verify the proposed methods. We consider the Van Der Pol dynamics

$$\dot{x}_1=x_2,\quad \dot{x}_2=(1-x_1^2)x_2-x_1+u. \quad (38)$$

For operator approximation, 10000 data points are uniformly sampled within the region $\mathbf{X}=[-5,5]\times[-5,5]$. gEDMD method is deployed in the approximation. Monomial basis with highest degree 9 is used. For the degree of polynomials, we choose $\deg(a(\mathbf{x})) = 4$, $\deg(c(\mathbf{x})) = 6$. The polynomial $b(\mathbf{x}) = 3.3784x_1^2 + 0.82843x_1x_2 + 2.6818x_2^2$, which is the result of an LQR controller for the system locally linearized around the origin. To avoid singularities, the controller is switched to this local LQR controller once the trajectory enters $\mathbf{X}_r$. We choose $\alpha = 4$ in (25). For state and control costs in (22), we choose $q(\mathbf{x}) = x_1^4 + x_2^4$ and $\mathbf{R} = 1$. Define different sets as

- $\mathbf{X}_1 \triangleq \{(x_1, x_2)\colon 4.2^2 \geq x_1^2 + x_2^2 \geq 0.1^2\}$,
- $\mathbf{X}_0^1 \triangleq \{(x_1, x_2)\colon 0.5^2 - (x_1 + 1.5)^2 - (x_2 - 2.5)^2 \geq 0\}$,
- $\mathbf{X}_0^2 \triangleq \{(x_1, x_2)\colon 0.5^2 - (x_1 - 1.5)^2 - (x_2 + 3)^2 \geq 0\}$,
- $\mathbf{X}_u^1 \triangleq \{(x_1, x_2)\colon 0.5^2 - (x_1 - 0.15)^2 - (x_2 - 1.0)^2 \geq 0\}$,
- $\mathbf{X}_u^2 \triangleq \{(x_1, x_2)\colon 0.5^2 - (x_1 + 0.3)^2 - (x_2 + 1.2)^2 \geq 0\}$,
- $\mathbf{X}_r \triangleq \{(x_1, x_2)\colon 0.4^2 - x_1^2 - x_2^2 \geq 0\}$.

We gradually increase the penalty constant $\bar{\lambda}$ starting from 0 (solely under the optimal control objective) and observe the system's performance in terms of obstacle avoidance. The results of the problems defined in (36) and (37) are shown in Figure 1 and Figure 2 respectively. We choose the weight on the control penalty $\beta = 5e^{-4}$ in (37). As shown in both the figures, when $\bar{\lambda} = 0$, the system trajectories starting from the two initial sets, $\mathbf{X}_0^1$ and $\mathbf{X}_0^2$, intersect with a large portion of the two unsafe sets, $\mathbf{X}_u^1$ and $\mathbf{X}_u^2$. As $\bar{\lambda}$ increases, the trajectories intersects less and less with the unsafe sets. When $\bar{\lambda}$ increases to 10^4 for problem (37) and $\bar{\lambda} = 5 \times 10^7$ for problem (36), trajectories completely avoid the unsafe sets and reach the reach set $\mathbf{X}_r$. The choice of $\bar{\lambda}$ is to find an appropriate value which enables the system to avoid the unsafe sets while preserving the original optimal control objectives.

VI. Conclusion

In this paper, we considered the optimal control problem with safety constraints for nonlinear dynamical systems. Studying the problem in the lifted space and using the Koopman and Perron Frobenius operator, a dual form of the original problem was obtained where the avoidance of the unsafe sets was expressed as zero occupancy. We leveraged the penalty function method to get a near-optimal solution for the infinite-dimensional constrained optimization problem. Furthermore, we obtained a convex formulation of the problem by focusing on the control-affine dynamical system and restricting the problem in the polynomial space. This problem was then solved with the SOS techniques. Future directions and applications of this work will involve more complex dynamical environment, and hardware experiments.

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