Estimating High Probability Reachable Sets using Gaussian Processes

Michael E. Cao, Matthieu Bloch, and Samuel Coogan

Abstract— **We present a method for computing reachable sets and forward invariant sets for systems with dynamics that include unknown components. Our main assumption is that, given any hyperrectangle of states, lower and upper bounds for the unknown components that hold with high probability are available. We then show that this assumption is well-suited when the unknown terms are modeled as state-dependent Gaussian processes. Under this assumption, we leverage the theory of mixed monotone systems and propose an efficient method for computing a hyperrectangular set that over-approximates the reachable set of the system with high probability. We then show a related approach that leads to sufficient conditions for identifying sets that are forward invariant for the dynamics with high probability. These theoretical results lead to practical algorithms for efficient computation of high probability reachable sets and invariant sets. A major advantage of our approach is that it leads to tractable computations for systems up to moderately high dimension that are subject to low dimensional uncertainty modeled as Gaussian Processes, a class of systems that appears often in practice. We demonstrate our results on an example of a six-dimensional model of a multirotor aerial vehicle.**

I. Introduction

To determine if a dynamical system satisfies a safety constraint or achieves certain control objectives, it is often required to compute reachable sets or forward invariant sets for the dynamics. However, such calculations often suffer from the curse of dimensionality. In addition, the true dynamics of the system may not be fully known, whether due to inaccuracies in the model itself or external disturbances. Recently, *mixed monotone* systems theory has been shown to be an effective tool for efficiently computing over-approximations of reachable and forward invariant sets for relatively high dimensional systems [1], with applications to control of practical systems with around ten state dimensions [2], [3]. Further, mixed monotone systems theory can integrate unknown disturbances into this over-approximation [4]. In this paper, we extend these ideas by applying Gaussian Process (GP) theory to efficiently calculate high-confidence bounds on unknown components of the dynamics in order to compute, with high probability, reachable sets and invariant sets. As these bounds tighten due to, *e.g.*, measurements of the GP, we show how improved set estimates can be achieved.

The authors are with the School of Electrical and Computer Engineering, Georgia Institute of Technology, Atlanta, 30332, USA {mcao34, sam.coogan}@gatech.edu, matthieu.bloch@ece.gatech.edu. S. Coogan is also with the School of Civil and Environmental Engineering, Georgia Institute of Technology, Atlanta, 30332, USA.

This research was supported in part by the National Science Foundation under awards #1836932 and #1924978 and the Air Force Office of Scientific Research under award FA9550-19-1-0015.

A system is mixed monotone if there exists a *decomposition function* that separates the vector field of the system into solely increasing and solely decreasing components [1], [5]–[7]. Given an n–dimensional system that is mixed monotone with respect to some decomposition function, a $2n$–dimensional *embedding system*, which is monotone with respect to a particular southeast order, is constructed from said decomposition function. This allows for the application of tools from monotone systems theory to the embedding system dynamics, which yields conclusions on the reachability and safety properties of the original system. In particular, if the original system is subjected to a p–dimensional disturbance input, the resulting embedding system is subject to a $2p$–dimensional disturbance input; considering the worst-case inputs of these disturbances allows for the computation of forward invariant sets of the original system by calculating equilibria of the embedding system [4].

These prior works did not consider disturbances arising from unknown but state-dependent uncertainty in the dynamics, although this is a common scenario in practice. To that end, GPs have been used to model unknown functions to great effect in statistics and machine learning [8], as they are able to model distributions over any continuous domain and provide confidence estimates over a given range of function values, even with few observations. We can consequently take advantage of these confidence estimates to form our high-confidence bounds on the disturbance, allowing these bounds to be updated as more observations are gathered.

The idea of applying learning in controls is not new; [9] provides a method for online tuning of controller parameters using GPs while fulfilling safety criteria, [10] describes a method for incorporating Reinforcement Learning using GPs into classical model reference adaptive control, [11], [12] explore the coverage control problem for estimating unknown spatial fields using GPs, and [13] derives a uniform error bound for GPs that is used to calculate safety bounds for unknown dynamical systems. In service of providing high probability safety guarantees, [14] uses Bayesian learning to obtain a distribution over the system dynamics, [15] presents a model predictive control formulation that incorporates GPs, and [16] implements reinforcement learning to model uncertainties within control barrier function and control Lyapunov function constraints.

In this paper, we present a method for computing reachable sets and forward invariant sets for systems whose dynamics include unknown components, building off of the previous literature regarding mixed monotone systems. We accomplish this by assuming high probability bounds on the unknown components of the system and show that, when GPs are used to model the unknown components, this assumption is particularly appropriate. We show that these bounds lead to the identification of high probability reachable and forward invariant sets, which leads to algorithms for efficient computation of such sets.

The approach proposed in this paper is particularly appropriate for systems with low dimensional uncertainty modeled using GPs that appears as unknown components in the dynamics of a higher dimensional system, a scenario that often occurs in practice. For this class of systems, bounds on the low dimensional uncertainty can be efficiently evaluated using update laws for GPs and direct sampling, while the theory of mixed monotone systems accommodates the higher dimensional dynamics, leading to tractable computations. In addition, in contrast to much of the prior work using GPs in control systems, we do not assume the dynamics are affine in the unknown components, and our approach is suitable for systems modeled in continuous time, though these results are also applicable to discrete-time systems.

This paper is organized as follows. In Section II, we introduce key notation. In Section III, we formally define the assumptions made and the problems to be solved. Subsequently, in Section IV we illustrate the key theoretical results that solve the previously defined problems, before detailing the theory that allows us to leverage GPs in Section V. Section VI showcases a demonstration on a model of a multirotor aerial vehicle subject to unknown wind forces, and the paper concludes with a discussion in Section VII.

II. Notation

Let (x, y) denote the vector concatenation of $x, y \in \mathbb{R}^n$, i.e., $(x, y) := [x^T\ y^T]^T \in \mathbb{R}^{2n}$. Additionally, $\preceq$ denotes the componentwise vector order, i.e. $x \preceq y$ if and only if $x_i \leq y_i$ for all $i \in \{1, ..., n\}$ where vector components are indexed via subscript.

Given $x, y \in \mathbb{R}^n$ such that $x \preceq y$, we denote the hyperrectangle defined by the endpoints x and y using the notation $[x, y] := \{z \in \mathbb{R}^n \mid x \preceq z \text{ and } z \preceq y\}$. Also, given $a = (x, y) \in \mathbb{R}^{2n}$ with $x \preceq y$, $[\![a]\!]$ denotes the hyperrectangle formed by the first and last n components of a, i.e., $[\![a]\!] := [x, y]$.

Finally, let $\preceq_{\text{SE}}$ denote the *southeast order* on $\mathbb{R}^n$ defined by $(x, x') \preceq_{\text{SE}} (y, y')$ if and only if $x \preceq y$ and $y' \preceq x'$. In particular, observe that when $x \preceq x'$ and $y \preceq y'$,

$$(x, x') \preceq_{\text{SE}} (y, y') \iff [y, y'] \subseteq [x, x']. \tag{1}$$

III. Problem Formulation

Consider the dynamical system

$$\dot{x} = f(x, w) \tag{2}$$

where $x \in \mathbb{R}^n$ is the system state and $w \in \mathbb{R}^p$ is an unknown, state-dependent component of the dynamics so that $w_i = g_i(x)$ where g_i is unknown. For example, g_i might account for higher order nonlinearities not explicitly captured in the model.

We make the following two fundamental assumptions throughout.

Assumption 1. *Each w_i, $i \in \{1, \ldots, p\}$ in (2) is state-dependent so that $w_i = g_i(x)$ for some unknown, Lipschitz continuous g_i.*

Further, there exist known, Lipschitz continuous functions $\underline{\gamma}_i(x, \hat{x})$ and $\overline{\gamma}_i(x, \hat{x})$ for all $i \in \{1, \ldots, p\}$ such that with probability at least $1 - \epsilon$

$$\underline{\gamma}_i(\underline{x}, \overline{x}) \leq g_i(x) \leq \overline{\gamma}_i(\underline{x}, \overline{x})\ \forall x \in [\underline{x}, \overline{x}] \tag{3}$$

for all $\underline{x}, \overline{x} \in \mathbb{R}^n$ with $\underline{x} \preceq \overline{x}$. Without loss of generality, we assume $\underline{\gamma}_i$ and $\overline{\gamma}_i$ satisfy the natural inclusion property that for all $\underline{x}^1 \preceq \underline{x}^2 \preceq \overline{x}^2 \preceq \overline{x}^1$ it holds that $\underline{\gamma}_i(\underline{x}^1, \overline{x}^1) \leq \underline{\gamma}_i(\underline{x}^2, \overline{x}^2) \leq \overline{\gamma}_i(\underline{x}^2, \overline{x}^2) \leq \overline{\gamma}_i(\underline{x}^1, \overline{x}^1)$.

In Section V, we present a method for computing functions $\underline{\gamma}_i(x, \hat{x})$ and $\overline{\gamma}_i(x, \hat{x})$ satisfying Assumption 1 when g_i is modeled as a GP, and we explicitly quantify the probability that (3) holds.

We denote by $g(x)$, $\underline{\gamma}$, and $\overline{\gamma}$ the vector concatenation of g_i, $\underline{\gamma}_i$, and $\overline{\gamma}_i$ for $i = 1, \ldots, p$.

Assumption 2. *The system (2) is mixed monotone with respect to a decomposition function $\delta(x, w, \hat{x}, \hat{w})$, that is, δ satisfies:*

1) *For all x and all w, $\delta(x, w, x, w) = F(x, w)$;*
2) *For all i, $j \in \{1, \cdots, n\}$ with $i \neq j$, $\frac{\partial \delta_i}{\partial x_j}(x, w, \hat{x}, \hat{w}) \geq 0$ for all x, $\hat{x}$ and all $w, \hat{w}$;*
3) *For all i, $j \in \{1, \cdots, n\}$, $\frac{\partial \delta_i}{\partial \hat{x}_j}(x, w, \hat{x}, \hat{w}) \leq 0$ for all $x, \hat{x}$ and all $w, \hat{w}$; and*
4) *For all $i \in \{1, \cdots, n\}$ and all $k \in \{1, \cdots, m\}$, $\frac{\partial \delta_i}{\partial w_k}(x, w, \hat{x}, \hat{w}) \geq 0$ and $\frac{\partial \delta_i}{\partial \hat{w}_k}(x, w, \hat{x}, \hat{w}) \leq 0$ for all $x, \hat{x}$ and all $w, \hat{w}$.*

A large class of systems have been shown to satisfy the above assumption; see [1] for further details and examples.

For initial condition $x_0 \in \mathbb{R}^n$, let $\phi(t, x_0)$ denote the resulting state trajectory of (2) when $w = g(x)$, that is, $\phi(t, x_0)$ satisfies $\frac{d}{dt}\phi(t, x_0) = f(\phi(t, x_0), g(\phi(t, x_0)))$. The *$T$-horizon reachable set from X_0* for (2) is the set of states reachable over the time horizon T from any initial condition $x_0 \in X_0$ and is denoted $R(T, X_0)$. That is,

$$R(T, X_0) = \{\phi(T, x_0) \mid x_0 \in X_0\}. \tag{4}$$

Even with full knowledge of the dynamics, computing exact reachable sets is generally not possible. Thus, we are interested in computing approximations of reachable sets. In particular, over-approximations are often preferred for, e.g., safety verification.

The focus of this paper is on the tractable computation of over-approximations for reachable sets of (2). Since $g(x)$ is unknown, and in light of Assumption 1, we specifically seek over-approximations that hold with probability at least $1 - \epsilon$.

Problem 1. *Given $X_0 = [\underline{x}_0, \overline{x}_0]$ for some $\underline{x}_0, \overline{x}_0 \in \mathbb{R}^n$ with $\underline{x}_0 \preceq \overline{x}_0$, compute $\hat{R}(T, X_0)$ such that $R(T, X_0) \subseteq \hat{R}(T, X_0)$ with probability at least $1 - \epsilon$.*

Closely related to the problem of computing reachable sets is the problem of computing forward invariant sets. A set $A \subseteq \mathbb{R}^n$ is *forward invariant* if $R(t, A) \subseteq A$ for all $t \geq 0$.

That is, A is forward invariant if any trajectory initialized in A always remains within A.

Problem 2. *Identify sets $S \subseteq \mathbb{R}^n$ that are forward invariant for* (2) *with probability at least $1-\epsilon$.*

In Section IV, we present solutions to Problems 1 and 2 using mixed monotone systems theory. Then, in Section V, we use the theory of GPs to derive a general approach to satisfying Assumption 1 and, in particular, obtaining the necessary functions $\underline{\gamma}$ and $\overline{\gamma}$ such that (3) holds with high probability.

IV. High Confidence Reachable and Invariant Sets

A key feature of mixed monotone systems is that hyperrectangular over-approximations of reachable sets are efficiently computed from trajectories of a $2n$–dimensional embedding system constructed from the decomposition function δ; however, existing results have only considered deterministic dynamics or dynamics with disturbances that have constant bounds. In this section, we extend this fundamental property to systems with state-dependent uncertainty satisfying Assumption 1. Due to page constraints, we omit full proofs of Theorems 1 and 2, as they are natural extensions of [1, Proposition 3] and [4, Theorem 1], respectively.

Theorem 1. *Consider* (2) *satisfying Assumptions 1 and 2. Let $X_0 = [\underline{x}_0, \overline{x}_0]$ for $\underline{x}_0, \overline{x}_0 \in \mathbb{R}^n$, with $\underline{x}_0 \preceq \overline{x}_0$, be a hyperrectangular set of initial conditions. Let $(x(t), \hat{x}(t))$ be the solution to the $2n$ dimensional system*

$$\begin{bmatrix}\dot{x}\\ \dot{\hat{x}}\end{bmatrix} = e(x,\hat{x}) := \begin{bmatrix}\delta(x, \underline{\gamma}(x,\hat{x}), \hat{x}, \overline{\gamma}(x,\hat{x}))\\ \delta(\hat{x}, \overline{\gamma}(x,\hat{x}), x, \underline{\gamma}(x,\hat{x}))\end{bmatrix} \tag{5}$$

with initial condition $(x(0), \hat{x}(0)) = (\underline{x}_0, \overline{x}_0)$. Then, with probability at least $1-\epsilon$, $R(T, X_0) \subseteq [x(T), \hat{x}(T)]$ for all $T \geq 0$.

Theorem 1 indicates that $\hat{R}(T, X_0) := [x(T), \hat{x}(T)]$, where $x(T), \hat{x}(T)$ are obtained as the solution to (5), provides a hyperrectangular over-approximation of the true reachable set $R(T, X_0)$ with probability at least $1-\epsilon$, thus solving Problem 1. The system (5) is called the *embedding system* for the mixed monotone system (2).

Theorem 2. *Consider* (2) *satisfying Assumptions 1 and 2. If $\underline{x}^*, \overline{x}^*, \underline{w}^*, \overline{w}^*$ with $\underline{x}^* \preceq \overline{x}^*$ and $\underline{w}^* \preceq \overline{w}^*$ are such that*

$$\underline{w}^* \preceq \underline{\gamma}(\underline{x}^*, \overline{x}^*) \text{ and } \overline{\gamma}(\underline{x}^*, \overline{x}^*) \preceq \overline{w}^* \tag{6}$$

and

$$\delta(\underline{x}^*, \underline{w}^*, \overline{x}^*, \overline{w}^*) \succeq 0 \text{ and } \delta(\overline{x}^*, \overline{w}^*, \underline{x}^*, \underline{w}^*) \preceq 0, \tag{7}$$

then with probability at least $1-\epsilon$, $[\underline{x}^*, \overline{x}^*]$ is forward invariant for (2).

We have the following useful corollary.

Corollary 1. *Consider* (2) *satisfying Assumptions 1 and 2. If $(\underline{x}^*, \overline{x}^*)$ is an equilibrium for the embedding system* (5)*, then with probability at least $1-\epsilon$, $[\underline{x}^*, \overline{x}^*]$ is forward invariant for* (2).

Corollary 1 suggests an immediate method for identifying high probability invariant sets for (2): compute equilibria of the embedding system (5) by, *e.g.*, initializing the embedding system dynamics at some point and simulating the dynamics to determine if the trajectory converges.

One difficulty of this method, however, is that the functions $\underline{\gamma}$ and $\overline{\gamma}$ must be evaluated at each point along the entire trajectory, which may be impractical in some cases. Instead, Theorem 2 offers an alternative method for identifying invariant sets that relies on evaluating $\underline{\gamma}$ and $\overline{\gamma}$ at a sequence of points and simulating the resulting embedding dynamics with $\underline{\gamma}$ and $\overline{\gamma}$ fixed to these evaluations.

To that end, consider an initial $\underline{x}^1 \preceq \overline{x}^1$ and construct the sequences $\{\underline{x}^k\}_{k=1}^{\infty}$, $\{\overline{x}^k\}_{k=1}^{\infty}$ according to the recursion

$$\underline{w}^k = \underline{\gamma}(\underline{x}^k, \overline{x}^k),\ \overline{w}^k = \overline{\gamma}(\underline{x}^k, \overline{x}^k) \tag{8}$$

and

$$(\underline{x}^{k+1}, \overline{x}^{k+1}) = \lim_{t\to\infty} (x^k(t), \hat{x}^k(t)) \tag{9}$$

provided the limit exists, where $(x^k(t), \hat{x}^k(t))$ is the solution to

$$\dot{x}^k = \delta(x^k, \underline{w}^k, \hat{x}^k, \overline{w}^k),\ \dot{\hat{x}}^k = \delta(\hat{x}^k, \overline{w}^k, x^k, \underline{w}^k) \tag{10}$$

with initial condition $x^k(0) = \underline{x}^k$, $\hat{x}^k(0) = \overline{x}^k$.

Theorem 3. *Consider* (2) *satisfying Assumptions 1 and 2. For any initial $\underline{x}^1 \preceq \overline{x}^1$, if the sequences $\{\underline{x}^k\}_{k=1}^{\infty}$, $\{\overline{x}^k\}_{k=1}^{\infty}$ constructed according to* (8)–(10) *are well-defined and converge, then $(\underline{x}^*, \overline{x}^*) := \lim_{k\to\infty}(\underline{x}^k, \overline{x}^k)$ constitutes an equilibrium of* (5) *and, hence, with probability at least $1-\epsilon$, $[\underline{x}^*, \overline{x}^*]$ is forward invariant for* (2).

In addition, if for some K it holds that

$$\underline{x}^K \preceq \underline{x}^{K+1} \text{ and } \overline{x}^{K+1} \preceq \overline{x}^K, \tag{11}$$

then for all $k \geq K$, it holds that $\underline{x}^k \preceq \underline{x}^{k+1}$ and $\overline{x}^{k+1} \preceq \overline{x}^k$ and the sequences $\{\underline{x}^k\}_{k=1}^{\infty}$, $\{\overline{x}^k\}_{k=1}^{\infty}$ converge. Moreover, with probability at least $1-\epsilon$, each $[\underline{x}^k, \overline{x}^k]$ for $k \geq K$ is forward invariant for (2).

Proof. For the first part of Theorem 3, construct the embedding system described by (8)–(10) for each iteration k

$$\begin{bmatrix}\dot{x}^k\\ \dot{\hat{x}}^k\end{bmatrix} = e^k(x^k, \hat{x}^k) := \begin{bmatrix}\delta(x^k, \underline{w}^k, \hat{x}, \overline{w}^k)\\ \delta(\hat{x}^k, \overline{w}^k, x^k, \underline{w}^k)\end{bmatrix}. \tag{12}$$

Since the limit $\lim_{t\to\infty}(x^k(t), \hat{x}^k(t))$ exists, $(\underline{x}^{k+1}, \overline{x}^{k+1})$ as defined by (9) must be such that

$$\begin{bmatrix}\dot{x}\\ \dot{\hat{x}}\end{bmatrix} = e^k(\underline{x}^{k+1}, \overline{x}^{k+1}) = 0, \tag{13}$$

i.e., $(\underline{x}^{k+1}, \overline{x}^{k+1})$ is an equilibrium for e^k.

Because the sequences $\{\underline{x}^k\}_{k=1}^{\infty}$, $\{\overline{x}^k\}_{k=1}^{\infty}$ converge, and because δ is Lipschitz continuous by Assumption 2, the Lipschitz continuous function $e^*(x, \hat{x}) = \begin{bmatrix}\delta(x, \underline{w}^*, \hat{x}, \overline{w}^*) & \delta(\hat{x}, \overline{w}^*, x, \underline{w}^*)\end{bmatrix}^T$ where $(\underline{w}^*, \overline{w}^*) := \lim_{k\to\infty}(\underline{w}^k, \overline{w}^k)$ satisfies $e^*(\underline{x}^*, \overline{x}^*) = 0$ where $(\underline{x}^*, \overline{x}^*) := \lim_{k\to\infty}(\underline{x}^k, \overline{x}^k)$, meaning that $(\underline{x}^*, \overline{x}^*)$ is an equilibrium of the embedding system $\begin{bmatrix}\dot{x} & \dot{\hat{x}}\end{bmatrix}^T = e^*(x, \hat{x})$, which we recall from Corollary 1 means that with probability at least $1-\epsilon$, $[\underline{x}^*, \overline{x}^*]$ is forward invariant for (2).

For the second part of Theorem 3, we note from the inclusion property in Assumption 2 that, for the K at which (11) holds, it must be true that $\underline{\gamma}(\underline{x}^K, \overline{x}^K) \preceq \underline{\gamma}(\underline{x}^{K+1}, \overline{x}^{K+1}) \preceq \overline{\gamma}(\underline{x}^{K+1}, \overline{x}^{K+1}) \preceq \overline{\gamma}(\underline{x}^K, \overline{x}^K)$, or, equivalently, $\underline{w}^K \preceq \underline{w}^{K+1} \preceq \overline{w}^{K+1} \preceq \overline{w}^K$. From (13), it also holds that $\delta(\underline{x}^{K+1}, \underline{w}^K, \overline{x}^{K+1}, \overline{w}^K) = 0$ and $\delta(\overline{x}^{K+1}, \overline{w}^K, \underline{x}^{K+1}, \underline{w}^K) = 0$. Thus, as an immediate consequence of property 4 in Assumption 2,

$$\delta(\underline{x}^{K+1}, \underline{w}^{K+1}, \overline{x}^{K+1}, \overline{w}^{K+1}) \succeq 0, \tag{14}$$

$$\delta(\overline{x}^{K+1}, \overline{w}^{K+1}, \underline{x}^{K+1}, \underline{w}^{K+1}) \preceq 0, \tag{15}$$

which subsequently means that $\underline{x}^{K+1} \preceq \underline{x}^{K+2}$ and $\overline{x}^{K+2} \preceq \overline{x}^{K+1}$ must also hold, which means that $\underline{w}^{K+1} \preceq \underline{w}^{K+2} \preceq \overline{w}^{K+2} \preceq \overline{w}^{K+1}$ also holds, and so on by induction. This also extends back one step to iteration K, i.e., it must also have been true that $\delta(\underline{x}^K, \underline{w}^K, \overline{x}^K, \overline{w}^K) \succeq 0$ and $\delta(\overline{x}^K, \overline{w}^K, \underline{x}^K, \underline{w}^K) \preceq 0$ in order for (11) to hold in the first place (though we note that $\underline{w}^{K-1} \preceq \underline{w}^K \preceq \overline{w}^K \preceq \overline{w}^{K-1}$ does not necessarily have to hold for this to be the case).

As a result, for all $k \geq K$, it holds that $\underline{x}^k \preceq \underline{x}^{k+1}$ and $\overline{x}^{k+1} \preceq \overline{x}^k$ and the sequences $\{\underline{x}^k\}_{k=1}^{\infty}$, $\{\overline{x}^k\}_{k=1}^{\infty}$ converge. Additionally, as $\delta(\underline{x}^k, \underline{w}^k, \overline{x}^k, \overline{w}^k) \succeq 0$ and $\delta(\overline{x}^k, \overline{w}^k, \underline{x}^k, \underline{w}^k) \preceq 0$ hold for all $k \geq K$, by Theorem 2 each $[\underline{x}^k, \overline{x}^k]$ for $k \geq K$ is forward invariant for (2) with probability at least $1-\epsilon$. ■

Theorem 2 and Corollary 1 indicate that the hyperrectangle $[\underline{x}^*, \overline{x}^*]$, such that $(\underline{x}^*, \overline{x}^*)$ is an equilibrium for the embedding system (5), is a forward invariant set for (2) with probability at least $1-\epsilon$. Additionally, Theorem 3 describes a computationally reasonable manner of calculating $[\underline{x}^*, \overline{x}^*]$. Thus, Theorems 2 and 3, and Corollary 1, solve Problem 2.

As detailed in the next section, the theory of GPs naturally leads to a methodology for modeling and obtaining $\underline{\gamma}$ and $\overline{\gamma}$ satisfying Assumption 2. In this case, it is further reasonable to envision updating the bounds $\underline{\gamma}$ and $\overline{\gamma}$ by incorporating newly collected data into estimation of the GPs, such that the bounds become tighter as the confidence of the GPs increase. This leads to tighter overapproximations of reachable and forward invariant sets, which in turn leads to more refined control of the system. We demonstrate this behavior in our Case Study outlined in Section VI.

V. Gaussian Processes for High Probability Uncertainty Bounds

We now propose an approach to construct functions $\underline{\gamma}$ and $\overline{\gamma}$ satisfying Assumption 1. The crux of the approach is to posit the existence of a specific probability distribution over the function space for each of the unknown functions $\{g_i\}_{i=1,\cdots,p}$ constituting the unknown part of the dynamics.

Assumption 3. *The unknown functions $\{g_i\}_{i\in\{1,\cdots,p\}}$, are independent realizations of a Gaussian Process $\mathcal{GP}(0, k(x,x'))$ with zero mean and kernel $k(\cdot,\cdot)$. In addition, observations of the GP are perturbed by additive i.i.d. Gaussian noise $\mathcal{N}(0,\sigma^2)$ with zero mean and variance σ^2.*

GPs are a form of non-parametric estimators [8] that are extremely powerful and have gained popularity in a broad range of applications including optimization and control [9]–[13], [17]. The kernel $k(\cdot,\cdot)$ is a hyper-parameter of the model that controls the correlation of the GP over its domain, which can be heuristically viewed as an assumption regarding the smoothness of the unknown function g_i.

Assumption 3 allows one to approximate the true unknown functions $\{g_i\}_{i=1,\cdots,p}$ using surrogate functions that 1) provide lower or upper bounds for the true functions with high probability; and 2) can be refined by acquiring additional observations of the GP. Specifically, given noisy observations $\{y_j\}_{j\in 1,\cdots,t}$ of the GPs at corresponding points $\{x_j\}_{j\in 1\cdots,t}$ the surrogate functions of interest to approximate g_i are

$$\forall i \in \{1,\cdots,p\} \quad \begin{cases} \overline{g}_i^{(t)}(x) := \mu_t(x) + \sqrt{\beta_t}\sigma_t(x) \\ \underline{g}_i^{(t)}(x) := \mu_t(x) - \sqrt{\beta_t}\sigma_t(x) \end{cases} \tag{16}$$

where β_t is to be specified later (see Theorem 4), $\mu_t(\cdot)$ is the posterior mean, and $\sigma_t(\cdot)$ is the posterior variance, computed according to the standard GP updates [8]:

$$\mu_t(x) := k_t(x)^T(K_t + \sigma^2 I)^{-1}k_t(x) \tag{17}$$

$$k_t(x,x') := k(x,x') = k_t(x)^T(K_t + \sigma^2 I)^{-1}k_t(x') \tag{18}$$

$$\sigma_t^2(x) := k_t(x,x). \tag{19}$$

where $k_t(x) := (k(x_1,x),\cdots,k(x_t,x))$ and $K_t = [k_t(x_i,x_j)]$. Intuitively, the bounds in (16) hold with high probability and can be used to create functions $\underline{\gamma}$ and $\overline{\gamma}$ as follows. For all $i \in \{1,\cdots,p\}$ and all $t \geq 1$

$$\forall \underline{x} \preceq \overline{x} \quad \begin{cases} \underline{\gamma}_i^{(t)}(\underline{x},\overline{x}) := \min_{x\in[\underline{x},\overline{x}]} \underline{g}_i^{(t)}(x), \\ \overline{\gamma}_i^{(t)}(\underline{x},\overline{x}) := \max_{x\in[\underline{x},\overline{x}]} \overline{g}_i^{(t)}(x). \end{cases} \tag{20}$$

By definition, the functions in (20) satisfy the natural inclusion property in Assumption 1. However, establishing that (3) holds requires a bit more care because the high probability statement has to hold for all states in a subset of $\mathbb{R}^n$ and for all times t at which updates are made to the GP. We introduce the following mild technical assumptions.

Assumption 4. *The states x are confined to a compact subset $\mathcal{D} \subset \mathbb{R}^n$ included in a hypercube of edge size r. In addition, there exist constants $a, b > 0$ such that*

$$\forall i \in \{1,\cdots,n\} \forall j \in \{1,\cdots,p\} \quad \Pr\left(\sup_{x\in\mathcal{D}} \left|\frac{\partial g_j}{\partial x_i}\right| > L\right) \leq a e^{-L^2/b^2}. \tag{21}$$

The first part of Assumption 4 is relatively mild since we can assume that the trajectories are confined into a (possibly) large hypercube when computing safe reachable sets as in Section VI. The second part of Assumption 4 is also mild and is satisfied by many kernels of interest [17]. By adapting the proof of [17, Theorem 2], we have the following.

Theorem 4. *Assume that the unknown functions $\{g_i\}_{i=1,\cdots,p}$ satisfy Assumptions 3 and 4. Pick $\epsilon \in (0,1)$ and set*

$$\beta_t := 2\log\left(\frac{pt^2\pi^2}{3\epsilon}\right) + 2n\log\left(t^2 nbr\sqrt{\log\left(\frac{4na}{\epsilon}\right)}\right). \tag{22}$$

At every step t of the GP update, define a uniform discretization $\mathcal{D}_t$ of the hypercube containing $\mathcal{D}$ with size τ_t^n where $\tau_t := nt^2br\sqrt{\log\left(\frac{2npa}{\epsilon}\right)}$. For every $x \in \mathcal{D}$, define

$$x^{(t,-)} := \sup\{y \in \mathcal{D}_t \mid y \preceq x\}, \tag{23}$$

$$x^{(t,+)} := \inf\{y \in \mathcal{D}_t \mid x \preceq y\}. \tag{24}$$

For all $i \in \{1,\cdots,p\}$ and all $t \geq 1$ define $\forall \underline{x} \preceq \overline{x}$

$$\underline{\gamma}_i^{(t)}(\underline{x},\overline{x}) := \min_{x\in[\underline{x}^{(t,-)},\overline{x}^{(t,+)}]\cap\mathcal{D}_t} \underline{g}_i^{(t)}(x) - \frac{1}{t^2}, \tag{25}$$

$$\overline{\gamma}_i^{(t)}(\underline{x},\overline{x}) := \max_{x\in[\underline{x}^{(t,-)},\overline{x}^{(t,+)}]\cap\mathcal{D}_t} \overline{g}_i^{(t)}(x) + \frac{1}{t^2}. \tag{26}$$

Then, with probability at least $1-\epsilon$,

$$\forall \underline{x} \preceq \overline{x} \quad \forall x \in [\underline{x},\overline{x}] \quad \forall t \geq 1 \quad \forall j \in \{1,\cdots,p\}$$
$$\underline{\gamma}_i^{(t)}(\underline{x},\overline{x}) \leq g_i(x) \leq \overline{\gamma}_i^{(t)}(\underline{x},\overline{x}). \tag{27}$$

The proof is omitted for brevity. Theorem 4 can be directly combined with the results of Section IV.

VI. Case Study: A Planar Multirotor

We consider the *planar multirotor* model for a multirotor aerial vehicle constrained to move in a vertical plane. The horizontal and vertical position of the multirotor are denoted y and z, the roll angle is denoted θ, and the six-dimensional state x of the system consists of y, z, θ, and their derivatives, $v_y = \dot{y}$, $v_z = \dot{z}$, $\omega = \dot{\theta}$, so that $x = \begin{bmatrix} y \ v_y \ z \ v_z \ \theta \ \omega \end{bmatrix}^T$. The two inputs are thrust u_1 acting at the center of mass in the direction $\begin{bmatrix} -\sin\theta & \cos\theta \end{bmatrix}^T$ perpendicular to the line segment connecting the rotors, and roll angular acceleration u_2. Aside from gravitational acceleration a_g, we assume the system is also subject to an unknown force due to wind. We assume this force affects acceleration in both the horizontal and vertical directions and is a function of altitude z. The resulting dynamics with normalized mass and moment of inertia are given by

$$\begin{aligned} \ddot{y} &= -u_1\sin\theta + g_1(z) \\ \ddot{z} &= u_1\cos\theta - a_g + g_2(z) \\ \ddot{\theta} &= u_2 \end{aligned} \tag{28}$$

where g_1 and g_2 constitute the unknown wind forces in the horizontal and vertical directions, respectively. We estimate g_1 and g_2 using Gaussian processes with a radial basis function kernel, and obtain high confidence bounds by considering posterior estimates up to two standard deviations from the mean.

To demonstrate our theoretical results, we consider a simple control objective of climbing to a nominal altitude and returning to the ground at $z = 0$. We suppose that position is not measurable during the maneuver so that the unknown wind force is capable of blowing the system off course. On the other hand, this force can be compensated by feedforward control using an estimate of the wind force. Given a horizontal displacement that can be safely tolerated during the maneuver, the theory developed in this paper is able to determine in advance if the proposed maneuver is safe with high probability.

To that end, given a target altitude and a time horizon T for the maneuver, we propose the following control strategy that does not require position measurements. We divide the time horizon into a uniform acceleration phase during time interval $[0, \frac{T}{4}]$, a uniform deceleration phase during $[\frac{T}{4}, \frac{3T}{4}]$, and a uniform acceleration phase from $[\frac{3T}{4}, T]$. The result is a desired vertical trajectory that is piecewise quadratic in time and reaches the peak target altitude at time $\frac{T}{2}$.

This desired vertical acceleration profile is converted to a desired thrust profile $u_1^*(t)$ and desired roll angle $\theta^*(t)$ computed from the dynamics (28) in order to counter the force due to gravity and the wind forces, where we use the mean estimated wind forces in place of the unknown g_1 and g_2. We then apply a proportional-derivative control so that $\theta(t)$ tracks $\theta^*(t)$, and we use directly $u_1^*(t)$ as the applied thrust. The closed-loop system results in dynamics that are mixed monotone after a state transformation of the closed-loop (θ,ω) coordinates into Jordan canonical form. We then obtain the system decomposition and embedding dynamics from the tight decomposition construction in [18].

Since the estimated wind forces are used to compute the input profile, the actual trajectory of the multirotor will differ from the planned profile. Given a safe horizontal displacement, Theorem 1 allows for efficiently computing a high probability reachable set for the system over the horizon T to determine if the system will remain safe with high probability during the duration of the maneuver.

Lastly, note that while the system has six state dimensions, the unknown wind force appears only in two entries of the vector field, those for $\dot{v}_y$ and $\dot{v}_z$, and is assumed only to be a function of altitude z. Therefore, it is computationally tractable to obtain the functions $\underline{\gamma}_i$ and $\overline{\gamma}_i$ for $i \in \{1,2\}$ by evaluating the Gaussian process mean and standard deviation functions via direct sampling. This emphasizes the main appeal of the methodology proposed in this paper: mixed monotone system theory, which is applicable to high dimensional systems, is combined with the theoretical guarantees of Gaussian process estimation, which is tractable in lower dimensions, to obtain high dimensional, high probability over-approximations of reachable sets.

We consider three scenarios. In the first scenario, the target altitude is $z = 50$, but the estimate of the wind force is poor and therefore the reachable set computed using Theorem 1, as well as the actual system trajectory, enters the unsafe region, which is the set of states such that $y \leq -20$ or $y \geq 20$. In the second scenario, we show that with the same poor wind force estimate, the system is able to safely climb to a lower target altitude of $z = 20$. Lastly, in the third scenario, the target altitude is again $z = 50$ but the estimate of the wind

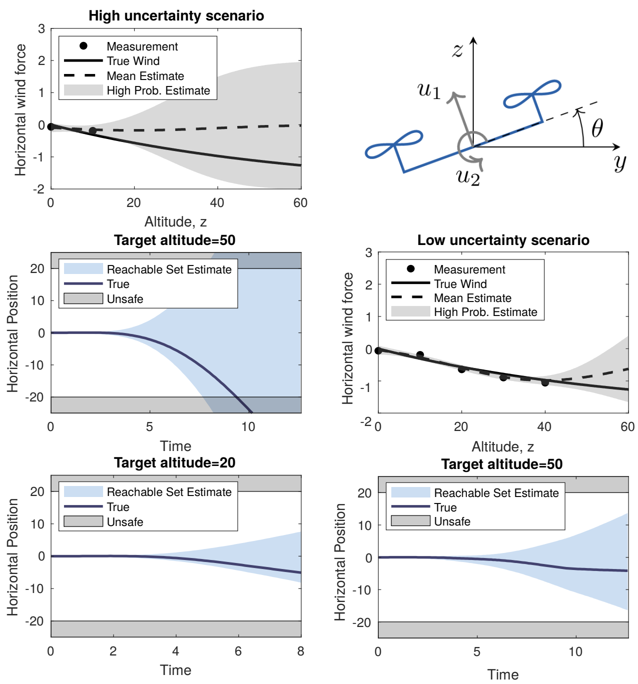

Fig. 1. The planar multirotor model (right, top) has horizontal position y, vertical position z, and roll angle θ. The inputs are thrust u_1 in the direction perpendicular to the line segment connecting the rotors and roll angle acceleration u_2. In the first two scenarios for the multirotor case study, the estimate of the wind force is poor (left, top). With a target altitude of 50, the high probability reachable set computed from this poor estimate using Theorem 1 enters the unsafe set, as does the true trajectory (left, middle). However, a lower target altitude of 20 maintains safety (left, bottom). In the third scenario, the estimate of the wind force is improved (right, middle). With a target altitude of 50, the high probability reachable set now remains safe (right, bottom).

force is more accurate with lower uncertainty. For example, wind measurements might be safely collected at successively higher altitudes, although we do not consider here explicitly the mechanism by which measurements are collected. In this scenario, the maneuver is now safe with high probability. In all scenarios, computing the reachable set of the six-dimensional system with MATLAB on a standard personal computer takes under one second. Figure 1 demonstrates these scenarios.

VII. Conclusion

We have presented a technique for computing reachable and forward invariant sets for dynamical systems with unknown components by modeling these components as GPs, which allows for the assumption of high probability bounds. For systems that are moderately high dimensional in the known component and lower dimensional in the unknown component, which occur often in practice, this assumption in turn enables tractable algorithms for determining reachable and forward invariant sets with high probability by leveraging tools from mixed monotone systems theory. As shown in the case study, this is achieved by sampling the GP over the relevant region of the state space to retrieve high probability bounds, then inputting these bounds into an embedding system, from which the reachable and forward invariant sets are calculated. Crucially, this method does not require the unknown components to be affine, and we are able to model the components in continuous time. Future directions of research include integrating techniques for efficient observation of the state space in order to more effectively tighten bounds on the unknown components.

References

[1] S. Coogan, “Mixed monotonicity for reachability and safety in dynamical systems,” in *2020 59th IEEE Conference on Decision and Control (CDC)*, pp. 5074–5085, 2020.

[2] S. Coogan, E. A. Gol, M. Arcak, and C. Belta, “Traffic network control from temporal logic specifications,” *IEEE Transactions on Control of Network Systems*, vol. 3, pp. 162–172, June 2016.

[3] M. Abate, M. Mote, E. Feron, and S. Coogan, “Verification and runtime assurance for dynamical systems with uncertainty,” in *Hybrid Systems: Computation and Control*, 2021, to appear.

[4] M. Abate and S. Coogan, “Computing robustly forward invariant sets for mixed-monotone systems,” in *2020 59th IEEE Conference on Decision and Control (CDC)*, pp. 4553–4559, 2020.

[5] G. Enciso, H. Smith, and E. Sontag, “Nonmonotone systems decomposable into monotone systems with negative feedback,” *Journal of Differential Equations*, vol. 224, no. 1, pp. 205–227, 2006.

[6] S. Coogan and M. Arcak, “Efficient finite abstraction of mixed monotone systems,” in *Proceedings of the 18th International Conference on Hybrid Systems: Computation and Control*, pp. 58–67, 2015.

[7] H. Smith, “Global stability for mixed monotone systems,” *Journal of Difference Equations and Applications*, vol. 14, no. 10-11, pp. 1159–1164, 2008.

[8] C. E. Rasmussen and C. K. I. Williams., *Gaussian Processes for Machine Learning*. Cambridge, Massachusetts: MIT Press, 2006.

[9] F. Berkenkamp, A. P. Schoellig, and A. Krause, “Safe controller optimization for quadrotors with Gaussian Processes,” pp. 491–496, May 2016.

[10] M. Liu, G. Chowdhary, B. C. da Silva, S.-Y. Liu, and J. P. How, “Gaussian Processes for learning and control: A tutorial with examples,” *IEEE Control Systems Magazine*, vol. 38, pp. 53–86, oct 2018.

[11] W. Luo, C. Nam, G. Kantor, and K. Sycara, “Distributed environmental modeling and adaptive sampling for multi-robot sensor coverage,” in *Proceedings of the 18th International Conference on Autonomous Agents and MultiAgent Systems*, AAMAS ’19, (Richland, SC), pp. 1488–1496, International Foundation for Autonomous Agents and Multiagent Systems, 2019.

[12] A. Benevento, M. Santos, G. Notarstefano, K. Paynabar, M. Bloch, and M. Egerstedt, “Multi-robot coordination for estimation and coverage of unknown spatial fields,” in *Proc. of IEEE International Conference on Robotics and Automation*, (Paris, France), pp. 7740–7746, May 2020.

[13] A. Lederer, J. Umlauft, and S. Hirche, “Uniform error bounds for Gaussian Process regression with application to safe control,” in *Advances in Neural Information Processing Systems* (H. Wallach, H. Larochelle, A. Beygelzimer, F. d'Alché-Buc, E. Fox, and R. Garnett, eds.), vol. 32, (Vancouver, Canada), Curran Associates, Inc., Dec. 2019.

[14] M. J. Khojasteh, V. Dhiman, M. Franceschetti, and N. Atanasov, “Probabilistic safety constraints for learned high relative degree system dynamics,” in *Proceedings of the 2nd Conference on Learning for Dynamics and Control*, vol. 120 of *Proceedings of Machine Learning Research*, pp. 781–792, PMLR, 10–11 Jun 2020.

[15] T. Koller, F. Berkenkamp, M. Turchetta, and A. Krause, “Learning-based model predictive control for safe exploration,” in *2018 IEEE Conference on Decision and Control (CDC)*, pp. 6059–6066, 2018.

[16] J. Choi, F. Castañeda, C. Tomlin, and K. Sreenath, “Reinforcement learning for safety-critical control under model uncertainty, using control lyapunov functions and control barrier functions,” in *Proceedings of Robotics: Science and Systems*, (Corvalis, Oregon, USA), July 2020.

[17] N. Srinivas, A. Krause, S. Kakade, and M. Seeger, “Gaussian Process optimization in the bandit setting: No regret and experimental design,” in *Proceedings of the 27th International Conference on Machine Learning*, (USA), pp. 1015–1022, 2010.

[18] M. Abate, M. Dutreix, and S. Coogan, “Tight decomposition functions for continuous-time mixed-monotone systems with disturbances,” *IEEE Control Systems Letters*, 2020.