Change-Of-Bases Abstractions For Non-Linear Hybrid Systems.

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Abstract

We present abstraction techniques that transform a given non-linear dynamical system into a linear system, or more generally, an algebraic system described by polynomials of bounded degree, so that invariant properties of the resulting abstraction can be used to infer invariants for the original system. The abstraction techniques rely on a change-of-bases transformation that associates each state variable of the abstract system with a function involving the state variables of the original system. We present conditions under which a given change-of-bases transformation for a non-linear system can define an abstraction. Furthermore, the techniques developed here apply to continuous systems defined by Ordinary Differential Equations (ODEs), discrete systems defined by transition systems and hybrid systems that combine continuous as well as discrete subsystems.

The techniques presented here allow us to discover, given a non-linear system, if a change-of-bases transformation involving degree-bounded polynomials yielding an algebraic abstraction exists. If so, our technique yields the resulting abstract system, as well. Our techniques enable the use of analysis techniques for linear systems to infer invariants for non-linear systems. We present preliminary evidence of the practical feasibility of our ideas using a prototype implementation.

Keywords: Hybrid Systems, Abstraction, Verification, Linearization, Invariants, Conservation Laws, Program Analysis, Abstract Interpretation.

1. Introduction

In this paper, we explore a class of abstractions for non-linear autonomous systems (continuous, discrete and hybrid systems) using *Change-of-Bases* (CoB) transformations. CoB transformations are obtained for a given system by expressing the dynamics of the system in terms of a new set of variables that relate to the original system variables by means of a transformation. Such a transformation is akin to studying the system under a new set of “bases”. We derive conditions on the transformations such that (a) the CoB transformations also define an *autonomous system* and (b) the resulting system abstracts the

original system: i.e., all invariants of the abstract system can be inverted to obtain invariants for the original system. Furthermore, we often seek abstract systems through CoB transformations whose dynamics are of a simpler form, more amenable to automatic verification techniques. For instance, it is possible to use CoB transformations that relate an ODE with non-linear right-hand sides to an affine ODE, or transformations that reduce the degree of a system with polynomial right-hand sides. If such transformations can be found, then safety analysis techniques over the simpler abstract system can be used to infer safety properties of the original system.

In this paper, we make two main contributions: (a) we define CoB transformations for continuous, discrete and hybrid systems and provide conditions under which a given transformation is valid; (b) we provide search techniques for finding CoB transformations that result in a polynomial system whose right-hand sides are degree limited by some limit $d \geq 1$. Specifically, the case $d = 1$ yields an affine abstraction; and (c) we provide experimental evidence of the application of our techniques to a variety of ordinary differential equations (ODEs) and discrete programs.

The results in this paper extend our previously published results that appeared in Hybrid Systems: Computation and Control (HSCC) 2011 [52]. The contributions of this paper include (a) an extension from linearizing CoB transformations to degree-bounded polynomial CoB transformations, (b) extending the theory from purely continuous system to purely hybrid systems, and (c) an improved implementation that can handle hybrid systems with some evaluation results over this implementation. On the other hand, our previous work also included an extension of the theory to differential inequalities and iterative techniques over cones. These extensions are omitted here. Finally, our work here is restricted to autonomous ODEs and programs without external inputs. All uncertainty in our system is restricted to the initial set of states, which are not considered explicitly in the process of abstracting the dynamics, as detailed in Section 2.2. Bounded disturbances can potentially be handled in a planned extension of this paper that considers iterations over cones rather than vector spaces [52].

1.1. Motivating Examples

In this section, we motivate the techniques developed in this paper by means of a few illustrative examples involving purely continuous ODEs and purely discrete programs.

Our first example concerns a continuous system defined by a system of Ordinary Differential Equations (ODEs):

Example 1.1. Consider a continuous system over $\{x, y\}$: $\dot{x} = xy + 2x$, $\dot{y} = -\frac{1}{2}y^2 + 7y + 1$, with initial conditions given by the set $x \in [0, 1]$, $y \in [0, 1]$. Using the transformation $\alpha : (x, y) \mapsto (w_1, w_2, w_3)$ wherein $\alpha_1(x, y) = x$, $\alpha_2(x, y) = xy$ and $\alpha_3(x, y) = xy^2$, we find that the dynamics over $\vec{w}$ can be written as

$$\dot{w}_1 = 2w_1 + w_2, \quad \dot{w}_2 = w_1 + 9w_2 + \frac{1}{2}w_3, \quad \dot{w}_3 = 2w_2 + 16w_3.$$

Its initial conditions are given by $w_1 \in [0, 1]$, $w_2 \in [0, 1]$, $w_3 \in [0, 1]$. We analyze the system using the TimePass tool as presented in our previous work [56] to obtain polyhedral invariants:

$$\begin{aligned} & -w_1 + 2w_2 \geq -1 \wedge w_3 \geq 0 \wedge w_2 \geq 0 \wedge \\ & -16w_1 + 32w_2 - w_3 \geq -17 \wedge 32w_2 - w_3 \geq -1 \wedge \\ & 2w_1 - 4w_2 + 17w_3 \geq -4 \wedge 286w_1 - 32w_2 + w_3 \geq -32 \wedge \\ & \dots \end{aligned}$$

Substituting back, we can infer polynomial inequality invariants on the original system including,

$$\begin{aligned} & -x + 2xy \geq -1 \wedge xy^2 \geq 0 \wedge -16x + 32xy - xy^2 \geq -17 \\ & x \geq 0 \wedge 2x - 4xy + 17xy^2 \geq -4 \wedge \dots \end{aligned}$$

Finally, we link the presence of affine change-of-bases abstractions with a set of conserved quantities (first integrals) of the original system (see Lemma 2.4 in page 21). Recall that a conserved quantity $f(\vec{x}, t)$ is a function whose value is constant over all trajectories: i.e, for all time trajectories of the system $f(\vec{x}(t), t) = f(\vec{x}(0), 0)$. For this example, we infer the following conserved quantity on the underlying non-linear system:

$$\begin{aligned} & \left(\frac{e^{-9t}}{51} + \frac{1}{102} (50 + 7\sqrt{51}) e^{(-9+\sqrt{51})t} + \frac{1}{102} (50 - 7\sqrt{51}) e^{-(9+\sqrt{51})t} \right) x + \\ & \left(-\frac{1}{102} e^{-9t-(9+\sqrt{51})t} \begin{pmatrix} 7e^{9t} - \sqrt{51}e^{9t} - 14e^{(9+\sqrt{51})t} + \\ 7e^{9t+(-9+\sqrt{51})t+(9+\sqrt{51})t} + \\ \sqrt{51}e^{9t+(-9+\sqrt{51})t+(9+\sqrt{51})t} \end{pmatrix} \right) xy + \\ & \left(\frac{1}{204} e^{-9t-(9+\sqrt{51})t} \left(e^{9t} - 2e^{(9+\sqrt{51})t} + e^{9t+(-9+\sqrt{51})t+(9+\sqrt{51})t} \right) \right) xy^2 \end{aligned}$$

Finally, if $x(0) \neq 0$, the map α is invertible and therefore, the ODE above can be integrated.

Note that not every transformation yields a linear abstraction. In fact, most transformations will not define an abstraction. The conditions for an abstraction are discussed in Section 2. $\blacktriangle$

Next, we motivate our approach on purely discrete programs, showing how CoB transformations can linearize a discrete program with non-linear assignments, modeled by a *transition system* [33]. In turn, we show how invariants of the abstract linearized program can be transferred back.

Example 1.2. Figure 1 shows an example proposed originally by Petter [43] that considers a program that sums up all squares from 1 to K^2 for some input $K \geq 0$. Consider a very simple change-of-bases transformation wherein we add a new variable “y2” that tracks the value of y^2 as the loop is executed. It is straightforward to write assignments for “y2” in terms of itself, x, y . Finally, the resulting program has affine guards and assignments, making it suitable for polyhedral abstract interpretation [15, 26]. The polyhedral analysis yields

<pre> proc computeP(int k) int x,y; assert(k > 0); x := y := 0; while (y < k){ x := x + y * y; y := y + 1; } end-function </pre>	<pre> proc computePAbs(int k) int x,y,y2; assert(k > 0); x := y := y2 := 0; while (y < k){ x := x + y2; y2 := y2 + 2 * y + 1; y := y + 1; } end-function </pre>
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Figure 1: Program showing a benchmark example proposed by Petter [43] and its abstraction obtained by a change-of-bases ($x \mapsto x, y \mapsto y, y2 \mapsto y^2$).

linear invariants at the loop head and the function exit in terms of the variables $x, y, y2$. We may safely substitute y^2 in place of $y2$ and obtain invariants over the original program. The non-linear invariants obtained at the function exit are shown below:

$$4x + 18y - 7y^2 \geq 11 \wedge 4 \leq 2x + 7y - 3y^2 \wedge 9 \leq x + 12y - 3y^2 \wedge 1 \leq y \wedge 3y - y^2 \leq 2 \wedge 5y - y^2 \leq 6 \wedge 6y - y^2 \leq 9 \wedge k = y$$

In this example, the change-of-bases to y^2 can be inferred from the syntax of this program. However, we demonstrate other situations in this paper, wherein the change-of-bases cannot be inferred from the expressions in the program using syntactic means.

The invariant

$$6x = 2k^3 + 3k^2 + k,$$

discovered by Petter and many other subsequent works such as the complete approach for P-solvable loops by Kovacs [29] can also be discovered by Karr's analysis when the term y^3 is introduced into the change-of-bases transformations in addition to y^2 .

1.2. Related Work

Many different types of *discrete abstractions* have been studied for hybrid systems [2] including predicate abstraction [59] and abstractions based on invariants [40]. The use of counter-example guided abstraction-refinement for iterative refinement has also been investigated in the past (Cf. Alur et al. [1] and Clarke et al. [11], for example). In this paper, we consider continuous abstractions for continuous systems specified as ODEs, discrete systems and hybrid systems using a change-of-bases transformation. As noted above, not all transformations can be used for this purpose. Our abstractions for ODEs bear similarities to the notion of topological semi-conjugacy between flows of dynamical systems [35].

Previous work on invariant generation for hybrid system by the author constructs invariants by assuming a desired template form (ansatz) with unknown parameters and applying the “consecution” conditions such as *strong consecution* and *constant scale* consecution [55]. Matringe et al. present generalizations of these conditions using morphisms [34]. Therein, they observe that strong and constant scale consecution conditions correspond to a linear abstraction of the original non-linear system of a restrictive form. Specifically, the original system is abstracted by a system of the form $\frac{dx}{dt} = 0$ for strong consecution, and a system of the form $\frac{dx}{dt} = \lambda x$ for constant-scale consecution. This paper builds upon this observation by Matringe et al. using fixed-point computation techniques to search for a general linear abstraction that is related to the original system by a change-of-bases transformation. Our work is closely related to the technique of differential invariants proposed by Platzer et al [44, 46]. A key primitive used in this technique can be cast as a search for abstractions of the form $\frac{dz}{dt} = 0$, wherein z stands for an expression involving the state variables of the system of interest. The basic differential invariant framework is extended to allow a larger set of rules involving so-called “cuts” in a subsequent extension [45]. It is shown that the power of differential invariants can be strictly improved by the addition of so-called auxilliary state variables. In contrast, here we attempt a different type of extension by using change-of-bases transformations, so that properties of the “abstract” system resulting from the change-of-bases can indeed be transferred back to the original system. In this regard, our approach allows us to use a rich set of known facts about the trajectories of linear systems that can be transferred back to reason about the original system.

Example 1.3. Consider, once again, our motivating example (Ex. 1.1). We wish to show that the set $x \geq 0 \wedge y \geq 0$ is a positive invariant for the system. However, neither $x \geq 0$ nor $y \geq 0$ can be established as a differential invariant. However, consider the linear system abstraction recalled below:

$$\begin{array}{rcl} \frac{dw_1}{dt} & = & 2w_1 + w_2 \\ \frac{dw_2}{dt} & = & w_1 + 9w_2 \\ \frac{dw_3}{dt} & = & 2w_2 + 16w_3 \end{array}$$

The system has the form $\frac{d\vec{w}}{dt} = A\vec{w}$ where A is a so-called *Metzler* matrix, i.e, a matrix whose nondiagonal entries are nonnegative [19]. It can be shown that e^{At} is a positive matrix for each $t \geq 0$. In turn, it follows that the first quadrant $w_1 \geq 0 \wedge w_2 \geq 0 \wedge w_3 \geq 0$ is positive invariant. This immediately shows that in the original co-ordinate system $x \geq 0 \wedge y \geq 0$ is a positive invariant.

Differential invariants are used inside a sophisticated verification framework for hybrid programs called Keymaera¹. On one hand, work here extends to more general abstractions that can involve multiple variables and can be system specific. However, the integration inside a framework such as Keymaera is an

¹Cf. <http://symbolaris.com/info/Keymaera.html>

important problem that is not addressed here. The approach presented here can be generalized to fixed-point computation over cones to search for generalized linear differential inequality abstractions.

Fixed point techniques for deriving invariants of differential equations have been proposed by the author in previous papers [56, 51]. These techniques have addressed the derivation of polyhedral invariants for affine systems [56] and algebraic invariants for systems with polynomial right-hand sides [51]. In this technique, we employ the machinery of fixed-points. Our primary goal is not to derive invariants, per se, but to search for abstractions of non-linear systems into linear systems.

There has been a large body of work focused on the use of algebraic techniques for deriving invariants of programs. Previous work by the author focuses on deriving polynomial equality invariants for programs, automatically, by setting up template polynomial invariants with unknown coefficients and deriving constraints on values of these coefficients to ensure invariance [55, 54]. Carbonell et al. present loop invariant generation techniques by solving recurrences and computing polynomial ideals to capture algebraic properties of the reachable states [50] and subsequently using the descending abstract interpretation over ideals with widening over ideals to ensure termination [49]. The approach is extended to polyhedral cones generated by polynomial inequalities to generate polynomial inequality invariants [4]. Another set of related techniques concern the use of linear invariant generation techniques for polynomial equality invariant generation. Müller-Olm and Seidl explore the use of linear algebraic techniques, wherein a vector space of matrices are used to summarize the transformation from the initial state of a program to a given location. This space is then used to generate polynomial invariants of the program [38]. Likewise, the work of Colón explores degree-bounded restrictions to Nullstellensatz to enable linear algebraic techniques to generate polynomial invariants [14]. More recently, the work of Kovacs uses sophisticated techniques for solving recurrence equations over so-called P-Solvable loops to generate polynomial invariants for them [29].

Finally, our approach is closely related to *Carleman embedding* that can be used to linearize a given differential equation with polynomial right-hand sides [30]. The standard Carleman embedding technique creates an infinite dimensional linear system, wherein, each dimension corresponds to a monomial or a basis polynomial. In practice, it is possible to create a linear approximation with known error bounds by truncating the monomial terms beyond a degree cutoff. Our approach for differential equation abstractions can be seen as a search for a “finite submatrix” inside the infinite matrix created by the Carleman linearization. The rows and columns of this submatrix correspond to monomials such that the derivative of each monomial in the submatrix is a linear combination of monomials that belong to the submatrix.

Organization: The rest of this paper presents our approach for Ordinary Differential Equations in Section 2. The ideas for discrete systems are presented in Section 3 by first presenting the theory for simple loops and then extending it to

arbitrary discrete programs modeled by transition systems. The extensions to hybrid systems are presented briefly by suitably merging the techniques for discrete programs with those for ODEs. Finally, Section 4 presents an evaluation of the ideas presented using our implementation that combines an automatic search for CoB transformations with polyhedral invariant generation for continuous, discrete and hybrid systems [15, 26, 56].

2. Abstractions for ODEs

We first present some preliminary definitions for continuous systems defined by Ordinary Differential Equations (ODEs).

2.1. Preliminaries: Continuous Systems

Let $\mathbb{R}$ denote the field of real numbers. Let $x_1, \dots, x_n$ denote a set of variables, collectively represented as $\vec{x}$. The set $\mathbb{R}[\vec{x}]$ denotes the ring of multivariate polynomials over $\mathbb{R}$.

A *power-product* over $\vec{x}$ is of the form $x_1^{r_1} x_2^{r_2} \dots x_n^{r_n}$, succinctly written as $\vec{x}^{\vec{r}}$, wherein each $r_i \in \mathbb{N}$. The *degree* of a monomial $\vec{x}^{\vec{r}}$ is given by $\sum_{i=1}^n r_i = \vec{1} \cdot \vec{r}$. A *monomial* is of the form $c \cdot m$ where $c \in \mathbb{R}$ and m is a power-product. A multivariate polynomial p is a sum of finitely many monomial terms: $p = \sum_{\vec{r} \in \mathbb{N}^n} c_{\vec{r}} \vec{x}^{\vec{r}}$. The degree of a multivariate polynomial p is the maximum over the degrees of all monomial terms m that *occur* in p with a non-zero coefficient.

We assume some basic familiarity with the basics of computational algebraic geometry [16] and elementary linear algebra [27].

Vector Fields: A *vector field* F over a manifold $M \subseteq \mathbb{R}^n$ is a map $F : M \mapsto \mathbb{R}^n$ from each $\vec{x} \in M$ to a vector $F(\vec{x}) \in \mathbb{R}^n$, wherein $F(\vec{x}) \in T_M(\vec{x})$, the tangent space of M at $\vec{x}$.

A vector field F is continuous if the map F is continuous. A *polynomial vector field* $F \in (\mathbb{R}[\vec{x}])^n$ is specified by a tuple $F(\vec{x}) = \langle p_1(\vec{x}), p_2(\vec{x}), \dots, p_n(\vec{x}) \rangle$, wherein $p_1, \dots, p_n \in \mathbb{R}[\vec{x}]$.

A system of (coupled) ordinary differential equations (ODE) specifies the evolution of variables $\vec{x} : (x_1, \dots, x_n) \in M$ over time t :

$$\frac{dx_1}{dt} = p_1(x_1, \dots, x_n), \dots, \frac{dx_n}{dt} = p_n(x_1, \dots, x_n),$$

The system implicitly defines a vector field $F(\vec{x}) : \langle p_1(\vec{x}), \dots, p_n(\vec{x}) \rangle$. We assume that all vector fields F considered in this paper are (locally) Lipschitz continuous over the domain M . In general, all polynomial vector fields are locally Lipschitz continuous, but not necessarily *globally* Lipschitz continuous over an unbounded domain X . The Lipschitz continuity of the vector field F , ensures that given $\vec{x} = \vec{x}_0$, there exists a time $T > 0$ and a unique time trajectory $\tau : [0, T) \mapsto \mathbb{R}^n$ such that $\frac{d\tau(t)}{dt} = F(\tau(t))$ for all $t \in [0, T)$ [35].

Definition 2.1. For a vector field $F : \langle f_1, \dots, f_m \rangle$, the *Lie derivative* of a smooth function $f(\vec{x})$ is given by

$$\mathcal{L}_F(f) = (\nabla f) \cdot F(\vec{x}) = \sum_{i=1}^n \left(\frac{\partial f}{\partial x_i} \cdot f_i \right)$$

Definition 2.2. A continuous system over variables $x_1, \dots, x_n$ consists of a tuple $\mathcal{S} : \langle X_0, \mathcal{F}, X_I \rangle$ wherein $X_0 \subseteq \mathbb{R}^n$ is the set of initial states, $\mathcal{F}$ is a vector field over the domain represented by a manifold $X_I \subseteq \mathbb{R}^n$.

Note that in the context of hybrid systems, the set X_I is often referred to as the *state invariant* or the *domain* manifold.

2.2. Change-of-Bases for Continuous Systems

In this section, we will present change-of-bases (CoB) transformations of continuous systems and some of their properties.

Consider a map $\alpha : \mathbb{R}^k \mapsto \mathbb{R}^l$. Given a set $S \subseteq \mathbb{R}^k$, let $\alpha(S)$ denote the set obtained by applying α to all the elements of S . Likewise, the inverse map over sets is $\alpha^{-1}(T) : \{s \mid \alpha(s) \in T\}$. Let $\mathcal{S} : \langle X_0, \mathcal{F}, X_I \rangle$ be a continuous system over variables $\vec{x} : (x_1, \dots, x_n)$, involving the vector field $\mathcal{F}$, and $\mathcal{T} : \langle Y_0, \mathcal{G}, Y_I \rangle$ be a continuous system over variables $\vec{y} : (y_1, \dots, y_m)$ involving the vector field $\mathcal{G}$.

Definition 2.3. We say that $\mathcal{T}$ *simulates* $\mathcal{S}$ iff there exists a smooth mapping $\alpha : \mathbb{R}^n \mapsto \mathbb{R}^m$ such that

1. $Y_0 \supseteq \alpha(X_0)$ and $Y_I \supseteq \alpha(X_I)$.
2. For any trajectory $\tau : [0, T) \mapsto X_I$ of $\mathcal{S}$, $\alpha \circ \tau$ is a trajectory of $\mathcal{T}$.

A simulation relation implies that any time trajectory of $\mathcal{S}$ can be mapped to a trajectory of $\mathcal{T}$ through α . However, since α need not be invertible, the converse need not hold: i.e, $\mathcal{T}$ may exhibit time trajectories that are not mapped onto by any trajectory in $\mathcal{S}$.

Let $\mathcal{S}$ and $\mathcal{T}$ be defined by Lipschitz continuous vector fields. The following theorem enables us to check given $\mathcal{S}$ and $\mathcal{T}$, if $\mathcal{T}$ simulates $\mathcal{S}$.

Theorem 2.1. $\mathcal{T}$ *simulates* $\mathcal{S}$ if the following conditions hold:

1. $Y_0 \supseteq \alpha(X_0)$.
2. $Y_I \supseteq \alpha(X_I)$.
3. $\mathcal{G}(\alpha(\vec{x})) = J_\alpha \cdot \mathcal{F}(\vec{x})$, wherein, J_α is the Jacobian matrix

$$J_\alpha(x_1, \dots, x_n) = \begin{bmatrix} \frac{\partial \alpha_1}{\partial x_1} & \dots & \frac{\partial \alpha_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial \alpha_m}{\partial x_1} & \dots & \frac{\partial \alpha_m}{\partial x_n} \end{bmatrix},$$

and $\alpha(\vec{x}) = (\alpha_1(\vec{x}), \dots, \alpha_m(\vec{x}))$, $\alpha_i : \mathbb{R}^n \mapsto \mathbb{R}$.

Proof. Let $\tau_x : [0, T) \mapsto \mathbb{R}^n$ be a trajectory over $\vec{x}$ for system $\mathcal{S}$. Note that at any time instant $t \in [0, T)$, $\frac{d\tau_x}{dt} = \mathcal{F}(\tau(t))$.

We wish to show that $\tau_y(t) = \alpha(\tau_x(t))$ is a time trajectory for the system $\mathcal{T}$. Since, $\tau_x(0) \in X_0$, we conclude that $\tau_y(0) = \alpha(\tau_x(0)) \in Y_0$. Since $\tau_x(t) \in X_I$ for all $t \in [0, T)$, we have that $\tau_y(t) = \alpha(\tau_x(t)) \in Y_I$. Differentiating τ_y we get,

$$\begin{aligned} \frac{d\tau_y}{dt} &= \frac{d\alpha(\tau_x(t))}{dt} = J_\alpha \cdot \frac{d\tau_x}{dt} = J_\alpha \cdot \mathcal{F}(\tau_x(t)) \\ &= \mathcal{G}(\alpha(\tau_x(t))) = \mathcal{G}(\tau_y(t)). \end{aligned}$$

Therefore $\tau_y = \alpha \circ \tau_x$ conforms to the dynamics of $\mathcal{T}$. By Lipschitz continuity of $\mathcal{G}$, we obtain that τ_y is the unique trajectory starting from $\alpha \circ \tau(0)$. $\square$

Theorem 2.1 shows that the condition

$$\mathcal{G}(\alpha(\vec{x})) = J_\alpha \cdot \mathcal{F}(\vec{x})$$

relating vector fields $\mathcal{F}$ and $\mathcal{G}$ suffices to guarantee that time trajectories (integral curves) of $\mathcal{F}$ are related to those in $\mathcal{G}$ through the map α . In differential geometric terms, this condition can be stated as $\mathcal{F}$ is α -related to $\mathcal{G}$ [32].

Note that, in general, a trajectory $\tau_y(t) = \alpha(\tau_x(t))$ may exist for a longer interval of time than the interval $[0, T)$ over which τ_x is assumed to be defined.

Theorem 2.2. *Let $\mathcal{T}$ simulate $\mathcal{S}$ through a map α . If $Y \subseteq Y_I$ is a positive invariant set for $\mathcal{T}$ then $\alpha^{-1}(Y) \cap X_I$ is a positive invariant set for $\mathcal{S}$.*

Proof. Assuming otherwise, let τ_x be a time trajectory that starts from inside $\alpha^{-1}(Y) \cap X_I$ and has a time instant t such that $\tau_x(t) \notin \alpha^{-1}(Y) \cap X_I$. Since we defined time trajectories so that $\tau_x(t) \in X_I$, it follows that $\tau_x(t) \notin \alpha^{-1}(Y)$. As a result, $\alpha(\tau_x(t)) \notin Y$. Therefore, corresponding to τ_x , we define a new trajectory $\tau_y = \alpha \circ \tau_x$ which violates the positive invariance of Y . This leads to a contradiction. $\square$

Given a constraint $\varphi[\vec{y}]$ that represents an invariant over Y , we can translate it back through α^{-1} simply by substituting $\alpha(\vec{x})$ for $\vec{y}$. As a result, $\varphi[\vec{y} \mapsto \alpha(\vec{x})]$ is the corresponding invariant over X . An application of this fact is illustrated in Example 1.1, wherein we transfer invariants inferred on the abstract system back in terms of the original system through the map α .

Example 2.1. Consider a mechanical system $\mathcal{S}$ expressed in generalized position coordinates (q_1, q_2) and momenta (p_1, p_2) defined using the following vector field:

$$F(p_1, p_2, q_1, q_2) : \langle -2q_1q_2^2, -2q_1^2q_2, 2p_1, 2p_2 \rangle$$

with the initial conditions: $(p_1, p_2) \in [-1, 1] \times [-1, 1] \wedge (q_1, q_2) : (2, 2)$. Using the transformation $\alpha(p_1, p_2, q_1, q_2) : p_1^2 + p_2^2 + q_1^2q_2^2$, we see that $\mathcal{S}$ is simulated by a linear system $\mathcal{T}$ over y , with dynamics given by $\frac{dy}{dt} = 0$, $y(0) \in [16, 18]$.

Incidentally, the form of the system $\mathcal{T}$ above indicates that α is an expression for a conserved quantity (in this case, the Hamiltonian) of the system.

The main goal of this work is to study CoB transformations that “simplify” the system’s dynamics either (a) casting a non-algebraic vector field into one defined algebraically or (b) reducing the degree of a given algebraic vector field by means of an abstraction. A special case consists of *linearizing CoB transformations* that map a non-linear system to one defined by affine dynamics.

Recall that a system $\mathcal{T}$ is algebraic if it is described by a polynomial vector field. Furthermore, $\mathcal{T}$ is *affine* if it is described by an affine vector field $\frac{d\vec{y}}{dt} = A\vec{y} + \vec{b}$ for an $m \times m$ matrix A and an $m \times 1$ vector $\vec{b}$.

Definition 2.4. Let $\mathcal{S}$ be a (non-linear) system. We say that α is an *algebraizing CoB transformation* if it maps $\mathcal{S}$ to an algebraic system $\mathcal{T}$.

We say that α is a *linearizing CoB transformation* if it maps each trajectory of $\mathcal{S}$ to that of an affine system $\mathcal{T}$.

Example 2.2. Consider the vector field $\mathcal{F}$

$$\frac{dx}{dt} = x^3 - 2x^2 + y^2 + xy, \quad \frac{dy}{dt} = 2x - 3x^2 + 2y^3.$$

Let $\alpha : (x, y) \rightarrow (w_1, w_2, w_3, w_4)$ be defined as

$$\alpha(x, y) : (x, y, x^2, y^2)$$

We can verify that using α , we note that $\mathcal{F}$ is simulated by the vector field $\mathcal{G}$:

$$\begin{aligned} \frac{dw_1}{dt} &= w_1w_3 - 2w_3 + w_4 + w_1w_2, & \frac{dw_2}{dt} &= 2w_1 - 3w_3 + 2w_2w_4 \\ \frac{dw_3}{dt} &= -4w_1w_3 + 2w_3^2 + 2w_1w_3 + 2w_1w_4, & \frac{dw_4}{dt} &= 4w_1w_2 - 6w_2w_3 + 4w_4^2 \end{aligned}$$

Note that while $\mathcal{F}$ is a cubic vector field over $\mathbb{R}^2$, $\mathcal{G}$ is a quadratic vector field over $\mathbb{R}^4$. ▲

Example 1.1 illustrates a linearizing CoB transformation.

The above definition of an algebraizing or linearizing CoB seems useful, in practice, only if α and $\mathcal{T}$ are already known. We may then use known techniques for reasoning over algebraic systems or affine systems for safely bounding the reachable set of an affine system, given some initial conditions, and transform the result back through α^{-1} to obtain a bound on the reachable set for $\mathcal{S}$.

We now present a technique that searches for a map α to obtain an algebraic system $\mathcal{T}$ that simulates a given system $\mathcal{S}$ through α such that the vector field describing $\mathcal{T}$ is degree bounded by some given degree limit $d > 0$. In particular, if the degree limit d is set to 1, then the resulting transformation α is linearizing.

We ignore the initial condition and invariant, for the time being, and simply focus on obtaining the dynamics of $\mathcal{T}$. In other words, we will search for a map $\alpha : (\alpha_1, \dots, \alpha_m)$ that maps $\mathbb{R}^n$ into $\mathbb{R}^m$ so that

$$J_\alpha(\vec{x}) \cdot \mathcal{F}(\vec{x}) = G(\alpha(\vec{x})).$$

Having found such a map, we may find appropriate over-approximate initial and invariance conditions for the simulating system $\mathcal{T}$, so that Definition 2.3

holds. Specifically, we are interested in finding transformations α that ensure that (a) G is a polynomial vector field and (b) the degrees of polynomials describing G are degree bounded by some given degree limit $d > 0$.

2.3. Multilinear Abstractions through Dimension Copying

We first show that any polynomial system of ODEs can be abstracted by a *multilinear* system. However, doing so may require α to have many repeated components wherein $\alpha_i(\vec{x}) = \alpha_j(\vec{x})$ for $i \neq j$. This result is well-known and has been used, for instance, to extend known results on invariant rectangles for multiaffine systems to arbitrary polynomial systems by Ben Sassi et al. [57].

Definition 2.5. A polynomial p is defined to be *multilinear* if and only if each power-product in p is of the form $x_1^{r_1} x_2^{r_2} \cdots x_n^{r_n}$ wherein each $r_i = 0$ or 1.

Example 2.3. As an example, the polynomial $p = 2x_1x_2x_3 + x_1x_3 + 4x_1 - 2x_2 - 1$ is multilinear. On the other hand, the polynomial $q = 2x_2^2 + x_1 + x_3$ is not, owing to the x_2^2 power product.

We first observe that any polynomial ODE may be equivalently written by means of a multilinear system using a suitably defined α .

Theorem 2.3. Let $\mathcal{F}$ be a polynomial vector field over $\vec{x} \in \mathbb{R}^n$. There is a transformation $\alpha : \mathbb{R}^n \rightarrow \mathbb{R}^m$, that maps $\mathcal{F}$ to a multilinear system $\mathcal{G}$.

Proof. Let us write $\mathcal{F}(\vec{x}) : (p_1, \dots, p_n)$ for multivariate polynomials $p_1, \dots, p_n$. We will assume that the vector field $\mathcal{F}$ is not already multi-linear. Therefore, some p_j has a power product that is divisible x_k^r for some $r \geq 2$. The idea is to use r different functions $\alpha_{k,1} = \alpha_{k,2} = \dots = \alpha_{k,r} = x_k$ so that in the transformed system the term x_k^r appears as a multilinear product $y_{k,1}y_{k,2} \cdots y_{k,r}$.

In the worst case, the transformation α involves $n \times K$ components, wherein $K = \max(\text{degree}(p_1), \dots, \text{degree}(p_n))$. Each component $\alpha_{i,k} : x_i$ is simply a “copy” of the variable x_i that ensures multilinearity of the transformed system. $\square$

Example 2.4. Consider the one dimensional system defined by

$$\frac{dx}{dt} = 2x^5 + 3x^2 + x - 5.$$

We use the transformation $\alpha : \mathbb{R} \rightarrow \mathbb{R}^5$ wherein $\alpha_1(x) = \alpha_2(x) = \dots = \alpha_5(x) = x$. Using this transformation, we derive an abstract system defined by the ODE

$$\frac{dy_j}{dt} = 2y_1y_2y_3y_4y_5 + 3y_1y_2 + y_1 - 5, \quad j = 1, 2, \dots, 5.$$

▲

Even though there are efficient algorithms for analyzing multi-linear systems [5], the transformation in Theorem 2.3 faces two problems: (a) the dimensionality of the transformed system $\mathcal{T}$ is often forbiddingly large, and (b)

forgetting the implicit equality relationships between the various dimensions results in a very coarse abstraction, while maintaining these equalities as state invariants of the transformed system may invalidate the special insights into the dynamics multi-linear systems that enable efficient reachability analysis.

2.4. Independent Transformations

The rest of this paper, will focus on *independent transformations* $\alpha : (\alpha_1, \dots, \alpha_N)$ wherein each α_i cannot be written as a linear combination of the remaining α_j s for $j \neq i$. Assuming independence automatically rules out the constructions used in Theorem 2.3.

In general, computing independent transformations α for any given ODE is a hard problem. In this paper, we will focus on solutions that involve searching for an appropriate map α , wherein α is specified to be the linear combination of some fixed, finite set of basis functions $g_1, \dots, g_N$. The initial basis is assumed to be given to our algorithm by the user. Starting from this initial basis of functions, our algorithm searches for transformations α whose components can be written as linear combinations $\sum_{i=1}^N \lambda_j g_j$.

The basis functions could be specified implicitly as the set of all power products over $\vec{x}$ of degree upto some limit $K > 0$ or the set of all power products involving the variables x_i and various non-algebraic functions $\sin(z)$, $\cos(z)$ and e^z applied to these power products. Having chosen a basis $B = \{g_1, \dots, g_N\}$ for α , we will cast the search for the map α as a vector space iteration.

Let $\alpha(\vec{x}) : (\alpha_1(\vec{x}), \dots, \alpha_m(\vec{x}))$ be a smooth mapping $\alpha : \mathbb{R}^n \mapsto \mathbb{R}^m$, wherein each $\alpha_i : \mathbb{R}^n \mapsto \mathbb{R}$. Recall that $\mathcal{L}_F(\alpha_i(\vec{x})) = (\nabla \alpha_i) \cdot \mathcal{F}(\vec{x})$ denotes the Lie derivative of the function $\alpha_i(\vec{x})$ w.r.t vector field $\mathcal{F}$.

Lemma 2.1. $J_\alpha \cdot \mathcal{F}(\vec{x}) = \begin{pmatrix} \mathcal{L}_F(\alpha_1(\vec{x})) \\ \mathcal{L}_F(\alpha_2(\vec{x})) \\ \vdots \\ \mathcal{L}_F(\alpha_m(\vec{x})) \end{pmatrix}.$

Proof. Recall the definition of the Jacobian matrix J_α :

$$J_\alpha(x_1, \dots, x_n) = \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \dots & \frac{\partial y_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial y_m}{\partial x_1} & \dots & \frac{\partial y_m}{\partial x_n} \end{bmatrix} = \begin{bmatrix} \nabla \alpha_1 \\ \vdots \\ \nabla \alpha_m \end{bmatrix}.$$

Therefore, $J_\alpha \cdot \mathcal{F} = \begin{pmatrix} (\nabla \alpha_1) \cdot (\mathcal{F}) \\ (\nabla \alpha_2) \cdot (\mathcal{F}) \\ \vdots \\ (\nabla \alpha_m) \cdot (\mathcal{F}) \end{pmatrix} = \begin{pmatrix} \mathcal{L}_F(\alpha_1(\vec{x})) \\ \mathcal{L}_F(\alpha_2(\vec{x})) \\ \vdots \\ \mathcal{L}_F(\alpha_m(\vec{x})) \end{pmatrix}. \quad \square$

Note: For the rest of this section, we will fix a vector field $\mathcal{F}$ belonging to a system $\mathcal{S}$ as the original system for which we seek an abstraction and use $\mathcal{L}_F$ to denote the Lie derivative according to $\mathcal{F}$.

2.5. Vector Space Closure

We first define the vector spaces that will be used in our search.

Definition 2.6. Let $B = \{g_1, \dots, g_k\}$ be some finite set of functions wherein $g_i : \mathbb{R}^n \rightarrow \mathbb{R}$ for $n > 0$. The *vector space* spanned by B denoted $Span(B)$ consists of all functions that are linear combinations of g_i :

$$Span(B) = \left\{ \sum_{i=1}^k \lambda_i g_i \mid \lambda_i \in \mathbb{R} \right\}.$$

We assume, without loss of generality, that the elements in B are linearly independent: i.e., no $g_i \in B$ can be written as a linear combination of the remaining $g_j \in B$, for $j \neq i$.

Let $\mathbf{1}$ represent the constant function $\mathbf{1}(\vec{x}) = 1, \forall \vec{x} \in \mathbb{R}^n$. Given a vector space $V = Span(B)$, we define the space of power products of V upto a degree limit $d \geq 1$ as

$$V^{(d)} = Span(\{g_{i_1} \times g_{i_2} \times \dots \times g_{i_d} \mid g_{i_1}, \dots, g_{i_d} \in B \cup \{\mathbf{1}\}\}).$$

In particular, note that $V^{(1)} = Span(V \cup \{\mathbf{1}\})$.

Example 2.5. Let $B = \{x, \sin(y)\}$ be our basis set. The vector space $V : Span(B)$ is given by $\{a_1 x + a_2 \sin(y) \mid a_1, a_2 \in \mathbb{R}\}$. The space $V^{(2)}$ is the set

$$\{a_0 + a_1 x + a_2 \sin(y) + a_3 x \sin(y) + a_4 x^2 + a_5 \sin^2(y) \mid a_0, \dots, a_5 \in \mathbb{R}\}.$$

This space is generated by the functions $\mathbf{1}, x, \sin(y), x \sin(y), x^2, \sin^2(y)$. It consists of all polynomials of degree at most 2 formed by the functions $x, \sin(y)$. The purpose of adding the function $\mathbf{1}$ is to enable terms of degree 1 and 0 to be considered. $\blacktriangle$

Roughly, the main idea behind our approach is to find a vector space U that satisfies the following closure property:

$$(\forall f \in U) \mathcal{L}_F(f) \in U^{(d)}.$$

In other words, we will search for a vector space U , such that taking the Lie derivative of any element of U yields an element in $U^{(d)}$. Such a vector space U will be called d -closed. Let $U = Span(\{h_1, \dots, h_m\})$ be a d -closed vector space. We will prove that $\alpha : (h_1, \dots, h_m)$ maps the original system $\mathcal{S}$ to an algebraic system $\mathcal{T}$ with a vector field of degree d .

Definition 2.7. A vector space V is said to be d -closed under the application of Lie derivatives iff $(\forall f \in V) \mathcal{L}_F(f) \in V^{(d)}$.

In order to check whether a given space $V = Span(B)$ is d -closed, it suffices to verify the property in Definition 2.7 for the elements in B .

Lemma 2.2. *A vector space $U = \text{Span}(\{h_1, \dots, h_m\})$ be d -closed under Lie derivatives if and only if $\mathcal{L}_F(h_i) \in U^{(d)}$ for $i \in \{1, \dots, m\}$.*

Proof. If U is d -closed under Lie derivatives then by definition, the Lie derivatives of its basis elements h_i should lie in $U^{(d)}$. We will prove the reverse direction. Let U be such that for each basis element h_i , we have $\mathcal{L}_F(h_i) \in U^{(d)}$. Any element of U can be written as $f = \sum_{j=1}^k a_j h_j$ for $a_j \in \mathbb{R}$. We have $\mathcal{L}_F(f) = \sum_{j=1}^k a_j \mathcal{L}_F(h_j)$. Since each $\mathcal{L}_F(h_j) \in U^{(d)}$, we have that $\mathcal{L}_F(f) \in U^{(d)}$. This completes the proof. $\square$

Next, we relate d -closed vector spaces to algebraizing CoB transformations. Let $B = \{h_1, \dots, h_m\}$ and $U = \text{Span}(B)$ be a d -closed vector space. Let α be the map from $\mathbb{R}^n \rightarrow \mathbb{R}^m$ defined as $\alpha : (h_1, \dots, h_m)$.

Theorem 2.4. *The map α formed by the basis elements of a d -closed vector field is an algebraizing transformation from the original system $\mathcal{S}$ to a system $\mathcal{T}$ defined by a polynomial vector field of degree at most d .*

Proof. Since U is d -closed, we note that for each h_i in the basis of U , we have $\mathcal{L}_F(h_i) \in U^{(d)}$. In other words, we may write $\mathcal{L}_F(h_i)$ as a linear combination of power products as shown below:

$$\mathcal{L}_F(h_i) : \sum_{j=1}^K a_{ij} h_{i,j,1} \times h_{i,j,2} \times \dots \times h_{i,j,d}, \text{ wherein } h_{i,j,k} \in B \cup \{1\} \quad (1)$$

We define the system $\mathcal{T}$ over variables $y_1, \dots, y_m$. We will use variable y_i to correspond to $h_i(\vec{x})$. The dynamics are obtained as

$$\frac{dy_i}{dt} = \sum_{j=1}^K a_{ij} y_{i,j,1} \times y_{i,j,2} \times \dots \times y_{i,j,k},$$

by substituting the variable y_j wherever the function h_j occurs in Equation (1). Let G be the resulting vector field on $\vec{y}$. It is easy to see that (a) G is a polynomial vector field and (b) of degree at most d .

From Lemma 2.1, we note that $J_\alpha \cdot \mathcal{F}(\vec{x}) = (\mathcal{L}_F(h_1), \dots, \mathcal{L}_F(h_m))$. We verify that $(\mathcal{L}_F(h_1), \dots, \mathcal{L}_F(h_m)) = G(h_1(\vec{x}), \dots, h_m(\vec{x}))$. This is directly evident from the construction of G from Equation (1). Thus, the key condition (3) of Theorem 2.1 is seen to hold. By finding the right sets Y_0, Y_I given α , we take care of the remaining conditions as well. $\square$

Note: The trivial space $V = \text{Span}(\{0\})$ consisting just of the constant function that maps all inputs to $\vec{0}$ is always d -closed. This space yields $\alpha : (0)$ that maps all states $\vec{x}$ to the zero vector. As such, the map α is not very useful in practice for inferring invariants.

Example 2.6. Consider the ODE from Example 1.1 recalled below:

$$\begin{aligned}\frac{dx}{dt} &= xy + 2x \\ \frac{dy}{dt} &= -\frac{1}{2}y^2 + 7y + 1\end{aligned}$$

We claim that the vector space V generated by the set of functions $\{x, xy, xy^2\}$ is 1-closed. To verify, we compute the Lie derivative of a function of the form $c_1x + c_2xy + c_3xy^2$ to obtain

$$c_1(xy + 2x) + c_2(\frac{1}{2}xy^2 + 9xy + x) + c_3(16xy^2 + 2xy)$$

which is seen to belong to $V^{(1)}$. As a result, we obtain the CoB abstraction $\alpha(x, y) : (x, xy, xy^2)$ that maps the vector field to an affine vector field (polynomial of degree 1).

The abstract system over $(w_1, w_2, w_3) \in \mathbb{R}^3$ has dynamics given by

$$\begin{aligned}\frac{dw_1}{dt} &= 2w_1 + w_2 \\ \frac{dw_2}{dt} &= \frac{1}{2}w_3 + 9w_2 + w_1 \\ \frac{dw_3}{dt} &= 16w_3 + 2w_2\end{aligned}$$

The mapping between original and abstract system is given by

$$w_1 \mapsto x, w_2 \mapsto xy, w_3 \mapsto xy^2.$$

▲

2.6. Finding Closed Vector Spaces

We will now describe a search technique for finding a map α and the associated abstraction $\mathcal{T}$, such that the dynamics of $\mathcal{T}$ are described by polynomials with degree bound d . If $d = 1$, the dynamics of $\mathcal{T}$ are affine. The inputs to our search procedure are

1. The original system $\mathcal{S}$ described by a vector field $\mathcal{F}$,
2. The degree limit d for the desired vector field $\mathcal{T}$, and
3. An initial basis $B_0 = \{h_1, \dots, h_N\}$ of continuous and differentiable functions. We may regard the linear combination

$$c_1h_1(\vec{x}) + c_2h_2(\vec{x}) + \dots + c_Nh_N(\vec{x}),$$

as an *ansatz* or a template for each component α_j of the map $\alpha : (\alpha_1, \dots, \alpha_m)$, that we are searching for. However, we do not fix the number of components m of the transformation α , *a priori*, or guarantee that a non-trivial α (with $m > 0$) can be found.

The initial basis B_0 is often specified as consisting of all power products of the variables in $\vec{x}$ with a given degree limit M . This limit M is chosen independent of the limit d for the desired abstraction $\mathcal{T}$.

Our overall approach is to start with the initial vector space $V_0 : \text{Span}(B_0)$ and iteratively refine V_0 to construct a sequence of spaces

$$V_0 \supseteq V_1 \supseteq V_2 \cdots \supseteq V_k = V_{k+1} = V^*$$

wherein, (1) $V_{j+1} \subseteq V_j$, for $j \in [1, k-1]$, and (2) $V_k = V_{k+1}$. The iterative scheme is designed to guarantee that the converged result V^* is d -closed. If V^* has a non-zero basis, then the basis elements of V^* form the components of the map α and the abstraction $\mathcal{T}$ whose dynamics have the desired form.

The main step of iteration is to derive V_{i+1} from V_i . This is performed as follows:

$$V_{i+1} = \{g \in V_i \mid \mathcal{L}_F(g) \in V_i^{(d)}\}. \quad (2)$$

In other words, V_{i+1} retains those functions $g \in V_i$ whose Lie derivatives also lie inside $V_i^{(d)}$.

Lemma 2.3. (1) V_{i+1} is a sub-space of V_i . (2) V_i is d -closed iff $V_i = V_{i+1}$.

Proof. We prove the two parts (1) and (2) as follows.

(1) Since by Eq. (2), $V_{i+1} \subseteq V_i$, it suffices to show that V_{i+1} is a vector space. Let $g_1, \dots, g_k \in V_{i+1}$. We have that $g_1, \dots, g_k \in V_i$. Furthermore, since V_i is a vector space, any linear combination $g : \sum_{j=1}^k \lambda_j g_j \in V_i$. The lie derivative $\mathcal{L}_F(g)$ can be written as $\sum_{j=1}^k \lambda_j \mathcal{L}_F(g_j)$. Since $\mathcal{L}_F(g_j) \in V_i^{(d)}$, we have $\mathcal{L}_F(g) = \sum_{j=1}^k \lambda_j \mathcal{L}_F(g_j) \in V_i^{(d)}$. Therefore, by definition $g \in V_{i+1}$ as well. The linear combination of any finite subset of elements from V_{i+1} also belongs to V_{i+1} , proving that it is a sub-space of V_i .

(2) If $V_i = V_{i+1}$, it is easy to check that V_i satisfies the definition of being d -closed. For the other direction, let us assume that V_i is d -closed. Then for each $g \in V_i$, we have $\mathcal{L}_F(g) \in V_i^{(d)}$. Thus $g \in V_{i+1}$. This proves that $V_{i+1} \supseteq V_i$. Combining with the fact that $V_{i+1} \subseteq V_i$, we obtain equality. $\square$

We now focus on calculating V_{i+1} from V_i . Let $V_i : \text{Span}(B_i)$ for a finite set B_i . Any element of V_i can be represented as $\sum_{h_j \in B_i} c_j h_j$ for some multipliers c_j . The Lie derivative is expressed as $\sum_{h_j \in B_i} c_j \mathcal{L}_F(h_j)$. The procedure for calculating V_{i+1} reduces to finding the set of multipliers $(c_1, \dots, c_M)$ where $M = |B_i|$ such that $\sum_{h_j \in B_i} c_j \mathcal{L}_F(h_j) \in V_i^{(d)}$.

The key challenge lies in comparing two elements of the form $\sum_j c_j \mathcal{L}_F(h_j)$ and $\sum_k d_k g_k$, for unknowns c_j and d_k , where $h_j \in B_i$ and $g_k \in V_i^{(d)}$. If both the functions are polynomials over $\vec{x}$, the comparison is performed by equating the coefficients of corresponding monomials. This is illustrated using the example below:

Example 2.7. Consider once again the ODE from Example 1.1 and 2.6. We seek to find an affine system $\mathcal{T}$ that abstracts this system. Let us consider the

space V_0 generated by the basis $B_0 : \{x, y, xy, x^2, y^2\}$ of all degree 2 monomials. Any element in V_0 can be written as

$$p(c_1, \dots, c_5) : c_1x + c_2y + c_3xy + c_4x^2 + c_5y^2.$$

Its Lie derivative is given by

$$\begin{aligned} & c_1(xy + 2x) + c_2(-\frac{1}{2}y^2 + 7y + 1) + c_3x(-\frac{1}{2}y^2 + 7y + 1) \\ & + c_3y(xy + 2x) + c_4(2x)(xy + 2x) + c_5(2y)(-\frac{1}{2}y^2 + 7y + 1) \end{aligned}$$

This can be simplified as

$$p'(c_1, \dots, c_5) : \begin{bmatrix} c_2 + (2c_1 + c_3)x + (7c_2 + 2c_5)y + (c_1 + 9c_3)xy + 4c_4x^2 + \\ (14c_5 - \frac{1}{2}c_2)y^2 + \frac{1}{2}c_3xy^2 + 2c_4x^2y - c_5y^3 \end{bmatrix}.$$

We require the Lie derivative to belong to $V^{(1)} = \text{Span}(B_0 \cup \{1\})$. This yields the constraints:

$$(\exists d_0, d_1, \dots, d_5) (\forall x, y) d_0 + d_1x + d_2y + d_3xy + d_4x^2 + d_5y^2 = p'(c_1, \dots, c_5).$$

We use the lemma that two polynomials are identical iff their coefficients on corresponding power-products are. This yields the following system of linear equations:

$$\begin{aligned} c_2 &= d_0, \quad 2c_1 + c_3 = d_1, \quad 7c_2 + 2c_5 = d_2, \quad c_1 + 9c_3 = d_3, \\ 4c_4 &= d_4, \quad 14c_5 - \frac{1}{2}c_2 = d_5, \quad c_3 = 0, \quad 2c_4 = 0, \quad c_5 = 0 \end{aligned}$$

Eliminating $d_0, \dots, d_5$, we obtain the constraints $c_3 = c_4 = c_5 = 0$. The new basis B_1 is $\{x, y\}$. ▲

On the other hand, if the basis B_i involves non-polynomials (trigonometric or exponential functions), then encoding equality by matching up coefficients of syntactically identical terms is *incomplete*: i.e, not all solutions can be found by equating coefficients of matching terms. In general, deciding if expressions involving trigonometric functions are identically zero is undecidable ² In practice, we may continue to handle trigonometric functions using the same syntactic matching technique that is complete for polynomials. If a d -closed basis is discovered this way, then it may be used to derive a valid abstraction. On the other hand, the process may be unable to find a vector space starting from the initial set of functions even if one such exists.

Example 2.8. Consider a simple example with the ODE

$$\frac{dx}{dt} = \sin(x + y), \quad \frac{dy}{dt} = x + y.$$

Consider the space V spanned by the basis

$$B = \{x, y, \sin(x), \sin(y), \cos(x), \cos(y)\}.$$

²This follows from Richardson's theorem [42].

To check if V is 3-closed, we note that any element of V can be written as

$$c_1x + c_2y + c_3 \sin(x) + c_4 \sin(y) + c_5 \cos(x) + c_6 \cos(y) .$$

Its Lie derivative can be written as

$$\begin{aligned} & c_1 \sin(x+y) + c_2(x+y) + c_3 \cos(x) \sin(x+y) + c_4 \cos(y)(x+y) \\ & - c_5 \sin(x) \sin(x+y) - c_6 \sin(y)(x+y) . \end{aligned}$$

Our goal is to check if the Lie derivative belongs to $V^{(3)}$. We note that a syntactic check for membership yields the constraints $c_1 = c_3 = c_5 = 0$. On the other hand, substituting the trigonometric identity

$$\sin(x+y) \equiv \sin x \cos y + \sin y \cos x ,$$

we may indeed verify that the Lie derivative of any element of V belongs to $V^{(3)}$. This yields a degree 3 algebraization given by $\alpha(x, y) : (x, y, \sin(x), \sin(y), \cos(x), \cos(y))$ with the abstract system having the dynamics

$$\begin{aligned} \frac{dw_1}{dt} &= w_3w_6 + w_4w_5 \\ \frac{dw_2}{dt} &= w_1 + w_2 \\ \frac{dw_3}{dt} &= w_3w_5w_6 + w_5^2w_4 \\ \frac{dw_4}{dt} &= w_6w_1 + w_6w_2 \\ \frac{dw_5}{dt} &= -w_3^2w_6 - w_3w_4w_5 \\ \frac{dw_6}{dt} &= -w_4w_1 - w_4w_2 \end{aligned}$$

Here $w_1, \dots, w_6$ correspond to the components of the map α above. ▲

Theorem 2.5. *Given an initial vector space V_0 and vector field $\mathcal{F}$, the iterative procedure using Eqn. (2) converges in finitely many steps to a subspace $V^* \subseteq V_0$. Let $\alpha_1, \dots, \alpha_m$ be the basis functions that generate V^* .*

1. *The transformation $\alpha : (\alpha_1, \dots, \alpha_m)$ generated by the basis functions of the final vector space leads to an abstract system whose dynamics are described by polynomials of degree at most d .*
2. *A limited form of completeness holds: Let $U \subseteq V_0$ be a subspace that is d -closed. It follows that $U \subseteq V^*$. In other words, if a d -closed CoB transformation exists whose functions are part of the initial space V_0 then it is also a part of the final result V^* .*

Proof. Let us represent the iterative sequence as

$$V_0 \supseteq V_1 \supseteq V_2 \cdots$$

The convergence of the iteration follows from the observation that if $V_{i+1} \subset V_i$, the dimension of V_{i+1} is at least one less than that of V_i . Since V_0 is finite dimensional, the number of iterations is upper bounded by the number of basis functions in V_0 .

The first statement follows directly from Theorem 2.4.

The next statement is proved by induction. Specifically, we prove by induction that $U \subseteq V_i$ for each i . The base case is true since $U \subseteq V_0$ by assumption.

Next, we show that if $U \subseteq V_i$ then $U \subseteq V_{i+1}$. This follows from Eq. 2 since for each $p \in U$, we have $p \in V_i$ and $\mathcal{L}_F(p) \in U^{(d)}$. This gives us $\mathcal{L}_F(p) \in V_i^{(d)}$. Therefore, $p \in V_{i+1}$.

As a result, we prove by induction that $U \subseteq V_i$ for each i . This also means that $U \subseteq V^*$. $\square$

Note that it is possible for the converged result V^* to be trivial. i.e, it is generated by the constant function $\mathbf{1}$.

Example 2.9. Consider the van der Pol oscillator whose dynamics are given by

$$\dot{x} = y, \quad \dot{y} = \mu(y - \frac{1}{3}y^3 - x).$$

Our search for polynomials ($\mu = 1$) of degree up to 20 did not yield a non-trivial transformation.

For a trivial system, the resulting affine system $\mathcal{T}$ is $\frac{dy}{dt} = 0$ under the map $\alpha(\vec{x}) = 0$. Naturally, this situation is not quite interesting but will often result, depending on the system $\mathcal{S}$ and the initial basis chosen V_0 . Section 2.7 discusses common situations where the vector space V^* obtained as the result is guaranteed to be non-trivial.

2.6.1. Complexity

For simplicity, we analyze the time complexity bounds when we search for a 1-closed subspace of the initial space V_0 .

There are two ways of representing vector spaces over polynomials: (a) through an explicit list of the basis elements, or alternatively, (b) using a parameteric polynomial form over n variables:

$$V(\vec{c}, \vec{x}) : \sum c_\alpha \vec{x}^\alpha$$

wherein c_α is a parameter corresponding to the monomial $\vec{x}^\alpha$, and an associated set of constraints $A\vec{c} = 0$ over $\vec{c}$. The former is often called a “generator” representation of the vector space, whereas the latter is a “constraint” representation.

We also note that the steps involved in this computation are remarkably similar to the so-called *Karr’s algorithm* used for generating linear equality invariants for programs originally studied by M. Karr in 1976 [28, 37].

Borrowing ideas from Muller-Olm and Seidl [37], our implementation of this iteration alternates between both the representations of the vector space during the process of computation. At the start of each iteration, we represent V_i as a list of polynomials that form its basis. Next, we construct a generic element of V_i as a parameteric linear combination of the basis elements:

$$p(\vec{c}, \vec{x}) : \sum_{p_j \in V_i} c_j p_j$$

We compute constraints $A\vec{c} = 0$ that are enforcing that the Lie derivative of p belongs back to V_i . This system is often rank deficient (or else $\vec{c} = 0$ and we obtain the trivial result). We compute a set of basis vectors for the nullspace of A . This immediately yields a basis for V_{i+1} .

The worst-case time complexity of the overall procedure is decomposed into two parts: (a) the worst-case time complexity of each iteration and (b) the number of iterations. For an ODE with n variables, let us start with an initial monomial basis that involves all terms of degree upto d . This yields the dimension of the initial vector space $\dim(V_0) = O(n^d)$. This also yields an upper bound on the number of iterations.

Each iteration involves computing the Lie derivative of each of the basis elements in the current vector space V_i , forming the system $A\vec{c} = 0$ and extracting the nullspace for A . The latter can be performed through a Gaussian elimination procedure, involving $O(\dim(V_i)^3)$ cost.

Combining, we obtain an overall complexity of $O(n^{4d})$ wherein n is the number of variables in the system and d is the maximum degree of monomials in the original basis V_0 . In our evaluation (see Section 4), we observe two important features that mitigate the high worst-case complexity: (a) our iterations converge in very few iterations even for large initial basis, and (b) the dimensions of the vector spaces reduces considerably yielding a much smaller dimension for the converged result in comparison with the original vector space.

2.7. Strong and Constant Scale Consecution

The notion of “strong” consecution, “constant scale” consecution and “polynomial scale” consecution were defined for equality invariants of differential equations in our previous work [55] and subsequently expanded upon by Matringe et al. [34] using the notion of morphisms. We now show that the techniques presented in this section can capture these notions, ensuring that all the systems handled by the techniques presented in our previous work [55] can be handled by the techniques here (but not vice-versa).

Definition 2.8. A function f satisfies the *strong scale* consecution requirement for a vector field $\mathcal{F}$ iff $\mathcal{L}_{\mathcal{F}}(f) = 0$. In other words, f is a conserved quantity.

Similarly, f satisfies the *constant scale* consecution iff $\exists \lambda \in \mathbb{R}, \mathcal{L}_{\mathcal{F}}(f) = \lambda f$.

The following theorem is a corollary of Theorem 2.5 and shows that the ideas presented in this section can capture the notion of strong and constant scale consecution without requiring quantifier elimination, solving an eigenvalue problem [55] or finding roots of a univariate polynomial [34].

Theorem 2.6. *The result of the iteration V^* starting from an initial space V_0 contains all the strong and constant scale invariant functions in V_0 .*

Proof. This is a direct consequence of Theorem 2.5 by noting that for a constant scale consecuting function f , the subspace $U \subseteq V_0$ spanned by f is closed under Lie derivatives. $\square$

Furthermore, if such functions exist in V_0 the result after convergence V^* is guaranteed to be a non-trivial vector space (of positive dimension). Finally, constant scale and strong scale functions can be extracted by computing the affine equality invariants of the linear system $\mathcal{T}$ that can be extracted from V^* .

2.7.1. Stability

We briefly address the issue of deducing stability (or instability) of a system $\mathcal{S}$ using an abstraction to a system $\mathcal{T}$. Since α satisfies the identity

$$\mathcal{G}(\alpha(\vec{x})) = J_\alpha \cdot \mathcal{F}(\vec{x}).$$

Every equilibrium of $\mathcal{S}$ ($\mathcal{F}(\vec{x}) = 0$) maps onto an equilibrium of $\mathcal{T}$ ($\mathcal{G}(\vec{x}) = 0$), but not vice-versa. Furthermore, the map $\alpha(\vec{x}) = (\mathbf{0}, \dots, \mathbf{0})$ is an abstraction from any non-linear system to one with an equilibrium at origin. Therefore, unless restrictions are placed on α , we are unable to draw conclusions on liveness properties for $\mathcal{S}$ based on $\mathcal{T}$. If α has a continuous inverse, then $\mathcal{T}$ is topologically diffeomorphic to $\mathcal{S}$ [35]. This allows us to correlate equilibria of $\mathcal{T}$ with those of $\mathcal{S}$. The preservation of stability under mappings of state variables has been studied by Vassilyev and Ul'yanov [61]. We are currently investigating restrictions that will allow us to draw conclusions about liveness properties of $\mathcal{S}$ from those of $\mathcal{T}$.

The issue of stability preserving maps between continuous and hybrid systems was recently addressed by the work of Prabhakar et al. [47].

2.8. Affine CoB Abstraction: Existence

We will now focus on the special case of CoB transformations that lead to linear abstractions of the form $\frac{d\vec{w}}{dt} = A\vec{w}$ (and affine abstractions of the form $\frac{d\vec{w}}{dt} = A\vec{w} + \vec{b}$).

Let $\mathcal{S}$ be a non-linear system over $\vec{x}$ that has a CoB transformation $\alpha : \mathbb{R}^n \rightarrow \mathbb{R}^m$ with $m > 0$ that maps to a linear system $\frac{d\vec{w}}{dt} = A\vec{w}$.

Lemma 2.4. *The system $\mathcal{S}$ has m conserved quantities given by the components of the vector valued function $e^{-tA}\alpha(\vec{x})$.*

Proof. Our goal is to prove that the Lie derivative of each component of $e^{-tA}\alpha(\vec{x})$ equals zero. Since α is a linearizing CoB, we have $\mathcal{L}_F(\alpha(\vec{x})) = A\alpha(\vec{x})$.

The Lie derivative of $e^{-tA}\alpha(\vec{x})$ is given by

$$e^{-tA}\mathcal{L}_F(\alpha(\vec{x})) + \partial_t e^{-tA}\alpha(\vec{x}) = e^{-tA}A\alpha(\vec{x}) - e^{-tA}A\alpha(\vec{x}) = 0.$$

Thus we see that the Lie derivative of $e^{-tA}\alpha(\vec{x})$ vanishes. Therefore, each component of $e^{-tA}\alpha(\vec{x})$ is a conserved quantity. $\square$

Conversely, whenever the original system $\mathcal{S}$ has conserved quantities, it trivially admits the linearization $\frac{d\vec{w}}{dt} = 0$ using a transformation α that is formed by its conserved quantity.

Theorem 2.7. *A system $\mathcal{S}$ has an independent, linearizing CoB transformation $\alpha : \mathbb{R}^n \mapsto \mathbb{R}^m$ if and only if it has m linearly independent conserved quantities.*

The theorem extends to affine CoB transformations that yield abstract systems of the form $\frac{d\vec{w}}{dt} = A\vec{w} + \vec{b}$. While conservative mechanical and electromagnetic systems naturally have conserved quantities (eg., conservation of momentum, energy, charge, mass), many systems encountered are dissipative. Such cases are handled by extending the approach presented here to differential inequality abstractions [52].

Furthermore, even in a setting where conservative quantities exist, the advantages of searching for a CoB transformation as opposed to directly searching for a conserved quantity from an ansatz are not clear at a first glance. The advantage of the techniques presented here lies in the fact that existing techniques that search for conserved quantities focus for the most part on finding polynomial conserved quantities. Whereas, searching for a CoB transformation allows us to implicitly obtain conserved quantities that may involve exponentials, sines and cosines in addition to polynomial conserved quantities by focusing purely on reasoning with vector spaces generated by polynomials.

Example 2.10. We observed the following conserved quantity for the system in Example 1.1

$$\begin{aligned} & \left(\frac{e^{-9t}}{51} + \frac{1}{102} (50 + 7\sqrt{51}) e^{(-9+\sqrt{51})t} + \frac{1}{102} (50 - 7\sqrt{51}) e^{-(9+\sqrt{51})t} \right) x + \\ & \left(-\frac{1}{102} e^{-9t-(9+\sqrt{51})t} \begin{pmatrix} 7e^{9t} - \sqrt{51}e^{9t} - 14e^{(9+\sqrt{51})t} + \\ 7e^{9t+(-9+\sqrt{51})t+(9+\sqrt{51})t} + \\ \sqrt{51}e^{9t+(-9+\sqrt{51})t+(9+\sqrt{51})t} \end{pmatrix} \right) xy + \\ & \left(\frac{1}{204} e^{-9t-(9+\sqrt{51})t} \left(e^{9t} - 2e^{(9+\sqrt{51})t} + e^{9t+(-9+\sqrt{51})t+(9+\sqrt{51})t} \right) \right) xy^2 \end{aligned}$$

This is one of the three conserved quantities obtained by computing $e^{-tA}\alpha(\vec{x})$, where

$$\alpha : (x, xy, xy^2) \text{ and } A = \begin{pmatrix} 2 & 1 & 0 \\ 1 & 9 & \frac{1}{2} \\ 0 & 2 & 16 \end{pmatrix}.$$

We are unaware of techniques that can directly generate such conserved quantities. ▲

2.9. Change-of-Bases For Improved Flowpipe Construction

Theorem 2.2 already establishes a key motivation behind our study of CoB abstractions for ODEs: any property established for the abstract system can, in fact, be transferred back to the original system. Motivating example 1.1 illustrates this property for the simple running example. We now briefly examine another application of this idea to improve the process of flowpipe construction for verifying (time bounded) reachability properties of continuous and hybrid systems.

Figure 2: Comparing the flowpipes constructed for Flow* for the system in Example 1.1. **(Left)** The original 2 state model and **(Right)** The augmented model including the original system and the linear abstraction.

Given an initial set of states X_0 for a system of differential equations $\dot{\vec{x}} = f(\vec{x})$, the goal of flowpipe construction is to find approximations for the set X_t of reachable states at time t , where $t \in [0, T]$ for a given time horizon $T > 0$. Approaches to flowpipe construction have been derived for the specific case of linear (affine) hybrid systems [23, 31, 21, 25, 22] and for nonlinear continuous-time and hybrid systems [62, 3, 58, 9, 48, 39, 10, 6]. The key question is whether CoB abstractions can help in the process of flowpipe construction. We will investigate this using a tool called Flow* that the author has been involved in [10]. Flow* represents approximations of the solution of a differential equation using a *Taylor model* [6]. Taylor models are used to approximate smooth functions over a compact set by means of a Taylor polynomial and an interval that overapproximates the error. Integration using Taylor model was originally proposed by Berz and Makino [7], and further refined by many in the interval analysis community. Flow* implements a form of Taylor model integration that employs adaptive step sizing and choice of polynomial degrees during the integration process. It also takes into account mode invariants that constraint the evolution of the ODE, and can handle multimodal hybrid dynamics specified by means of switching surfaces and reset maps [9, 10].

Let $\mathcal{G}$ be an affine system that simulates our original nonlinear system $\mathcal{F}$ through a CoB transformation $\vec{w} = \alpha(\vec{x})$. We created an augmented system $\mathcal{FG}$ over the system of variables $(\vec{x}, \vec{w})$ linked by the constraint $\vec{w} = \alpha(\vec{x})$, that is added as an “invariant” to constrain the state-space of the system. The augmented dynamics include the original dynamics $\frac{d\vec{x}}{dt} = f(\vec{x})$ and the affine system $\frac{d\vec{w}}{dt} = A\vec{w}$. On one hand, augmenting the original system through the affine abstraction does not change the set of trajectories for the original system. In fact, it is easy to see that the $\vec{w}$ variables are superfluous, in this sense. However, in the context of an interval analysis, the augmentation helps because it adds back extra constraints that must be respected along all trajectories of

the system.

Example 2.11. Consider, once again, the system from Ex. 1.1, recalled below:

$$\dot{x} = xy + 2x, \quad \dot{y} = -\frac{1}{2}y^2 + 7y + 1$$

and the abstraction discovered through the transformation $\alpha : (x, y) \mapsto (w_1, w_2, w_3)$ wherein $\alpha_1(x, y) = x$, $\alpha_2(x, y) = xy$ and $\alpha_3(x, y) = xy^2$ and the affine dynamics:

$$\dot{w}_1 = 2w_1 + w_2, \quad \dot{w}_2 = w_1 + 9w_2 + \frac{1}{2}w_3, \quad \dot{w}_3 = 2w_2 + 16w_3$$

The augmented system has variables (x, y, w_1, w_2, w_3) and its dynamics are given by simply combining the original system dynamics with the abstraction, above. We also relate the variables by adding the invariants $w_1 = x \wedge w_2 = xy \wedge w_3 = xy^2$. The initial conditions $(x, y) \in [0, 1] \times [0, 1]$ for the original system translate to $(w_1, w_2, w_3) \in [0, 1]^3$ for the additional variables.

Figure 2 compares the results of running Flow* for a time horizon $T = 0.4$. Flow* analyzes the original system 0.8 seconds on a Macbook air laptop with 1.8GHz Intel(tm) processor and 8 GB RAM, running OSX 10.9. The augmented system takes 78.5 seconds to run on the same system, yielding a more accurate result. For instance, the augmented flowpipe correctly infers that all reachable states belong to the first quadrant $x \geq 0, y \geq 0$. Furthermore, it yields a tighter overall range for the given time horizon.

This example demonstrates that even though augmenting the original system using a CoB abstraction does not modify the trajectories of the original system, it can potentially improve the precision of flowpipe construction techniques that rely on interval analysis. Section 4 compares the performance of the Flow* tool on the original versus the augmented system for more examples.

3. Abstractions for Discrete and Hybrid Systems

In this section, we will discuss how the techniques of the previous sections can be extended to find CoB transformations of purely discrete programs. In particular, our focus will be on transforming loops in programs to infer abstractions that are of a simpler form. Our presentation will first focus on simple loops consisting of a single location. The combination of loops with multiple locations and continuous dynamics will be handled in the subsequent section.

3.1. Transition System Models

We will first define transition system models and the action of CoB transformations on these models. Let $\vec{x} \in X$ represent real valued system variables, where $X \subseteq \mathbb{R}^n$. Transition systems will form our basic models for loops in programs [33]. The process of transforming a given imperative program to a transition system representation is related to the idea of control flow graph (CFG) construction, that is implemented in most compilers [36].

Figure 3: Transition system model for the loop in Example 1.2.

Definition 3.1. A *transition system* Π is defined by a tuple $\langle X, L, \mathcal{T}, X_0, \ell_0 \rangle$, wherein,

1. $X \subseteq \mathbb{R}^n$ represents the continuous state-space. We will denote the system variables by $\vec{x} \in \mathbb{R}^n$.
2. L denotes a finite set of *locations*.
3. $\mathcal{T}$ represents a finite set of *transitions*. Each transition $t_j \in \mathcal{T}$ is a tuple $\langle \ell_j, m_j, G_j, F_j \rangle$, where
 - $\ell_j \in L$ is the pre-location of the transition, and $m_j \in L$ is the post-location.
 - $G_j \subseteq \mathbb{R}^n$ is the guard condition on the system variables $\vec{x}$.
 - $F_j : \mathbb{R}^n \rightarrow \mathbb{R}^n$ is the update function.
4. $X_0 \subseteq X$ represents the possible set of initial values and $\ell_0 \in L$ represents the starting location.

Example 3.1. Figure 3 shows an example of a transition system derived from a simple program that computes the sum of the first k squares. The transition system consists of a single location ℓ_0 , transitions $t_1 : (\ell_0, \ell_0, G_1, F_1)$ and $t_2 : (\ell_0, \ell_0, G_2, F_2)$. ▲

A *state* of the transition system is a tuple $\sigma : \langle \ell, \vec{x} \rangle$ where ℓ is the *current* location and $\vec{x} \in X$ are the values of the continuous variables.

A *run* is a finite or infinite sequence of states

$$\sigma_0 \xrightarrow{t_0} \sigma_1 \xrightarrow{t_1} \cdots \rightarrow \sigma_j \xrightarrow{t_j} \sigma_{j+1} \cdots,$$

where each $\sigma_j : (\ell_j, \vec{x}_j)$ is a state and t_j a transition, satisfying the following conditions:

1. The starting state $\sigma_0 : (\ell_0, \vec{x}_0)$ is initial: i.e., ℓ_0 is the initial location of Π and $\vec{x}_0 \in X_0$.
2. The state $\sigma_{i+1} : (\ell_{i+1}, \vec{x}_{i+1})$ is related to the state $\sigma_i : (\ell_i, \vec{x}_i)$ in the following way:
 - (a) The transition $t_i \in \mathcal{T}$ is of the form $(\ell_i, \ell_{i+1}, G_i, F_i)$, leading from ℓ_i to ℓ_{i+1} .
 - (b) The valuation $\vec{x}_i$ of the continuous variables satisfy the guard G_i and the valuation $\vec{x}_{i+1}$ is obtained by executing the assignments in F_i on $\vec{x}_i$:

$$\vec{x}_i \in G_i \text{ and } \vec{x}_{i+1} = F_i(\vec{x}_i).$$

A special class of “simple loop” transition systems that have a single location.

Definition 3.2. A transition system Π is called a *simple loop* if it has a single location: i.e., $L = \{\ell\}$. All transitions of a simple loop are self-loops around this location ℓ .

The transition system in Example 3.1 is a simple loop. It consists of a single location. In general, simple loops can have multiple transitions that “loop” around this single location.

We will now discuss the pre-image operator FPRE induced by a transition. Let $g(\vec{x})$ be some function over the state variables and $t : (\ell, m, G, F)$ be a transition.

Definition 3.3. The *functional pre-image* $\text{FPRE}(g, t)$ is defined as $g(F(\vec{x}))$.

Note: The standard precondition operator works over assertions over the state variables, involving computing the pre-image using F and computing the intersection of the result with the guard. The functional precondition defined here is defined over functions $g(\vec{x})$ over the state variables.

Example 3.2. Consider the transition

$$t : (\ell, m, G, F), \text{ wherein } G : \{(x, y) \mid x \geq y\}, F(x, y) : (x^2, y^2 - x^2).$$

The functional pre-image of the function $g(x, y) : x + y$, denoted $\text{FPRE}(x + y, \rho)$, is given by

$$\text{FPRE}(x + y, t) : (x^2) + (y^2 - x^2) = y^2.$$

To contrast with the standard pre-condition operator, which applies to assertions over states, let us consider the assertion $x + y \geq 0$. We have

$$\text{PRE}(x + y \geq 0, \rho) : y^2 \geq 0 \wedge x \geq y.$$

▲

We now show that FPRE is a linear operator over functions.

Lemma 3.1. *For any transition t and functions g_1, g_2, g over $\vec{x}$, we have $\text{FPRE}(g_1 + g_2, t) = \text{FPRE}(g_1, t) + \text{FPRE}(g_2, t)$ and further, $\text{FPRE}(\lambda g) = \lambda \text{FPRE}(g)$ for any $\lambda \in \mathbb{R}$.*

Proof. Proof follows by directly applying Def. 3.3. $\square$

Let us consider any run of the transition system

$$r : \sigma_0 \xrightarrow{t_0} \sigma_1 \rightarrow \cdots \rightarrow \sigma_i \xrightarrow{t_i} \sigma_{i+1} \cdots$$

Let $t_i : (\ell_i, \ell_{i+1}, G_i, F_i)$ denote the transition between $\sigma_i : (\ell_i, \vec{x}_i)$ and $\sigma_{i+1} : (\ell_{i+1}, \vec{x}_{i+1})$. Finally, let $g(\vec{x})$ be any function over the state variables of the transition system.

Lemma 3.2. *The following identity holds for all successive pairs of states $(\ell_i, \vec{x}_i) \xrightarrow{t_i} (\ell_{i+1}, \vec{x}_{i+1})$ encountered in a run of the transition system and for all functions $g(\vec{x})$:*

$$\text{FPRE}(g(\vec{x}), t_i) \equiv g(\vec{x}_{i+1})$$

Proof. We may write $h(\vec{x}) = g(F(\vec{x}))$. We know that $\vec{x}_{i+1} = F(\vec{x}_i)$. Therefore, $g(\vec{x}_{i+1}) = g(F(\vec{x}_i)) = h(\vec{x}_i)$. $\square$

We will now discuss change-of-basis abstractions for transition systems. The discussion will focus on defining change-of-basis abstractions for simple loops, which are represented by a transition system with a single location ℓ (Cf. Definition 3.2). The subsequent sections will extend this concept to arbitrary transition systems.

3.2. CoB Abstractions For Simple Loops

Consider a simple loop Π over $\vec{x} \in \mathbb{R}^n$ with a single location ℓ , transitions $\{t_1, \dots, t_k\}$, and initial condition X_0 . We seek to abstract Π with another simple loop Ξ over $\vec{y} \in \mathbb{R}^d$ with a single location m , transitions $\{t'_1, \dots, t'_k\}$ and initial condition Y_0 .

Definition 3.4. Simple loop Ξ is a CoB abstraction of Π iff there is a continuous function $\alpha : \mathbb{R}^n \rightarrow \mathbb{R}^d$ such that

1. The initial condition $Y_0 \supseteq \alpha(X_0)$,
2. For each transition $t_i : (\ell, \ell, G_i, F_i)$ in Π , there is a corresponding transition $t'_i : (m, m, G'_i, F'_i)$ in Ξ such that
 - (a) $G'_i \supseteq \alpha(G_i)$,
 - (b) $\forall \vec{x} \ F'_i(\alpha(\vec{x})) = \alpha(F_i(\vec{x}))$.

We will now present an example of CoB abstraction for simple loops.

Example 3.3. Consider the simple loop from Example 3.1 (also Fig. 3). We note that the map

$$\alpha : \mathbb{R}^3 \rightarrow \mathbb{R}^4, \text{ where } \alpha : (x, y, k, y^2),$$

yields an abstract transition system Ξ over variables $\vec{w} : (w_1, w_2, w_3, w_4)$. Informally, the variables (w_1, w_2, w_3, w_4) are placeholders for the expressions (x, y, k, y^2) , respectively. The resulting transition system Ξ is

$$\begin{aligned} \vec{w} & : (w_1, \dots, w_4) \\ L & : \{m\} \\ \mathcal{T} & : \{t'_1 : (m, m, G'_1, F'_1), t'_2 : (m, m, G'_2, F'_2)\} \\ X_0 & : w_1 = w_2 = w_4 = 0 \wedge w_3 \geq 1 \\ G'_1 & : \{\vec{w} \mid w_2 < w_3\} \\ G'_2 & : \{\vec{w} \mid w_2 \geq w_3\} \\ F'_1(\vec{w}) & : (w_1 + w_4, w_2 + 1, w_3, w_4 + 2w_2 + 1) \\ F'_2(\vec{w}) & : \vec{w} \end{aligned}$$

The various requirements laid out in Definition 3.4 can be easily verified. We will verify the requirement for F'_1 : $F'_1(\alpha(x, y, k)) = \alpha(F_1(x, y, k))$, as follows:

$$\begin{aligned} F'_1(\alpha(x, y, k)) & = F'_1(x, y, k, y^2) & = \underbrace{(x + y^2)}_{w_1 + w_4}, \underbrace{(y + 1)}_{w_2 + 1}, \underbrace{k}_{w_3}, \underbrace{(y^2 + 2y + 1)}_{w_4 + 2w_2 + 1} \\ & = \alpha(x + y^2, y + 1, k) & = \alpha(F_1(x, y, k)) \end{aligned}$$

▲

The definition of CoB abstraction immediately admits the following key theorem.

Theorem 3.1. *For any run*

$$\sigma_0 : (\ell, \vec{x}_0) \xrightarrow{t_0} (\ell, \vec{x}_1) \xrightarrow{t_1} (\ell, \vec{x}_2) \xrightarrow{t_2} \dots$$

the corresponding sequence of Ξ -states

$$\gamma_0 : (m, \alpha(\vec{x}_0)) \xrightarrow{t'_0} (m, \alpha(\vec{x}_1)) \xrightarrow{t'_1} (m, \alpha(\vec{x}_2)) \xrightarrow{t'_2} \dots,$$

is a run of Ξ .

Proof. Proof uses the property that whenever the move $(\ell, \vec{x}_j) \xrightarrow{t_j} (\ell, \vec{x}_{j+1})$ is possible in Π then the move $(m, \alpha(\vec{x}_j)) \xrightarrow{t'_j} (m, \alpha(\vec{x}_{j+1}))$ is possible in Ξ .

Let t_j be described by the guard G_j and the functional update F_j . Likewise, let t'_j be described by G'_j and F'_j . We note that $\alpha(G_j) \subseteq G'_j$. Since $\vec{x}_j$ satisfies the guard of t_j , $\alpha(\vec{x}_j)$ satisfies that of t'_j . The state obtained after the transition is given by $\vec{x}'_{j+1} = F'_j(\alpha(\vec{x}_j))\alpha(F_j(\vec{x}_j)) = \alpha(\vec{x}_{j+1})$.

We have proved that whenever the move $(\ell, \vec{x}_j) \xrightarrow{t_j} (\ell, \vec{x}_{j+1})$ is possible in Π then the move $(m, \alpha(\vec{x}_j)) \xrightarrow{t'_j} (m, \alpha(\vec{x}_{j+1}))$ is possible in Ξ . The rest of the proof extends this to trace containment through induction over prefixes of the traces. $\square$

As a direct consequence, we may state a theorem that corresponds to Theorem 2.2 for the case of vector fields. Given a formula $\varphi[\vec{x}]$, we use $[[\varphi]]$ to denote the set of valuations to $\vec{x}$ that satisfy φ .

Theorem 3.2. *Let $[[\varphi]]$ be an invariant set for the abstract system Ξ . Then, $\alpha^{-1}(\varphi)$ is an invariant of the original system Π .*

Proof. First, we note from Theorem 3.1 that if $(\ell, \vec{x})$ is reachable in Π then $(m, \alpha(\vec{x}))$ is reachable in Ξ . Since φ is an invariant for Ξ , we have $(m, \alpha(\vec{x})) \in [[\varphi]]$. Therefore for any reachable state $(\ell, \vec{x})$ in Π , we have $(\ell, \vec{x}) \in \alpha^{-1}([[\varphi]])$. Thus $\alpha^{-1}([[\varphi]])$ is an invariant set for Ξ . $\square$

Given an invariant $\varphi[\vec{y}]$ for Ξ in the form of an assertion, the invariants for the original system are obtained simply by substituting $\alpha(\vec{x})$ in the place of $\vec{y}$ in φ .

Example 3.4. Consider the transition system Π from Example 3.1 and its abstraction Ξ in Example 3.3. We note that Ξ has affine guards and updates. Therefore, we may use a standard polyhedral analysis tool to compute invariants over Ξ [15, 26, 53]. Some of the invariants obtained include

$$\begin{aligned} 13w_4 \leq 9w_1 + 24w_2 \ \wedge \ 7w_4 \leq 6w_1 + 11w_2 \ \wedge \ 4w_1 + 7w_2 - 7w_4 + 11w_3 \geq 11 \\ 2w_1 + 3w_2 - 3w_4 + 4w_3 \geq 4 \ \wedge \ w_4 \leq 2w_1 + w_2 \ \wedge \ 3w_4 \leq w_1 + 12w_2 \\ 9 - w_1 - 3w_2 + 3w_4 - 9w_3 \leq 0 \ \wedge \ w_2 \geq 0 \ \wedge \ 1 \leq w_3 \ \wedge \ w_2 - w_3 \leq 0 \end{aligned}$$

By substituting $w_1 \mapsto x, w_2 \mapsto y, w_3 \mapsto k, w_4 \mapsto y^2$ on these invariants, we conclude invariants for the original system. For instance, we conclude facts such as

$$13y^2 - 24y - 9x \geq 0 \ \wedge \ 7y^2 - 11y - 6 \geq 0 \ \wedge \ 11k - 7y^2 + 7y + 4x \geq 11.$$

▲

The goal, once again, is to find an abstraction α and an abstract system Ξ starting from a description of the system Π . Furthermore, we require that the update functions F'_j in Ξ are all polynomials whose degrees are smaller than some given limit $d > 0$. In particular, if we set $d = 1$, we are effectively requiring all the updates in Ξ to be affine functions over $\vec{y}$.

Our strategy will be to find a map $\alpha : \mathbb{R}^n \rightarrow \mathbb{R}^k$. For convenience, we will write α as $(\alpha_1, \dots, \alpha_k)$, wherein each component function $\alpha_j : \mathbb{R}^n \rightarrow \mathbb{R}$. Let V be the vector space spanned by the components of α , i.e, $V = \text{Span}(\{\alpha_1, \dots, \alpha_k\})$. Our goal will be to ensure that for each transition t in Π ,

$$\forall \vec{x}, \text{FPRE}(\alpha_i(\vec{x}), t) \in V^{(d)}. \quad (3)$$

Let V be a vector space that satisfies Eq. (3) for each transition t in Π . We will say that the space V is *d-closed* w.r.t Π .

Theorem 3.3. *Let $V : \text{Span}(g_1, \dots, g_k)$ be d -closed w.r.t Π for continuous functions $g_1, \dots, g_k$. The map $\alpha : (g_1, \dots, g_k)$ is a CoB transformation defining an abstract system Ξ , wherein each transition of Ξ has a polynomial update function involving polynomials of degree at most d .*

Proof. We construct the abstract system Ξ with variables $w_1, \dots, w_k$ representing the functions $g_1, \dots, g_k$ in the original system. Ξ has a single location m and for each transition $t_i \in \Pi$, we construct a corresponding transition $t'_i \in \Xi$ as follows.

Let G_i, F_i be the guard and update sets for t_i . The guard set for t'_i is given by $\alpha(G_i)$ or an over-approximation thereof. Likewise, the update F'_i for t'_i is derived as follows. We note that

$$\text{FPRE}(g_j, t_i) = \sum_r c_{r_1, r_2, \dots, r_k} g_1^{r_1} g_2^{r_2} \cdots g_k^{r_k},$$

wherein $0 \leq r_1 + r_2 + \dots + r_k \leq d$. The corresponding update for w_j in the abstract system is given by

$$F'_i(w_j) = \sum_r c_{r_1, r_2, \dots, r_k} w_1^{r_1} w_2^{r_2} \cdots w_k^{r_k}.$$

Note that each function $F'_i(w_j)$ is a polynomial of degree at most d over $w_1, \dots, w_k$. $\square$

Since the operator FPRE used to define the closure in Eq. (3) is a linear operator (Cf. Lemma 3.1), we may check the closure property for a given vector space V by checking if its basis functions satisfy the property.

Lemma 3.3. *The vector space $V : \text{Span}(\{g_1, \dots, g_k\})$ is d -closed w.r.t Π iff for each basis element g_i of V , and for each transition t in Π , $\text{FPRE}(g_i, t) \in V^{(d)}$.*

Proof. For the non-trivial direction, let V be a space where for each basis element g_i of V , and for each transition t in Π , $\text{FPRE}(g_i, t) \in V^{(d)}$. An arbitrary element $g \in V$ can be written as a linear combination of its basis elements: $g = \sum_j \lambda_j g_j$. We have $\text{FPRE}(g, t) = \sum_j \lambda_j \text{FPRE}(g_j, t)$ from Lemma 3.1. Since $\text{FPRE}(g_j, t) \in V^{(d)}$, which is a vector space itself, we have that $\text{FPRE}(g, t)$ is a linear combination of elements in $V^{(d)}$ and thus $\text{FPRE}(g, t) \in V^{(d)}$. Thus V is d -closed. $\square$

Example 3.5. Once again, consider the system Π in Example 3.1 and the map $\alpha : (x, y, k, y^2)$ from Example 3.3. The components of this map are the functions $\alpha_1 : x, \alpha_2 : y, \alpha_3 : k$, and $\alpha_4 : y^2$. We may verify that the vector space $V : \text{Span}(\{x, y, k, y^2\})$ satisfies the closure property in Eq. (3) for $d = 1$. The table below shows the results of applying FPRE on each of the basis elements.

Basis function g_j	$\text{FPRE}(g_j, t_1)$	$\text{FPRE}(g_j, t_2)$
x	$x + y^2$	x
y	$y + 1$	y
k	k	k
y^2	$y^2 + 2y + 1$	y^2

Thus, $\text{FPRE}(g_j, t_k)$ belongs to $V^{(1)} = \text{Span}(\{1, x, y, k, y^2\})$. ▲

Searching for Abstractions: The procedure for finding abstractions is identical to that used for vector fields with the caveat that closure under Lie-derivative is replaced by closure under $\text{FPRE}(\cdot, t_j)$ for every transition t_j in the system. The procedure takes as input an initial basis of functions B_0 and iteratively refines the vector space $V_i : \text{Span}(B_i)$ by removing all the functions that do not satisfy the closure property.

Example 3.6. Consider the system Π in Example 3.1 and the initial basis consisting of all monomials of degree at most 2 over variables x, y, k . We obtain the basis $B_0 : \{x, y, k, x^2, y^2, k^2, xy, yk, xk\}$ and the space $V_0 : \text{Span}(B_0)$. An element of V_0 can be written as

$$p : \begin{bmatrix} c_1x + c_2y + c_3k + c_4x^2 + c_5y^2 + c_6k^2 \\ + c_7xy + c_8yk + c_9xk \end{bmatrix}$$

We consider the transition t_1 with update $F_1(x, y, k) : (x + y^2, y + 1, k)$. Transition t_2 is ignored as its update is simply the identity relation. We have $\text{FPRE}(p, t_1)$ as

$$\text{FPRE}(p, t_1) : \begin{bmatrix} (c_2 + c_5) + (c_1 + c_7)x + (c_2 + 2c_5)y + (c_3 + c_8)k + c_4x^2 + \\ (c_1 + c_5 + c_7)y^2 + c_6k^2 + c_7xy + c_7y^3 + c_4y^4 + 2c_4xy^2 + \\ c_8yk + c_9xk + c_9y^2k \end{bmatrix}$$

The “overflow” terms c_7y^3 , c_4y^4 , c_9y^2k immediately yield the constraints $c_4 = c_7 = c_9 = 0$. The refined basis is $B_1 : \{x, y, k, y^2, k^2, yk\}$. The iterative process converges with $V_1 : \text{Span}(B_1)$ yielding a linearization. ▲

Complexity: The process of computing the vector space iterates and the overall complexity are quite the same as for the case of ODEs 2.6.1. The major change is that the computation of Lie derivatives is replaced with computing preconditions.

3.3. Abstractions for General Transition Systems

Thus far, we have presented CoB abstractions for simple loops consisting of a single location. The ideas seamlessly extend to systems with multiple locations with a few generalizations that will be described in this section.

Let Π be a system with a set of locations $L = \{\ell_1, \dots, \ell_k\}$ and transitions $\mathcal{T}$. We will assume that $|L| \geq 2$ so that the system is no longer a simple loop. The main idea behind change-of-bases (CoB) transformations for systems with multiple locations is to allow a different map for each location. In other words, the abstraction is defined by a maps $\alpha_\ell(\vec{x})$ for each location $\ell \in L$.

The maps for two different locations ℓ_1 and ℓ_2 are of the type $\alpha_{\ell_1} : \mathbb{R}^n \rightarrow \mathbb{R}^{m_1}$ and $\alpha_{\ell_2} : \mathbb{R}^n \rightarrow \mathbb{R}^{m_2}$. In general, we may assume that $m_1 \neq m_2$. This discrepancy can be remedied by padding each α_{ℓ_i} with extra components that

Figure 4: An example program fragment with multiple locations and its transition system.

map to the constant function 0. While, this transformation violates the linear independence requirement between the various components in α , it makes the resulting abstract system easier to describe. Without loss of generality, we assume that all the maps α_ℓ for each $\ell \in L$ are of the form $\alpha_\ell : \mathbb{R}^n \rightarrow \mathbb{R}^m$ for a fixed $m > 0$.

Definition 3.5. A system Ξ is a CoB abstraction of Π through a collection of maps $\alpha_{\ell_1}, \dots, \alpha_{\ell_k}$ each of the type $\mathbb{R}^n \rightarrow \mathbb{R}^m$, corresponding to locations $\ell_1, \dots, \ell_k$, iff

1. Ξ has locations m_j corresponding to $\ell_j \in L$ for $1 \leq j \leq k$, and transitions t'_i corresponding to transition $t_i \in \mathcal{T}$.
2. For each transition $t_i : \langle \ell_{pre}, \ell_{post}, G_i, F_i \rangle$ in Π , the corresponding transition $t'_i : \langle m_{pre}, m_{post}, G'_i, F'_i \rangle$ is such that
 - (a) m_{pre} and m_{post} correspond to ℓ_{pre} and ℓ_{post} , respectively,
 - (b) $G'_i \supseteq \alpha_{\ell_{pre}}(G_i)$,
 - (c) $(\forall \vec{x}) F'_i(\alpha_{\ell_{pre}}(\vec{x})) = \alpha_{\ell_{post}}(F_i(\vec{x}))$.

We note that for a simple loop with a single location, the definition above is identical to Def. 3.4.

Example 3.7. Figure 4 shows an example of a transition system with multiple locations. Consider the following CoB transformation:

$$\begin{aligned}
\alpha_{\ell_1} &: (z^2, yz, xz, z, y^2, xy, y, x^2, x) \\
\alpha_{\ell_2} &: (z^2, yz + xz, z, y, y^2 + 2xy + x^2, x, 0, 0, 0) \\
\alpha_{\ell_3} &: (z^2, yz, xz, z, y^2, xy, y, x^2, x)
\end{aligned}$$

The transformation yields an abstraction Ξ of the original system. The abstract system has 9 variables $w_0, \dots, w_8$. The structure of Ξ mirrors that of Π with

three locations m_1, m_2, m_3 corresponding to ℓ_1, ℓ_2, ℓ_3 , respectively and three transitions t'_1, t'_2 and t'_3 corresponding to t_1, t_2 and t_3 in Π . The guards and updates of the transition t'_1 are

$$\begin{aligned} G'_1 &: \{(w_0, \dots, w_8) \mid w_8 + w_6 - w_3 \leq 100\}, \\ F'_1 &: (w_0, w_1 + w_2, w_3, w_1 - w_2 + w_6, w_4 + 2w_5 + w_7, -w_1 + w_2 + w_8, 0, 0, 0) \end{aligned}$$

We verify the key condition that ensures that t'_1 is an abstraction of t_1 :

$$\alpha_{\ell_2}(F_1(x, y, z)) = F'_1(\alpha_{\ell_1}(x, y, z)).$$

The LHS $\alpha_{\ell_2}(F_1(x, y, z)) = \alpha_{\ell_2}(x + zx - zy, y + zy - zx, z)$ is given by

$$(z^2, zx + zy, z, y + zy - zx, x^2 + 2xy + y^2, x + zx - zy, 0, 0, 0).$$

The RHS $F'_1(\alpha_{\ell_1}(x, y, z)) = F'_1(z^2, yz, xz, z, y^2, xy, y, x^2, x)$ is given by

$$(z^2, xz + yz, z, y - zx + zy, y^2 + 2xy + x^2, x + zx - zy, 0, 0, 0).$$

The identity of LHS and RHS is thus verified. ▲

Our goal once again is to search of a collection of transformations α_ℓ , for each $\ell \in L$ such that the resulting system is described by polynomial updates of degree at most d . The case where $d = 1$ corresponds to affine updates. Once again, we generalize the notion of a d -closed vector space. Consider a collection of vector spaces $V_\ell : \text{Span}(B_\ell)$ for each location $\ell \in L$.

Definition 3.6. We say that the collection $V_\ell, \ell \in L$ is d -closed for transition system Π if and only if for each transition $t_j : \langle \ell_{pre}, \ell_{post}, G_j, F_j \rangle$ and for each element $p \in V_{post}$, we have $\text{FPRE}(p, t_j) \in V_{pre}^{(d)}$.

The notion of d -closed vector spaces can be related to CoB transformations and resulting abstractions whose updates are defined by means of polynomials of degree at most d .

Theorem 3.4. *Let $V_\ell, \ell \in L$ be a collection of vector spaces that are d -closed for a system Π . The basis elements of V_ℓ yields a collection of maps $\alpha_\ell, \ell \in L$ that relate Π to a CoB abstraction Ξ . The update maps of Ξ are all polynomials of degree at most d .*

Example 3.8. Consider the transition system described in Example 3.7 and Figure 4. We wish to discover an affine abstraction for this system automatically. Starting from the initial collection of vector spaces that maps each location to the space of all polynomials of degree at most 2 over x, y, z , we obtain the transformations $\alpha_{\ell_1}, \alpha_{\ell_2}, \alpha_{\ell_3}$ described in the same example. This yields an abstract system over variables $w_0, \dots, w_8$.

3.4. Combining Discrete and Continuous Systems

As a final step, we extend our approach to hybrid systems that combine discrete and continuous dynamics. We define hybrid systems briefly and extend the results from Sections 2 and 3 to address hybrid systems.

Definition 3.7. A hybrid system consists of a discrete transition system $\Pi : \langle X, L, \mathcal{T}, X_0, \ell_0 \rangle$ and a mapping that associates each location $\ell_i \in L$ with a continuous subsystem $\mathcal{S}_i : \langle \mathcal{F}_i, X_i \rangle$ over the state-space X , consisting of a vector field $\mathcal{F}_i$ and location invariant X_i .

A state σ of the hybrid system consists of a tuple $\langle \ell, \vec{x}, t \rangle$ where $\ell \in L$ is the current location, valuations to the continuous variables $\vec{x} \in X$ and the current time $t \geq 0$.

Given a time $\delta \geq 0$, we write $\langle \ell, \vec{x}, T \rangle \rightsquigarrow_{\delta} \langle \ell, \vec{y}, T + \delta \rangle$ to denote that starting from state $\langle \ell, \vec{x}, T \rangle$ the hybrid system *flows* continuously according to the continuous subsystem $\mathcal{S}_{\ell}$ corresponding to the location ℓ . Likewise, we write $\langle \ell, \vec{x}, T \rangle \xrightarrow{t_j} \langle \ell', \vec{x}', T \rangle$ to denote a *jump* between two states upon taking a discrete transition t_j from ℓ to ℓ' . Note that no time elapses upon taking a jump.

A run R of the hybrid system is given by a countable sequence of alternating flows (evolution according to the ODE inside a location) and jumps (discrete transition to a different location) starting from an initial state:

$$\sigma_0 : \langle \ell_0, \vec{x}_0, 0 \rangle \rightsquigarrow_{\delta_0} \sigma'_0 : \langle \ell_0, \vec{y}_0, \delta_0 \rangle \xrightarrow{t_1} \sigma_1 : \langle \ell_1, \vec{x}_1, \delta_0 \rangle \rightsquigarrow_{\delta_1} \sigma'_1 : \langle \ell_1, \vec{y}_0, \delta_0 + \delta_1 \rangle \xrightarrow{t_2} \dots$$

To avoid Zenoness, we require that the summation of the dwell times in the individual modes $\sum_{j=0}^{\infty} \delta_j$ diverges.

We now define CoB abstractions for hybrid systems. Our definitions simply combine aspects of the definition for transition systems 3.5 and continuous systems 2.3.

A CoB abstraction of the hybrid system is obtained through a collection of maps $\alpha_{\ell_1}, \dots, \alpha_{\ell_k}$ corresponding to the locations $\ell_1, \dots, \ell_k$ of the hybrid system. It is assumed that by padding with 0s, we obtain each α_{ℓ_i} as a function $\mathbb{R}^n \rightarrow \mathbb{R}^m$.

Definition 3.8. A system Ξ is a CoB abstraction of Π through a collection of maps $\alpha_{\ell_1}, \dots, \alpha_{\ell_k}$ each of the type $\mathbb{R}^n \rightarrow \mathbb{R}^m$, corresponding to locations $\ell_1, \dots, \ell_k$, iff

1. Ξ has locations m_j corresponding to $\ell_j \in L$ for $1 \leq j \leq k$, and transitions t'_i corresponding to transition $t_i \in \mathcal{T}$. Each location m_j in Ξ has an associated continuous system $\mathcal{T}_j$.
2. For each corresponding location pair ℓ_j, m_j , the system $\mathcal{T}_j$ is a CoB abstraction of $\mathcal{S}_j$ through the transformation α_{ℓ_j} .
3. For each transition $t_i : \langle \ell_{pre}, \ell_{post}, G_i, F_i \rangle$ in Π , the corresponding transition $t'_i : \langle m_{pre}, m_{post}, G'_i, F'_i \rangle$ are such that

- (a) m_{pre} and m_{post} correspond to ℓ_{pre} and ℓ_{post} , respectively,
- (b) $G'_i \supseteq \alpha_{\ell_{pre}}(G_i)$,
- (c) $(\forall \vec{x}) F'_i(\alpha_{\ell_{pre}}(\vec{x})) = \alpha_{\ell_{post}}(F_i(\vec{x}))$.

Once again, we focus on searching for an abstraction Ξ of a given hybrid system wherein the continuous abstraction for each location and that of each transition is expressed by means of polynomials degree bounded by some fixed bound d . The case where the bound is $d = 1$ specifies an affine hybrid abstraction Ξ . We translate this into a d -closure condition for vector spaces. Consider a collection of vector spaces $V_\ell : \text{Span}(B_\ell)$ for each location $\ell \in L$.

Definition 3.9. We say that the collection $V_\ell, \ell \in L$ is d -closed for transition system Π if and only if

1. For each location $\ell \in L$, the corresponding vector space V_ℓ is d -closed w.r.t to the vector field $\mathcal{F}_\ell$ defining the continuous subsystem $\mathcal{S}_\ell$.
2. For each transition $t_j : \langle \ell_{pre}, \ell_{post}, G_j, F_j \rangle$ and for each element $p \in V_{\ell_{post}}$, we have $\text{FPRE}(p, t_j) \in V_{\ell_{pre}}^{(d)}$.

Once again, the approach for finding a d -closed collection $V_\ell, \ell \in L$ starts from an initial basis $V_\ell^{(0)}$ at each location ℓ and refines the basis. Two types of refinements are applied (a) refinement of V_ℓ to enforce closure w.r.t the Lie derivative of its basis elements for the vector field $\mathcal{F}_\ell$ and (b) refinement of V_m w.r.t a transition $t : \langle \ell, m, G, F \rangle$ incoming at location m .

Abstracting Guard and Invariant Sets: We finally mention that a key difficulty for hybrid systems involves the process of abstracting guards and invariant sets. For instance, suppose the original system has a simple switching guard of the form $x \leq c$, it can be transformed by the abstraction process into a more complicated (nonlinear) guard on the resulting abstract hybrid system with affine dynamics. Similarly, polyhedral mode invariants can become general semi-algebraic invariants for the abstract system. The solution to this problem involves over-approximating guards and invariants through polyhedral sets. This over-approximation can however be quite coarse, introducing many spurious behaviors and also hard to compute, in general.

4. Implementation and Evaluation

We have implemented the ideas described in this paper to derive affine abstractions for (a) continuous systems described by ODEs with polynomial right-hand sides, (b) discrete systems with assignments that have polynomial RHS and (b) hybrid systems with polynomial ODEs and discrete transition updates. Our approach takes as inputs the system description, a degree limit $k > 0$ that is used to construct the initial basis. Starting from this initial basis, our approach iteratively applies refinement until convergence. Upon convergence, we print the basis inferred along with the resulting abstraction.

Figure 5: Comparing the flowpipes constructed for Flow* for the system in Toda-2 lattice. **(Left)** The original 6 state model and **(Right)** The augmented model with 12 state variables including the original system and the linear abstraction.

Currently, our implementation does not abstract the guard sets of the transitions and the invariant sets of the ODEs. However, once the basis is inferred using quantifier elimination techniques (which is quite expensive in practice) [12, 13, 18] or techniques such as SOS programming [41]. Our implementation currently relies on manual translation of invariant and guard assertions into the new basis to form the abstract transition system.

If a non-trivial abstraction is discovered by our iterative scheme, we may use a linear invariant generator on the resulting affine system to infer invariants that relate to the original transition system.

4.1. Continuous Systems

We first describe experimental results obtained for continuous systems described by ODEs. Table 1 summarizes the results on continuous system benchmarks. We collected nearly 15 benchmark systems and ran our implementation to search for a linearizing CoB transformation. We report on the degree of the monomials in the initial basis, time taken to converge and the number of polynomials in the final basis that form the transformation to the abstract system.

Trivial Transformations Found: Some of the benchmarks attempted resulted in trivial final transformations. Examples include the well-known Fitzhugh-Nagumo neuron model, the vanderpol oscillators and similar small but complex systems that are known to be non-integrable. There is as yet no characterization of systems that admit a non-trivial CoB transformation to an affine system.

We now highlight some of the interesting results, while summarizing all benchmarks in Table 1.

Toda Lattice with Boundary Particles: The Toda lattice models an infinite array of point particles such that the position and velocity of the n^{th} particle

are affected by its neighbours the $(n - 1)^{th}$ and $(n + 1)^{th}$ particle for $n \in \mathbb{Z}$ ³. We consider a finite version of this lattice with 2 fixed boundary particles that are constrained to have a fixed position and zero velocity and K particles in the middle. The dynamics for $K = 2$ non-fixed particles are given by position variables y_1, y_2 , velocities v_1, v_2 and extra state variables u_1, u_2 to model the interaction with neighbours.

$$\begin{aligned} \frac{dx_1}{dt} &= v_1 & \frac{dv_1}{dt} &= v_1(u_1 - u_2) & \frac{du_1}{dt} &= -v_1 \\ \frac{dx_2}{dt} &= v_2 & \frac{dv_2}{dt} &= v_2 u_2 & \frac{du_2}{dt} &= v_1 - v_2 \end{aligned}$$

In addition, we add time t as a variable to the model with dynamics $\frac{dt}{dt} = 1$. Our approach initialized with polynomials of degree 2 discovers a basis with 10 polynomials:

$$\begin{aligned} w_1 : & -2v_2 - 2v_1 - u_2^2 + 2x_1u_1 + x_2^2, \\ w_2 : & -2v_2 - 2v_1 - u_2^2 + u_1u_2 + x_2u_1 + x_1u_2 + x_1u_1 + x_1x_2 \\ w_3 : & -2v_2 - 2v_1 + 2u_1u_2 + 2x_2u_2 + 2x_2u_1 + x_2^2, \quad w_4 : u_1 + x_1, \\ w_5 : & 2v_2 + 2v_1 + u_1^2 + u_2^2, \quad w_6 : u_2 + x_2 - x_1, \quad w_7 : t, \\ w_8 : & u_1t + x_1t, \quad w_9 : u_2t + u_1t + x_2t, \quad w_{10} : t^2 \end{aligned}$$

The resulting abstract system has linear dynamics given by:

$$\frac{dw_j}{dt} = 0, \quad 1 \leq j \leq 6, \quad \frac{dw_7}{dt} = 1, \quad \frac{dw_8}{dt} = w_4, \quad \frac{dw_9}{dt} = w_4 + w_6, \quad \frac{dw_{10}}{dt} = 2w_7.$$

Results for larger instances are reported in Table 1.

Once again, we augment the original system with six additional variables $w_1, \dots, w_6$, ignoring time dependent variables $w_7, \dots, w_{10}$. The initial set X_0 is given by

$$x_1 \in [0, 0.1], \quad x_2 \in [1, 1.1], \quad v_1 \in [-0.1, 0], \quad v_2 \in [0, 0.1], \quad (u_1, u_2) \in [0, 0.1]^2$$

Figure 5 contrasts the original flowpipe for time horizon $T = 2$. The original model has 6 state variables and Flow* analyzes this model in 64.5 seconds. The augmented system has 12 state variables and requires 336.5 seconds for Flow* flowpipe construction. However, the figure clearly shows that the augmented system's flowpipe establishes a tighter range over the values of the state variables (x_1, x_2) over the time horizon when compared to the original system's flowpipe.

Quadratic Fermi-Pasta-Ulam-Tsingou System: Consider a system considered by Fermi et al. [20]. The system consists of a chain of particles at positions $x_1, \dots, x_N$ with fixed boundary particles $x_0 = 0$ and $x_{N+1} = N + 1$. The dynamics are given by

$$\frac{d^2x_i}{dt^2} = (x_{i+1} + x_{i-1} - 2x_i) + \alpha((x_{i+1}^2 - x_i^2) - (x_i - x_{i-1})^2), \quad 1 \leq i \leq N$$

³See description by Göktaş and Hereman [24] and references therein.

Figure 6: Comparing the flowpipes constructed for Flow* for the Fermi et al. system. **(Left)** The original 7 state model and **(Right)** The augmented model with 8 state variables.

We consider an instantiation with $N = 3$, searching for CoB transformations with an initial basis of monomials of degree upto 4. We obtain a transformation representing a conserved quantity

$$\frac{1}{2}(v_1^2 + v_2^2 + v_3^2) + x_1^2 + x_2^2 + x_3^2 - 3x_3(1 + 3a - ax_3) - x_2x_3(1 + ax_3 - ax_2) - x_1x_2(1 + ax_2 - ax_1) .$$

The abstract system is given by $\frac{dw_1}{dt} = 0$.

Figure 6 shows the Flow* comparison of the original system and the augmented one. Whereas the Flow* terminated in 18 seconds for the original system, it required 1292.5 seconds for the augmented system. In our experience, this extra time is not entirely due to the single additional variable but chiefly includes the time taken for the domain contraction operation that is required for enforcing mode invariants [9]. The Flowpipe for the augmented system is, in fact, somewhat more accurate especially comparing the upper bounds for x_1 established by both Flowpipes.

Two Mass Spring System: Consider the dynamics of two masses connected by a spring to each other and to two fixed walls. The state variables are (x_1, x_2, v_1, v_2) indicating the position and velocity of the masses while the spring constant k is a parameter. The dynamics are given by

$$\begin{aligned} \frac{dx_1}{dt} &= v_1 & \frac{dx_2}{dt} &= v_2 \\ \frac{dv_1}{dt} &= kx_2 - 2kx_1 & \frac{dv_2}{dt} &= k(x_1 - x_2) \end{aligned}$$

Our procedure yields a change-of-bases transformation

$$w_1 : v_2^2 + v_1^2 + kx_2^2 - 2kx_1x_2 + 2kx_1^2, \quad w_2 : v_1v_2 - \frac{1}{2}v_1^2 - \frac{1}{2}kx_2^2 + 2kx_1x_2 - \frac{3}{2}kx_1^2$$

Both w_1, w_2 represent conserved quantities, yielding the abstraction

$$\frac{dw_1}{dt} = \frac{dw_2}{dt} = 0 .$$

Figure 7: Comparing the flowpipes constructed for Flow* for the two mass spring system. **(Left)** The original 5 state model and **(Right)** The augmented model with 7 state variables.

We applied Flow* to this system with initial states

$$x_1 \in [1, 2], x_2 \in [3, 4], v_1 \in [0, 0.1], v_2 \in [-0.1, 0], k \in [0.5, 1.2].$$

Flow* requires 8.8 seconds for the original model and 660.5 seconds to analyze the augmented model. The comparison is shown in Figure 7. The flowpipe constructed for the augmented model is clearly more accurate.

Biochemical reaction network: We consider a biochemical reaction network benchmark from Dang et al. [17]. The ODE along with the values are parameters in our model coincide with those used by Dang et al. The ODE consists of 12 variables and roughly 14 parameters. Our search for degree bound ≤ 3 discovers a transformation generated by five basis functions (in roughly 3 seconds). The model itself is too large to be directly analyzed by Flow*.

Collision Avoidance We consider the algebraic abstraction of the roundabout mode of a collision avoidance system analyzed recently by Platzer et al. [46] and earlier by Tomlin et al. [60]. The two airplane collision avoidance system consists of the variables (x_1, x_2) denoting the position of the first aircraft, (y_1, y_2) for the second aircraft, (d_1, d_2) representing the velocity vector for aircraft 1 and (e_1, e_2) for aircraft 2. ω, θ abstract the trigonometric terms. In addition, the parameters a, b, r_1, r_2 are also represented as system variables. The dynamics are modeled by the following differential equations:

$$\begin{array}{llll} x'_1 = d_1 & x'_2 = d_2 & d'_1 = -\omega d_2 & d'_2 = \omega d_1 \\ y'_1 = e_1 & y'_2 = e_2 & e'_1 = -\theta e_2 & e'_2 = \theta e_1 \\ a' = 0 & b' = 0 & r'_1 = 0 & r'_2 = 0 \end{array}$$

A search for transformations of degree 2 yields a closed vector space with 27 basis functions within 0.2 seconds. The basis functions include a, b, r_1, r_2 and all degree two terms involving these. Removing these from the basis, gives us 14 basis functions that yield a transformation to a 14 dimensional affine ODE.

Table 1: Experimental evaluation results on non linear polynomial ODE benchmarks at a glance. Legend: $|V|$ denotes number of system variables + parameters, **Deg.**: max. degree of the system RHS, $|D_0|$: *degree limit for monomials* in the initial basis, **Time**: timing in seconds, $|B^*|$: number of polynomials in the final basis, †: some elements of the basis involving just the parameters were discarded from the count and **dnf**: did not finish in 2hrs or out of memory crash. **S?**: Did the process succeed in discovering an affine ODE abstraction? X indicates failure, whereas ✓ indicates success.

ID	$ V $	Deg.	$ D_0 $	Time	$ B^* $	$ D_0 $	Time	$ B^* $	S?
Brusselator	2	3	3	0.01	0	25	2.8	0	X
Fitz-Nag.	2	3	3	0.01	0	25	2.6	0	X
Vandepol	2	3	3	0.01	0	25	1.9	0	X
Proj-drag	4	2	3	0.02	8	10	9.7	64	✓
Circular	4	2	3	6	0.01	10	10.6	83	✓
Hamiltonian	5 + 1	2	3	0.02	5†	5	1.3	20†	✓
Two-spring	4 + 1	2	3	0.03	2†	5	0.5	6†	✓
Toda-2	7	2	3	0.1	22	5	4.6	82	✓
Toda-3	10	2	3	0.5	38	5	95	169	✓
Toda-5	16	2	3	6	90	5	6373	559	✓
Toda-10	31	2	3	301.5	375	5		dnf	✓
FPUT-3	6 + 1	3	3	0.05	0†	5	3.7	2 †	✓
FPUT-5	10 + 1	3	3	0.4	0	5	231	2	✓
Bio-network	13	2	3	0.07	5	5	4800	20	✓
Roundabout	10 + 4	2	3	1.5	68†	5	890	≥ 600 †	✓

4.2. Discrete Systems

We now describe experimental results on some discrete programs. We used a set of benchmark programs that require non-linear invariants to prove correctness compiled by Enric Carbonell⁴. Our evaluation focuses on a subset of benchmarks that have non-linear assignments or guards in them. The methods presented here converge in a single step with the initial basis whenever the program being considered already has affine updates.

Fermat Factorization. Figure 8 shows a program for finding a factor of a number N near its square root taken from a book by Bressoud [8]. Our analysis initialized with monomials of degree upto 2 over the program variables yields a final basis consisting of 17 polynomials. The resulting affine system is analyzed by a polyhedral analyzer using abstract interpretation to yield invariants. The invariants obtained at the loop head are shown in Figure 8. The equality invariant

$$4r + v^2 - 2v - u^2 + 2u + 4N = 0$$

⁴The benchmark instances are available on-line at http://www.lsi.upc.edu/~erodri/webpage/polynomial_invariants/list.html.

<pre> int fermat(int N, int R) pre (N >= 0 && R >= 0); int u,v,r; u := 2*R -1; v := 1; r := R*R -N; 1: while (r != 0){ 2: while (r > 0) (r,v) := (r-v, v+2); 3: while (r < 0) (r,v) := (r+u, u+2); } end </pre>	$ \begin{aligned} & -4r - v^2 - 4Nv + 2v + u^2 - 2u \leq 0 \wedge \\ & -r - Nu \leq 0 \wedge 1 - v^2 \leq 0 \wedge \\ & 1 - uv \leq 0 \wedge -Rv + R \leq 0 \wedge \\ & 1 - v \leq 0 \wedge 1 - u^2 \leq 0 \wedge \\ & -Ru + 2R^2 + R \leq 0 \wedge -Nu \leq 0 \wedge \\ & 1 - u \leq 0 \wedge -R^2 \leq 0 \wedge -NR \leq 0 \wedge \\ & -R \leq 0 \wedge -N^2 \leq 0 \wedge \\ & v^2 - 2v - u^2 + 2u \leq 0 \wedge \\ & 1 + r - u - R^2 \leq 0 \wedge 1 + 4r - u^2 \leq 0 \wedge \\ & 4r + v^2 - 2v - u^2 + 2u \leq 0 \wedge \\ & 2 + 6r - uv - u^2 - 2R^2 \leq 0 \wedge \\ & 4r + v^2 - 2v - u^2 + 2u + 4N = 0 \end{aligned} $
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Figure 8: Fermat’s algorithm for prime factorization taken from Bressoud [8] and invariants computed at location 1 using polyhedral analysis of the linearization.

is obtained at locations 1, 2 and 3 in the program. This forms a key part of the program’s partial correctness proof.

Product of Numbers: Consider the benchmark shown in Figure 9 that seeks to compute the product of its arguments x, y . Our approach initialized using degree 2 monomials computes an abstract system with 20 basis polynomials that in turn yields an affine transition system with 20 variables. Figure 9 shows the invariants computed using polyhedral abstract interpretation. The invariant $q - abp = 0$ cannot be established by our technique with degree 2 monomials. On the other hand, it can be established by considering degree 3 monomials in the initial basis. The resulting system however has 60 variables, making polyhedral analysis of the system as a whole hard.

Geometric Summation: Consider the geometric summation program in Figure 10. Our approach computes a linearization with 5 variables in the abstract system. Polyhedral analysis of the resulting program yields the invariant $(1 - r)s = a - p$. This invariant together with the invariant $p = ar^k$ (which cannot be obtained through algebraic reasoning) suffices to prove the partial correctness of the program.

5. Conclusion and Future Directions

Thus far, we have presented an approach that uses Change-Of-Bases transformation for inferring abstractions of continuous, discrete and hybrid systems. We have explored the theoretical underpinnings of our approach, its connections to various invariant generation techniques presented earlier. Our previous work presents an extension of the approach presented in this paper to infer differential inequality abstractions [52]. Similar extensions for discrete systems remain unexplored. Furthermore, the use of the abstractions presented here to establish

<pre> int productBR(int x, int y) pre (x >= 0 && y >= 0); int a,b,p,q; (a,b,p,q) := (x,y,1,0); 1: while (a >= 1 && b >= 1){ if (a mod 2 == 0 && b mod 2 == 0) (a,b,p) := (a/2, b/2, 4 * p); elseif (a mod 2 == 1 && b mod 2 == 0) (a,q) := (a-1, q+ b*p); elseif (a mod 2 == 0 && b mod 2 == 1) (b,q) := (b-1, q + a*p); else (a,b,p) := (a-1, b-1, q + (a+b-1)*p); } end </pre>	$ \begin{aligned} &1 - p^2 \leq 0 \wedge -yp + y \leq 0 \wedge \\ &-xp + x \leq 0 \wedge 1 - p \leq 0 \wedge \\ &-1 - b \leq 0 \wedge -1 - a \leq 0 \wedge \\ &-y \leq 0 \wedge -x \leq 0 \wedge \\ &2ap - xp - 2a + x \leq 0 \wedge \\ &7ap - xp - 7a - 14x \leq 0 \wedge \\ &7ap - xp + 8a - 14x \leq 0 \wedge \\ &16ap - 3xp - 16a - 12x \leq 0 \wedge \\ &2bp - yp - 2b + y \leq 0 \wedge \\ &7bp - yp - 7b - 14y \leq 0 \wedge \\ &7bp - yp + 8b - 14y \leq 0 \wedge \\ &16bp - 3yp - 16b - 12y \leq 0 \end{aligned} $
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Figure 9: A multiplication algorithm and loop invariant computed using polyhedral analysis on the linearization.

<pre> int geoSum(int a, int r, int n) int s := 0; int p := a; int k := 0; while (k < n) s := s + p; p := p * r; k := k + 1; end </pre>	$ \begin{aligned} &-k^2 + k \leq 0 \wedge -2 - k^2 + 3k \leq 0 \wedge \\ &-6 - k^2 + 5k \leq 0 \wedge -9 - k^2 + 6k \leq 0 \wedge \\ &-k \leq 0 \wedge -r^2 \leq 0 \wedge -n \leq 0 \wedge \\ &-1 + k - n \leq 0 \wedge -p + s - rs + a = 0 \end{aligned} $
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Figure 10: Geometric summation program and computed loop invariant.

termination for transition systems is also a promising line of future research. Future research will also focus on the use of Lie symmetries to reduce the size of the ansatz or templates used in the search for conserved quantities and CoB transformations [24].

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Table 2: Timings for computing abstractions of discrete systems and analyzing the resulting abstractions. Legend: $|\mathbf{V}|$ denotes number of system variables, **Trs**: number of transitions, **Deg.**: max. degree of the RHS, $|\mathbf{D}_0|$ degree limit for monomials in the initial basis, **Time**: timing in seconds, $|\mathbf{B}^*|$: number of elements in the final basis, **#I**: invariants computed and **DNF**: did not finish in 2hrs or out of memory crash.

System				Linearization			Analysis	
ID	#V	#Trs	Deg	$ \mathbf{D}_0 $	$ \mathbf{B}^* $	Time	Time	#I
Petter2	2	1	2	2	3	0.02	≤ 0.01	10
Petter3	2	1	2	3	1	0.02	≤ 0.01	2
Petter3	2	1	3	3	4	0.02	≤ 0.01	25
Geo	6	2	2	2	6	0.02	≤ 0.01	9
Fermat	5	6	2	2	17	0.04	0.5	26
Prodrbr	7	5	2	2	20	0.06	2.0	19
Euclidex1	11	5	2	2	51	0.66	DNF	

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