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Data-driven Reachability of Non-linear Systems via Optimization of Chen-Fliess Series

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Abstract

A reachable set is the set of all possible states produced by applying a set of inputs, initial states, and parameters. The fundamental problem of reachability is checking if a set of states is reached provided a set of inputs, initial states, and parameters, typically, in a finite time. In the engineering field, reachability analysis is used to test the guarantees of the operation's safety of a system. In the present work, the reachability analysis of nonlinear control affine systems is studied by means of the Chen-Fliess series. Different perspectives for addressing the reachability problem, such as interval arithmetic, mixed-monotonicity, and optimization, are used in this dissertation. The first two provide, in general, an overestimation of the reachable set that is not guaranteed to be the smallest. To improve these methods and obtain the minimum bounding box of the reachable set, the derivative-based optimization of Chen-Fliess series is developed. To achieve this, the closed form of the Gâteaux and Fréchet derivatives of Chen-Fliess series and several other tools from analysis are obtained. To provide a representation of these tools practically and systematically, an abstract algebraic derivative acting on words of a monoid is defined. Three nonconvex optimization algorithms are implemented for Chen-Fliess series. The problem of computing an inner approximation of the reachable set via Chen-Fliess series is also solved by means of convex analysis tools. Furthermore, a method for the computation of the backward reachable set of an output set is also provided. In this case, different from forward reachability analysis, the feasibility problem represents a challenge and requires using the Positivestellensatz. Examples and simulations are provided for every method presented. The application of control barrier functions via Chen-Fliess series is outlined. Finally, the future work and conclusions are stated in the last chapter.

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Chapter 1

Introduction

1.1 Motivation

As technology and industry advance, systems become more complex and aspects such as stability, controllability, liveness, and safety become more difficult to analyze. In many situations, for the correct operation of the system, the output is only allowed to lie in a certain region of the output space called *safety region*. A way to verify the compliance of these operating constraints is by computing the output generated by the inputs and checking if the set lies inside the safety region. In another scenario, the unsafety outputs are known and the set of inputs that generated them need to be identified. For example, in civilian air traffic control [66, 67], the aircraft have to keep a safe distance from each other to avoid accidents. With the distance known, the pilots adjust the inputs such as the acceleration and the angle of the steering wheel to remain in the safety region. An example regarding the energy field is the safe operation of a power system [36]. In [69], the dynamics of Type-4 wind turbines are analyzed to the electric disturbances that occur between a wind power plant and an electric grid. For this, the set of all currents and voltages output of the turbines are computed and checked whether or not lie in the safe region to guarantee the stability of the electric grid.

The set of outputs of a control system as a response to a set of inputs and initial conditions is called a *reachable set*, and the study of them is called *reachability analysis* which has its origins in model-checking and system verification in which the goal is to provide a systematic way of verifying if the reachable set or the input set is contained in a particular safety or unsafety set instead of simulating each possible outcome. In general, and for the type of systems considered in this manuscript, input and initial condition sets with infinite elements generate a set of infinite outcomes. This work is concerned with three categories of reachability analysis. In *forward reachability*, the focus is on the reachable set at a fixed time, while in *backward reachability* is on the input set at a fixed time. In *tube reachability*, the verification must be satisfied for a given time horizon.

Computing the actual reachable set has been proved undecidable even for simple cases like linear systems with inputs constrained to affine subspaces [23], and some methods such as the ones that rely on the Minkowski sum of polyhedra easily become burdensome for high-dimensional systems. Because of this, alternatives to the reachable set are preferred to compute, such as *overapproximations*, which are bigger sets that contain the reachable set, but they are easier to compute. For the same reason, underapproximations are also used. A particular overapproximating set is a box, also known as a bounding box. In particular, it is preferred to have the smallest bounding box called *minimum bounding box* (MBB) as it provides the most accurate box representation of the reachable set. In the literature, there are ways to compute overapproximations of the reachable set of a control system for a given set of inputs and initial conditions when the output is equal to the state. For linear systems having zonotopes as initial conditions and the input sets, the Minkowski sum provides a method to compute their overapproximating set [3]. This extends naturally to non-linear systems by linearizing the dynamics. A second approach for non-linear systems is mixed-monotonicity (MM), which makes use of an auxiliary dynamical system and the preservation of a partial order to obtain a bounding box of the reachable set [15, 74]. A third approach computes the reachable set by interpreting the non-linear system with disturbances as a differential game whose solution leads to the Hamilton-Jacobi-Bellman equation [26, 48]. The Koopman operator provides another method of linearization of systems used to obtain an overapproximation of the reachable set of polynomial systems [65]. Finally, neural networks combined with mixed-monotonicity are also employed to compute overapproximations of the reachable set [72].

1.2 Problem Description

This manuscript deals with the computation of reachable sets of non-linear control affine systems using Chen-Fliess series. Figure 1.1 shows an input-output representation of a system where a set of inputs enter the system and produce a set of outputs. In the literature, a set of states and parameters also enter the system but in the present work, only a set of inputs is considered. In reachability analysis, the goal is to compute the actual reachable set but in many cases, this is computationally expensive and an overestimation is preferred as long as it is faster computationally.

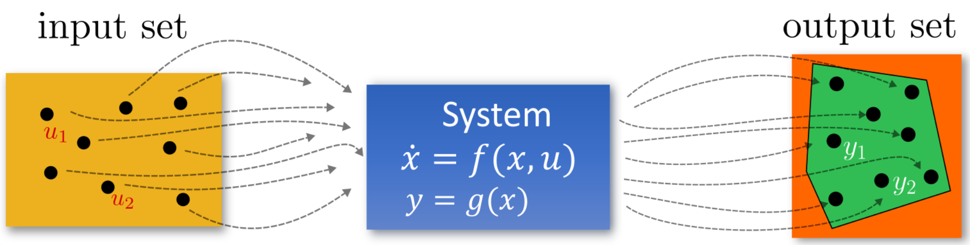


Figure 1.1: Reachable Set (green) and Overestimation (orange).

The computation of two types of reachable sets is addressed in this work: the forward and backward reachable. The use of them depends on the particular application. If the output of the system is compact, the minimum bounding box can be written in terms of two corners of the box. These two corners are formed by the maxima and the minima of the coordinates. Since the output is represented by the Chen-Fliess series, the problem translates into the problem of optimization of Chen-Fliess series as shown in (1.1) where $\mathcal{U}$ is a box. Figure 1.2 explains this idea.

$$\min_{u \in \mathcal{U}} F_c[u](t), \tag{1.1}$$

The backward reachable set of an output set at a fixed time is the set of input functions such that when they are applied to the system, all outputs lie inside the assumed output set. Equation (1.2) describes the optimization problem.

$$\begin{aligned} \min_{u \in B} \quad & u_i \\ \text{s.t.} \quad & F_c[u](t) \in \mathcal{U}. \end{aligned} \tag{1.2}$$

Assuming constant inputs, both (1.1) and (1.2) are non-convex optimization problems. The feasibility of the backward-reachability problem is non-trivial and its anal-

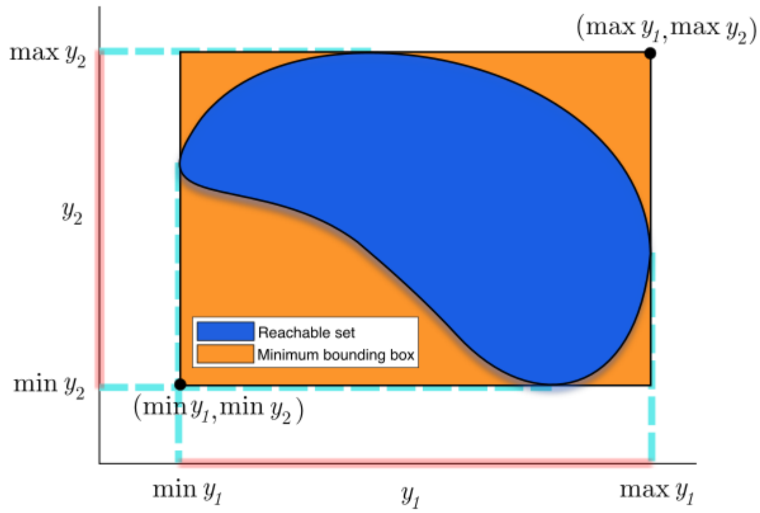


Figure 1.2: The graph shows the output reachable set of a non-linear affine system and its minimum bounding box (MBB).

ysis uses the Positivestellensatz.

1.3 Literature Review

1.3.1 Reachability Analysis

In the current section, three main techniques of reachability analysis are described. These are the Hamilton-Jacobi, mixed-monotonicity, and set-based methods.

1.3.1.1 Hamilton-Jacobi

This method analyzes the reachability of general non-linear systems (not necessarily control affine) and hybrid systems with inputs and disturbances. Consider the problem of computing the backward reachable set of a target set. In this case, the problem is modeled as a differential game [34]. The use of game theory in control theory can be traced back to [42]. The game is a *game of kind* for which the goal is to reach the target set at the determined time. Player 1 is the controller, and Player 2 is the disturbance. The goal is Boolean and described as an indicator function of the target region [63]. This is transformed into a *game of degree* by using the level set method [45]. The backward reachable set is given by the solution of the game by dynamical programming which is obtained from the Hamilton-Jacobi-Isaacs PDE as formulated originally in [66, 67] to address the problem of air traffic management. The problem of computing the forward reachable set is performed in a similar manner but with a change in the direction of the time variable, and the reachable tube is computed by first minimizing the objective function over the time horizon.

In [7], the authors provide a big picture of the method, and in [12] an updated review is given. According to [12], the computation of the reachable set by the Hamilton-Jacobi method is intractable for systems of dimension 5 or higher with exponential complexity. A way to overcome this drawback is to decouple the system into self-contained subsystems that are possibly coupled through common states, controls, and disturbances. Then, compute the reachable set of the subsystems and recombine them to construct the whole system. Other types of decompositions are proposed in the literature [13, 37, 38, 46].

Currently, there are two main toolboxes for reachability analysis. The Level Set Toolbox (toolboxLS) [47] in MATLAB solves PDEs with the level set method and the Berkeley Efficiency API in C++ for Level Set methods (BEACLS), which is designed for fast computation.

1.3.1.2 Mixed-Monotonicity

This method has its roots in monotone dynamical systems [62] which are systems whose flow preserves the partial order of the state space. The property is characterized in terms of the partial derivatives of the vector field. The most important aspect of this type of systems is that most solutions converge to the equilibrium [39]. This definition was extended to control systems in [2].

A mixed-monotone system is decomposed into a non-increasing and a non-decreasing part [28]. In [14], a characterization of this property is given in terms of the monotonicity of the vector field and this is bounded by the decomposition function to obtain an overestimation of the one-step reachable set. In [74], a relationship between the definitions of mixed-monotonicity was provided and new criteria was given to prove that a system is mixed-monotone in terms of the bounded variation of the vector field. A decomposition is tight among all the decompositions if it provides the smallest representation of the system. A tight decomposition for discrete systems was given in [73] and for continuous systems in [15] where the reachable set is overapproximated by the dynamics of the *embedding system*. This associated system is written in terms of the decomposition function and its realization provides the northeast and southwest points of the overapproximating box.

1.3.1.3 Set-based Methods

Another important tool to perform reachability is set-based methods. Different types of sets have different advantages in the computation of reachable sets. Examples of these sets are boxes, intervals, polytopes, ellipsoids and zonotopes. In [3] reachable sets are computed for linear systems using set-based methods. Also, the complexity of the operations for specific sets depends on their representation. For example, the hyperplane representation of a polytope requires a different amount of real numbers to represent than its vertex representation. An important operation for set-based reachability analysis is the Minkowski sum which is computationally expensive for polytopes [5]. Because of the good scalability of the state space models and cheap computation, zonotopes are preferred [27].

A way to overapproximate reachable sets is by using support functions [24,32,43]. Given a compact convex set, a finite number of vectors and their associated support functions are only necessary to provide the overapproximation. In the case of linear systems, if the set of inputs is closed and convex, then the corresponding reachable set also preserves these properties. Thus, reachable sets of non-linear systems can be computed by linearizing the system and using the Taylor polynomial along with set operations. In the literature, TIRA [44] and CORA [4] are two of the most popular toolboxes used to compute reachable sets with a set-based approach. The first is based on intervals, and the second on zonotopes, polytopes, and intervals.

1.3.2 Chen-Fliess Series

A Chen-Fliess series is a weighted sum of iterated integrals whose coefficients belong to a real coordinate domain. An iterated integral of a vector function at a particular time is defined recursively as the nested integral of the first coordinate function times the integral of the remaining coordinate functions. Because of this combinatoric nature, the Chen-Fliess series is indexed by words from formal languages. The mathematical structure that defines these words and their rules of formation is called a *monoid*.

A Chen-Fliess series provides an input-output representation of nonlinear affine control systems under certain conditions [21, 22, 35]. Applications of this methodology include data-driven identification [68], interconnected systems representation [31], and control [18]. Although the behavior of a Chen-Fliess series is intrinsically local, its advantage lies in that under a proper setup, its coefficients are learned online. That is, the Chen-Fliess series does not necessarily rely on a state-space model representation of the system [68]. This is useful since systems in the engineering field are, each time, more complex and challenging to represent. A more detailed account of the concepts associated with Chen-Fliess series are provided in [29]. In the present manuscript, Chen-Fliess series are used to present another methodology to compute overestimations of reachable sets of non-linear control affine systems.

1.4 Contribution

In Chapter 3, interval arithmetics is used to compute the overestimation of the output reachable sets of nonlinear control affine systems represented by the input-output Chen-Fliess formalism and whose inputs lie in a box. Specifically, this box is the cartesian product of an interval with itself as many times as the dimension of the input vector function. To obtain the overestimation of the output reachable set, first, the arithmetic product of intervals is defined and the closed form of an arbitrary power of an interval is obtained. Then, the closed form of the overestimation of the output reachable set of a single iterative integral is calculated. The relationship between the output reachable set of an iterative integral and its associated state-space representation is described. Next, all the overestimating boxes of the output reachable set corresponding to the iterative integrals associated with a Chen-Fliess series are added up to obtain the overestimating box of the output reachable set. Simulations and an example in which this straightforward methodology computes the actual reachable set and not an overestimation are provided.

In Chapter 4, the notion of mixed-monotonicity (MM) of systems whose outputs are described by a Chen-Fliess series is extended introducing the notion of input-output mixed-monotonicity (IOMM). In the state-space version, this definition relies on a decomposition function of the vector field that is defined in an extended domain and has monotone characteristics. In the input-output case, a way of obtaining this function is by expressing the Chen-Fliess series of a sum of two input functions in terms of the sum of two series. A partial order is defined to provide the monotone behavior of the new decomposition function. It is shown that any convergent Chen-Fliess series is input-output mixed-monotone. Next, the overestimating box is obtained using the decomposition function on each orthant of the input domain. Examples and simulations are provided.

In Chapter 5, the minimum bounding box of output reachable sets of systems represented by Chen-Fliess series is calculated by performing first-order optimization of Chen-Fliess series. For this, the closed form of the Fréchet and Gâteaux derivatives and the gradient are obtained. A proof of the mean value theorem by algebraic means is given. Specifically, the closed form of the derivative of the sum of two inputs is used instead of the proof from the books by the chain rule. The gradient descent algorithm is implemented for Chen-Fliess series, allowing the optimization and computation of the minimum bounding box. Examples and numerical simulations are provided.

In Chapter 6, three contributions are presented. First, the concept of differential languages is introduced. This is inspired by *differential fields* in [16] with the purpose of making the derivatives of Chen-Fliess series easy to represent. Second, the second-order Gâteaux derivative of a Chen-Fliess series is used to provide a finer approximation by its Taylor series. The closed form of the Hessian is obtained and differs slightly from the one for real functions on real coordinate domains. The second-order optimality conditions follow naturally from this. The third contribution consists of using the Hessian along with the Newton algorithm to optimize a Chen-Fliess series to obtain the minimum bounding box of the output reachable set. Then the trust region optimization algorithm is used to overcome the ill-posed cases. Examples and simulations are provided showing the efficiency of the trust regions method on Chen-Fliess series. The examples and simulations are presented in Chapter 7.

In Chapter 8, a discussion on the backward reachable set of an output set is presented. The goal is to describe two possible approaches to output backward reachability. Then assuming the convexity of the output set, an inner approximation of the output reachable set is obtained. Both problems are expressed and solved as optimization problems.

As a summary, a list of the contributions is given:

1. Different approaches for the computation of the forward reachable set using Chen-Fliess series:
   - Interval arithmetics: appears in [56].
   - Gradient descent: appears in [54].
   - Newton: appears in [55].
   - Trust regions: appears in [58].
2. Inner and backward reachable set using Chen-Fliess series: appears in [59].

3. Chen-Fliess calculus:

    - Gâteaux derivative: the closed-form is obtained and proved in [54].
    - Fréchet derivative: the closed-form is obtained and proved in the Transactions on System and Control Letters Journal [57].
    - Hessian: the closed-form is obtained in [55].
    - Differential monoids: introduced in [55].

Chapter 2

Preliminaries

In this section, Chen-Flies series are presented as a tool that provides an input-output representation of a type of nonlinear systems. Its definition is given in terms of iterated integrals indexed by words. Because of this, concepts of formal language theory such as words and formal power series along with the results that guarantee the Chen-Fliess series's convergence to the system's output are presented. Then, the theory of mixed-monotonicity is presented as a tool to approximate the set of outputs of a system as a result of a set of inputs and initial conditions acting on the system. This approximation is given in terms of an embedded system whose trajectory preserves certain partial order with respect to the inputs and initial conditions of the original system.

2.1 Formal Languages

Formal languages have applications in many fields such as the automata, programming languages, linguistic and logic fields. The objective of this section is to introduce the *monoid* structure, which describes what a word from an alphabet is. In the literature, Chen-Fliess series are represented by means of formal languages. In the present work, these concepts are also used to represent the differential tools of Chen-Fliess series. In principle, formal languages help index series of iterative integrals in a much more informative manner than just enumerating the elements of the series with the naturals, for example. This is mainly because of the structure of the iterative integral. This is will be clear when the Chen-Fliess series is defined. The first concept of formal language is the alphabet.

Definition 1 *An alphabet is a finite set of symbols, and its elements are called letters.*

In this manuscript, by convention, the alphabet is denoted $X = \{x_0, x_1, \cdots, x_m\}$ for an $m \in \mathbb{N}$. With an alphabet, one can form words.

Definition 2 *A word over an alphabet is a finite string of zero or more letters. The word consisting of zero letters is called the empty word.*

In general, a word over X has the form $\eta = x_{i_k} \cdots x_{i_1}$. Naturally, two words are the same if they have the same number of non-empty letters and all their letters are the same, this is, $\eta = x_{i_1} \cdots x_{i_r}$ and $\nu = x_{j_1} \cdots x_{j_s}$ are such that $\eta = \nu$ if and only if $r = s$ and $x_{i_k} = x_{j_k}$ for $k \in \{1, \cdots, r\}$. A useful characteristic of a word is its length.

Definition 3 *Consider the alphabet $X = \{x_0, \cdots, x_m\}$ for an $m \in \mathbb{N}$. The length of the word $|\cdot|$ is equal to the number of letters that compose the word. For the word $\eta = x_{i_1} \cdots x_{i_k}$, the length is $|\eta| = k$.*

The number of times the letter x_i appears in the word η is denoted $|\eta|_{x_i}$, the empty word is denoted $\emptyset$ and has zero length $|\emptyset| = 0$. The symbol X^k denotes the set of all words of length k, X^* is the set of words of any length, and X^+ denotes the set of all words with positive length.

Definition 4 *Any subset of X^* is called language.*

To formalize the formation of words, the concatenation operation on words is defined. This operation is associative, noncommutative, and the empty word works as the neutral element.

Definition 5 *The concatenation product on X^* is the associative mapping $\mathcal{C} : X^* \times X^* \to X^*$*

$$(\eta, \xi) \mapsto \eta\xi$$

The successive concatenation of a word is denoted as the power of the word $\eta^k = \eta \cdots \eta$ where η appears k times. With all the previous definitions, the following structure can be establish.

Definition 6 *A free monoid refers to triplet $(X^*, \mathcal{C}, \emptyset)$.*

In the present section, the concept of monoid was introduced. This set the foundations for studying real functions from a monoid which can also be represented as series.

2.2 Formal Power Series

In the previous section concepts from formal language were given. In the present section, those concepts are used to define formal power series.

Definition 7 *Consider the alphabet X, a formal power series c is a function that maps the set of all words to a real coordinate domain $c : X^* \to \mathbb{R}^\ell$. Denoting the image of the function c as (c, η), the function is represented as the formal sum*

$$c = \sum_{\eta \in X^*} (c, \eta)\eta$$

If the coefficients of a power series c lie in a real coordinate domain with dimension $\ell \geq 1$, the power series of the coordinates are called the component series of $c \in \mathbb{R}^\ell\langle\langle X \rangle\rangle$ and are denoted

$$c_i = \sum_{\eta \in X^*} (c, \eta)_i \eta,$$

where the i-th coordinate of $(c, \eta) \in \mathbb{R}^\ell$ is denoted $(c, \eta)_i$. The set of all formal power series over the alphabet X is denoted $\mathbb{R}^\ell\langle\langle X \rangle\rangle$. The next definition helps define a particular class of formal power series. The set of words in the series with associated non-zero coefficients is called the support of the power series.

Definition 8 *The support of a power series c is the set of words whose image under c is non-zero. This is,*

$$\text{supp}(c) := \{\eta \in X^* : (c, \eta) \neq 0\}.$$

A formal power series c with finite support is called a *polynomial* and the set of all polynomials is denoted $\mathbb{R}^\ell\langle X \rangle$. A couple of characteristics of a power series are its order and degree defined next.

Definition 9 *The order of a power series c is the smallest length of its words. This* *is,*

$$ord(c) = \begin{cases} \min\{|\eta| : \eta \in \operatorname{supp}(c)\} & , c \neq 0, \\ \infty & , c = 0 \end{cases}$$

A proper series c is such that $\operatorname{ord}(c) > 0$.

Definition 10 *The degree of a polynomial is given by the biggest length of the word*

$$\deg(p) = \begin{cases} \max\{|\eta| : \eta \in \operatorname{supp}(p)\} & , p \neq 0 \\ -\infty & , p = 0 \end{cases}$$

Finally, another important concept used in the definition of a differential monoid, introduced in this dissertation, as seen later, is given next.

Definition 11 *Consider the language $L \subset X^*$. The characteristic series $char(L)$ of L is equal to the formal sum of its elements. This is,*

$$char(L) = \sum_{\nu \in L} \nu.$$

As seen in the following sections, a Chen-Fliess series is associated to a formal power series. In the present section, formal power series were defined among other concepts that describe them. Next, an important set and operation for the whole present work is addressed.

2.3 The Shuffle Set and Product

In this section, useful tools on monoid are presented. These are the shuffle set and product. These objects possess, intrinsically, a combinatorial nature. The shuffle set is the set of all possible ways two words can be shuffled. In the same way as shuffling a deck of cards, but instead of having two parts of the deck, one has two words. The second concept is the shuffle product of two words and provides a polynomial whose monomials are the outcomes of the shuffle. Both definitions are extended to formal power series, and the product makes $\mathbb{R}\langle\langle X\rangle\rangle$ an algebra and an integral domain.

Definition 12 *The shuffle of two words $\eta, \xi \in X^*$ is defined to be the language*

$$\mathbb{S}_{\eta,\xi} = \{\nu \in X^* : \nu = \eta_1\xi_1\eta_2\xi_2\cdots\eta_n\xi_n,\ \eta_i, \xi_i \in X^*,$$
$$\eta = \eta_1\eta_2\cdots\eta_n,\ \xi = \xi_1\xi_2\cdots\xi_n,\ n \geq 1\}.$$

In particular, $\mathbb{S}_{\eta,\emptyset} = \{\eta\}$ and $\mathbb{S}_{\emptyset,\xi} = \{\xi\}$. Notice that this is a set, and as a set, all elements appear only once. For example, consider the language $X = \{x\}$, then $\mathbb{S}_{x,x} = \{x^2\}$.

Definition 13 *The shuffle product of two words is*

$$(x_i\eta) \sqcup\!\sqcup (x_j\xi) = x_i(\eta \sqcup\!\sqcup (x_j\xi)) + x_j((x_i\eta) \sqcup\!\sqcup \xi)$$

where $x_i, x_j \in X$, $\eta, \xi \in X^*$ and with $\eta \sqcup\!\sqcup \emptyset = \emptyset \sqcup\!\sqcup \eta = \eta$.

It is easy to notice that the shuffle product and the shuffle set are related through the support function by the identity $\mathbb{S}_{\eta,\xi} = \mathrm{supp}(\eta \sqcup\!\sqcup \xi)$.

Given the set of all words of length n with a fixed number of letters in the alphabet, this is, $L = \{\eta \in X^n \text{ s.t. } |\eta|_{x_0} = n_0, \ldots, |\eta|_{x_m} = n_m\}$, a helpful way to represent its characteristic polynomial is by means of the shuffle product as

$$\text{char}(L) = x_0^{n_0} ⧢ \cdots ⧢ x_n^{n_m}, \tag{2.1}$$

Moreover,

$$\text{char}(X^n) = \sum_{n_0+\cdots+n_m=n} x_0^{n_0} ⧢ \cdots ⧢ x_n^{n_m}.$$

It is seen later that there is an important relationship between the shuffle product and the product of iterated integrals. In the next section, Chen-Fliess series are presented.

2.4 Chen-Fliess Series

The purpose of the current section is to introduce the concept of Chen-Fliess series. These are weighted sums of iterated integrals. First, the domain of the input functions is specified. Then, the definitions are given along with Fliess' representation theorem of nonlinear control affine systems.

Consider $\mathfrak{p} \in \mathbb{N}$ such that $\mathfrak{p} \geq 1$ and $t_0, t_1 \in \mathbb{R}$ such that $t_0 < t_1$. The input vector functions $u : [t_0, t_1] \to \mathbb{R}^m$, where $u(t) = (u_1(t), \cdots, u_m(t))$, considered in this section are Lebesgue measurable. The norm in this input space is $\|u\|_{\mathfrak{p}} = \max\{\|u_i\|_{\mathfrak{p}} : 1 \leq i \leq m\}$, where $\|u_i\|_{\mathfrak{p}}$ is the usual $L_{\mathfrak{p}}$-norm of the measurable real-valued coordinate function, u_i, defined on $[t_0, t_1]$. Let $L_{\mathfrak{p}}^m[t_0, t_1]$ denote the set of all measurable functions defined on $[t_0, t_1]$ having a finite $\|\cdot\|_{\mathfrak{p}}$ norm and define the closed ball of radius R as the set $B_{\mathfrak{p}}^m(R)[t_0, t_1] := \{u \in L_{\mathfrak{p}}^m[t_0, t_1] : \|u\|_{\mathfrak{p}} \leq R\}$. Denote $C[t_0, t_1]$ as the subset of continuous functions in $L_1^m[t_0, t_1]$.

Definition 14 *An iterated integral is defined inductively for each word $\eta = x_i\bar{\eta} \in X^*$ as the map $E_\eta : L_1^m[t_0, t_1] \to C[t_0, t_1]$ by setting $E_\emptyset[u] = 1$ and letting*

$$E_{x_i\bar{\eta}}[u](t, t_0) = \int_{t_0}^{t} u_i(\tau) E_{\bar{\eta}}[u](\tau, t_0)\, d\tau, \tag{2.2}$$

where $x_i \in X$, $\bar{\eta} \in X^*$, and $u_0 = 1$.

Definition 15 *[21, 22]A Chen-Fliess series, is a causal m-input, ℓ-output operator, F_c, associated with a formal power series $c \in \mathbb{R}^\ell\langle\langle X\rangle\rangle$ such that*

$$y(t) = F_c[u](t) = \sum_{\eta \in X^*} (c, \eta)\, E_\eta[u](t, t_0).s \tag{2.3}$$

It is assumed hereafter without loss of generality that $t_0 = 0$, which allows denoting $E_\eta[u](t, t_0)$ as $E_\eta[u](t)$. Consider $|z| := \max_i |z_i|$ when $z \in \mathbb{R}^\ell$.

Definition 16 *A Chen-Fliess series is locally convergent if there exists $K, M \geq 0$ reals such that*

$$|(c, \eta)| \leq K M^{|\eta|}\, |\eta|!, \quad \forall \eta \in X^*.$$

The set of all locally convergent series is denoted $\mathbb{R}^\ell_{LC}\langle\langle X\rangle\rangle$.

In this case (2.3) converges absolutely and uniformly for sufficiently small $R, T > 0$ and is a well defined mapping from $B_{\mathfrak{p}}^m(R)[t_0,\ t_0 + T]$ into $B_{\mathfrak{q}}^\ell(S)[t_0,\ t_0 + T]$, where the numbers $\mathfrak{p}, \mathfrak{q} \in [1, +\infty]$ are conjugate exponents, i.e., $1/\mathfrak{p} + 1/\mathfrak{q} = 1$ [30].

Definition 17 *A Chen-Fliess series is globally convergent if there exists $K, M \geq 0$ reals such that*

$$|(c, \eta)| \leq KM^{|\eta|}, \ \ \forall \eta \in X^*.$$

The set of all globally convergent series is denoted $\mathbb{R}^{\ell}_{GC}\langle\langle X\rangle\rangle$.

In this case, (2.3) converges on the extended space $L^m_{\mathfrak{p},e}(t_0)$ into $C[t_0, \infty)$, where $L^m_{\mathfrak{p},e}(t_0) := \bigcup_{T>0} L^m_{\mathfrak{p}}[t_0, t_0 + T]$. Thus, (2.3) is well-defined for all times. A deeper discussion of the convergence of Chen-Fliess series is presented in [70].

Definition 18 *Given a locally convergent Chen-Fliess series F_c defined on $B^m_{\mathfrak{p}}(R)[t_0, t_0 + T]$ and having finite Lie Hankel rank. The series F_c is realizable by a system of the form*

$$\dot{z}(t) = g_0(z(t)) + \sum_{i=1}^{m} g_i(z(t))\, u_i(t), \ \ z(t_0) = z_0, \tag{2.4a}$$

$$y_j(t) = h_j(z(t)), \ \ j = 1, 2, \ldots, \ell, \tag{2.4b}$$

if $y_j(t) = F_{c_j}[u](t) = h_j(z(t))$, $t \in [t_0, t_0 + T]$, $j = 1, 2, \ldots, \ell$ where each g_i is analytic on some neighborhood $\mathcal{W}$ of $z_0 \in \mathbb{R}^n$, and each h_j is an analytic function on $\mathcal{W}$ such that (2.4a) has a well defined solution $z(t)$, $t \in [t_0, t_0 + T]$ for any given input $u \in B^m_{\mathfrak{p}}(R)[t_0, t_0 + T]$.

Theorem 1 *[61, 64] Given a realizable Chen-Fliess series F_c of the system in (2.4), then for any $\eta = x_{i_k} \cdots x_{i_1} \in X^*$ the coefficients of the corresponding Chen-Fliess* *series can be written as*

$$(c_j, \eta) = L_{g_\eta} h_j(z_0) := L_{g_{i_1}} \cdots L_{g_{i_k}} h_j(z_0), \tag{2.5}$$

where $L_{g_i} h_j$ *is the* Lie derivative *of* h_j *with respect to* g_i *[21, 35, 50].*

In [68], it is shown that a Chen-Fliess series can be defined independently of a state space model and thus can be used for data-driven analysis and control.

Definition 19 *The Chen series of the input vector* $u \in B_{\mathfrak{p}}(R)[0, t]$ *refers to the following object*

$$P[u](t) = \sum_{\eta \in X^*} E_\eta[u](t)\eta$$

It is also known [21, 29] that the Chen-Fliess series can be written as

$$F_c[u](t) = (c, P[u](t)) = \left(\sum_{\eta \in X^*} (c, \eta)\eta, \sum_{\eta \in X^*} E_\eta[u](t)\eta \right). \tag{2.6}$$

The following is an important result linking the shuffle product and the iterated integral.

Lemma 1 *For any* $\eta, \xi \in X^*$

$$E_\eta[u](t) E_\xi[u](t) = E_{\eta \sqcup\!\sqcup \xi}[u](t).$$

2.5 Convex Analysis

In the current section, basic concepts of convex analysis are presented. The goal is to provide the tools to understand that a compact and convex set in a real coordinate domain can be described in terms of the half-spaces of all its support hyperplanes. The convexity of functions is desirable in optimization problems since, in this case, a local optimum is, in fact, the global optimum. In the present dissertation, Chen-Fliess series are optimized, and even when restricting the input vector function to a constant vector, the Chen-Fliess series is not a convex function, in general. This is the reason the focus of this section is on convex sets and not on functions. The second reason is that, later, the inner approximation of a set is obtained via Chen-Fliess series for convex sets. The content is based on [11, 33].

Definition 20 *A set* $S \subset \mathbb{R}^n$ *is convex if for all* $x, y \in S$, $\alpha x + (1-\alpha)y \in S$ *for* $\alpha \in [0,1]$.

Definition 21 *A convex combination of elements* $x_1, \cdots, x_k$ *in* $\mathbb{R}^n$ *is an element of the form*

$$\sum_{i=1}^{k} \alpha_i x_i \quad \textit{where} \quad \sum_{i=1}^{k} \alpha_i = 1 \quad \textit{and} \quad \alpha_i \geq 0 \quad \textit{for} \quad i = 1, \cdots, k.$$

A way to generate convex sets is by taking the convex combinations of the elements of a set. This is the convex hull of a set, which, alternatively, can be defined as follows

Definition 22 *Consider a nonempty set* $C \subset \mathbb{R}^n$. *The convex hull* $\operatorname{co} C$ *is the intersection of all convex sets containing* C.

The following fundamental result characterizes the elements of the convex hull of a set in terms of the original set.

Theorem 2 (C. Caratheodory) *Any* $x \in co\ S \subset \mathbb{R}^n$ *can be represented as a convex combination of* $n+1$ *elements of* S*.*

The extreme points of a set are the ones that cannot be written in terms of the convex combination of two other points. An alternative definition is given next.

Definition 23 *Consider* $C \subset \mathbb{R}^n$ *convex. An element* $x \in C$ *is an extreme point of* C *if* $C \setminus \{x\}$ *is convex.*

Another fundamental result states that knowing the extreme points of a certain set is enough to reconstruct the original set exactly.

Theorem 3 (H. Minkowski) *Consider* $C \subset \mathbb{R}^n$ *compact and convex, then* $C = co(ext\ C)$*.*

The next tool is used later to provide a description of a convex set.

Definition 24 *An affine hyperplane* $H_{s,r}$ *supports the set* C *when* C *is entirely contained in one of the two closed half-spaces determined by* $H_{s,r}$*. This is,*

$$s \cdot y \leq r, \text{ for all } y \in C.$$

the hyperplane supports C *at* $x \in C$ *if, additionally,* $x \in H_{s,r}$ *which means that* $s \cdot x = r$*.*

The following result is known as the supporting hyperplane theorem.

Theorem 4 *Consider the convex set* $S \subset \mathbb{R}^n$*, and* $x \in \partial C$*, there exists a hyperplane supporting* C *at* x*.*

The next definitions appear in [32, 43] and are used to characterize the inner-approximation of the a of sets.

Definition 25 *The support function of a compact convex set* $A \subset \mathbb{R}^n$ *is the function is defined as* $\sigma_A : \mathbb{R}^n \to \mathbb{R}$

$$\sigma_A(v) = \max_{x \in A} x \cdot v.$$

Definition 26 *The support vectors of a compact convex set* $A \subset \mathbb{R}^n$ *are defined as*

$$\nu_A(v) = \arg\max_{x \in A} x \cdot v.$$

The supporting hyperplane theorem represents a convex set in terms of the half-spaces. This is called the dual representation of a convex set. In general, the supporting hyperplanes for this representation are not finite. If only a finite amount of these hyperplanes are taken, then an overestimation of the set is provided.

2.6 Mixed-Monotonicity of State Space Models

In section 1.3, mixed-monotonicity was briefly explained. In the current section, a more detailed account is provided. First, a partial order is specified, then the decomposition function of a vector field is defined, and with this a system associated with the original dynamics is used to compute an overestimation of a reachable set.

Definition 27 *A partial order is a relation that satisfies the properties of reflexivity, transitivity, and antisymmetry.*

A natural partial order is provided next.

Definition 28 *Let $\leq$ be the componentwise partial order on $\mathbb{R}^n$. This is, for $x = (x_1, \cdots, x_n)$ and $y = (y_1, \cdots, y_n) \in \mathbb{R}^n$, $x \leq y$ if and only if $x_i \leq y_i$ for $i \in \{1, \cdots, n\}$.*

Consider the vectors $x, \hat{x}, y, \hat{y} \in \mathbb{R}^n$ and the concatenated vectors $(x, \hat{x})$ and $(y, \hat{y})$ in $\mathbb{R}^{2n}$.

Definition 29 *The southeast (SE) partial order $\leq_{SE}$ on $\mathbb{R}^{2n}$ is defined as $(x, \hat{x}) \leq_{SE} (y, \hat{y})$ if and only if $x \leq y$ and $\hat{y} \leq \hat{x}$.*

This is equivalently written in terms of the componentwise partial order as $(x, \hat{x}) \leq_{SE} (y, \hat{y})$ if and only if $(x, -\hat{x}) \leq (y, -\hat{y})$.

Definition 30 *Consider $a, b \in \mathbb{R}^n$, an extended hyper-rectangle is defined as the set $[a, b] := \{x \in \mathbb{R}^n : \; a \leq x \leq b\} \subset \mathbb{R}^n$.*

Another way used to define a hyper-rectangle in $\mathbb{R}^n$ is by considering a single point $a = (b, \hat{b})$ in $\mathbb{R}^{2n}$ that is the concatenation of the vectors $b, \hat{b} \in \mathbb{R}^n$ and setting $[\![a]\!] := [b, \hat{b}]$. The southeast partial order in $\mathbb{R}^{2n}$ helps represent a partial order relation on the set of hyper-rectangles in $\mathbb{R}^n$. To observe this, consider the nested hyper-rectangles $[a, b] \subset [c, d] \subset \mathbb{R}^n$ where $c \leq a$ and $b \leq d$. This inclusion relation of

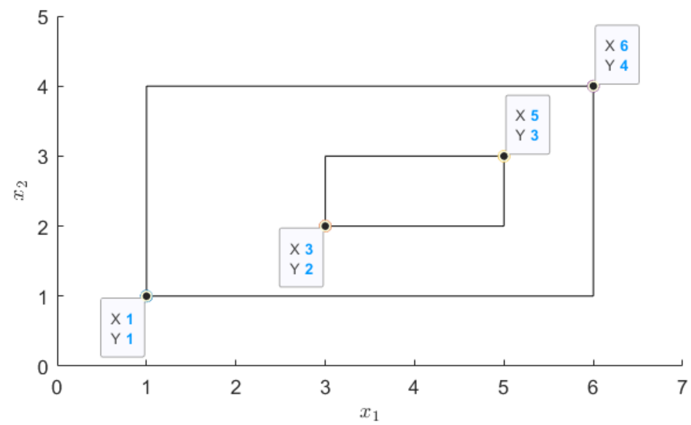


Figure 2.1: The hyper-rectangles $[(3,2),(5,3)]$ *and* $[(1,1),(6,4)]$ *in* $\mathbb{R}^2$ *satisfy* $((1,1),(6,4)) \leq_{SE} ((3,2),(5,3))$ *in* $\mathbb{R}^4$.

hyper-rectangles in $\mathbb{R}^n$ is equivalently written as $(c,d) \leq_{SE} (a,b)$ in $\mathbb{R}^{2n}$. Figure 2.1 illustrates the SE order as defined in this section.

Consider the hyper-rectangles $\mathcal{X} \subset \mathbb{R}^n$ and $\mathcal{U} \subset \mathbb{R}^m$ and the locally Lipschitz continuous function in each argument $f : \mathcal{X} \times \mathcal{U} \to \mathbb{R}^n$. The continuous-time dynamical system is defined

$$\begin{aligned} \dot{x}(t) &= f(x(t), u(t)) \\ x(0) &= x_0, \end{aligned} \tag{2.7}$$

where $x_0 \in \mathcal{X}$ and $u : [0,T] \to \mathcal{U}$. Given an input function $u(t)$ and an initial condition x_0, the trajectory function $\phi(t,u,x_0)$ of (2.7) satisfies the dynamical system and represents the state of the system at time t. Next, the set of states reached at a certain time by the dynamics is defined.

Definition 31 *Consider the system described by (2.7). The reachable set of the system subject to a set of inputs* $\mathcal{U} = [\underline{u}, \overline{u}]$ *and a set of initial states* $\mathcal{X}_0 = [\underline{x}, \overline{x}]$ *is the* *set*

$$\mathit{Reach}(\mathcal{X}_0,\mathcal{U})(T) := \Big\{\phi(T,u,x_0) \in \mathbb{R}^n : \textit{for some } u : [0,t] \to \mathcal{U}, x_0 \in \mathcal{X}_0\Big\}.$$

The next definition generalizes the concept of monotone system by embedding the vector field of the dynamics into the diagonal of a new function called *decomposition function*. This function has monotone properties in each argument.

Definition 32 *[15] Let* $d : \mathcal{X} \times \mathcal{U} \times \mathcal{X} \times \mathcal{U} \to \mathbb{R}^n$ *be a locally Lipschitz continuous function. The function* d *is said to be the decomposition function of (2.7) if the following holds:*

i. For all $x \in \mathcal{X}$ *and all* $u \in \mathcal{U}$, $d(x,u,x,u) = f(x,u)$.

ii. For all $i,j \in \{1,\cdots,n\}$ *with* $i \neq j$, $\frac{\partial d_i}{\partial x_j}(x,u,\hat{x},\hat{u}) \geq 0$ *for all* $x,\hat{x} \in \mathcal{X}$ *and for all* $u,\hat{u} \in \mathcal{U}$ *whenever the derivative exists.*

iii. For all $i,j \in \{1,\cdots,n\}$,

$$\frac{\partial d_i}{\partial \hat{x}_j}(x,u,\hat{x},\hat{u}) \leq 0$$

for all $x,\hat{x} \in \mathcal{X}$ *and for all* $u,\hat{u} \in \mathcal{U}$ *whenever the derivative exists.*

iv. For all $i \in \{1,\cdots,n\}$ *and all* $k \in \{1,\cdots,m\}$,

$$\frac{\partial d_i}{\partial u_k}(x,u,\hat{x},\hat{u}) \geq 0,\ \frac{\partial d_i}{\partial \hat{u}_k}(x,u,\hat{x},\hat{u}) \leq 0$$

for all $x,\hat{x} \in \mathcal{X}$ *and for all* $u,\hat{u} \in \mathcal{U}$ *whenever the derivative exists.*

The system (2.7) is said to be *mixed-monotone* if there exists a decomposition function of its vector field. The definition suggests that the decomposition function of a system is not unique. In fact, a system may have several decompositions. The next theorem provides one decomposition function of any vector field described in (2.7).

Theorem 5 *[15] Given an arbitrary system of the form (2.7). The system is mixed-monotone with respect to the following decomposition function d:*

$$d_i(x, u, \hat{x}, \hat{u}) = \begin{cases} \min\limits_{\substack{y \in [x, \hat{x}] \\ y_i = x_i \\ z \in [u, \hat{u}]}} f_i(y, z), \;\; x \leq \hat{x}, \;\; u \leq \hat{u}, \\ \\ \max\limits_{\substack{y \in [\hat{x}, x] \\ y_i = x_i \\ z \in [\hat{u}, u]}} f_i(y, z), \;\; \hat{x} \leq x, \;\; \hat{u} \leq u. \end{cases} \tag{2.8}$$

The decomposition function is used to compute an overapproximation of a reachable set of the system (2.7) by making it the vector field of system called *embedding system*.

Definition 33 *Consider the mixed-monotone system (2.7) with decomposition function d, the embedding system is defined as*

$$\begin{bmatrix} \dot{x} \\ \dot{\hat{x}} \end{bmatrix} = \varepsilon(x, u, \hat{x}, \hat{u}) := \begin{bmatrix} d(x, u, \hat{x}, \hat{u}) \\ d(\hat{x}, \hat{u}, x, u) \end{bmatrix}, \tag{2.9}$$

where $(x, \hat{x}) \in \mathcal{X} \times \mathcal{X} \subset \mathbb{R}^{2n}$ *and input* $(u, \hat{u}) \in \mathcal{U} \times \mathcal{U} \subset \mathbb{R}^{2m}$*.*

The following definition helps establish

Definition 34 *[1] A tight decomposition function D of (2.7) is such that for any decomposition d, it follows that that*

$$d(x, w, \hat{x}, \hat{w}) \leq D(x, w, \hat{x}, \hat{w}),$$
$$D(\hat{x}, \hat{w}, x, w) \leq d(\hat{x}, \hat{w}, x, w)$$

for $x \leq \hat{x}$ and $w \leq \hat{w}$.

The decomposition provided in Theorem 5 is the tightest in the sense that any other decomposition function generates no smaller hyper-rectangle that contains the true reachable set [15]. It is important to highlight that obtaining a closed-form of (2.8) is nontrivial and in general, requires solving a non-convex optimization problem.

Let $\Phi^{\varepsilon}(t, (x_0, \hat{x}_0), (u, \hat{u}))$ denote the state trajectory of (2.9) at time t when the initial state is $(x_0, \hat{x}_0) \in \mathcal{X} \times \mathcal{X}$ and the inputs are $u, \hat{u} : [0, \infty[\rightarrow \mathcal{U} = [\underline{u}, \overline{u}]$. When the inputs are of the form $u(t) = \underline{u}$ and $\hat{u}(t) = \overline{u}$, the state trajectory of (2.9) is denoted $\Phi^{e}(t, (x_0, \hat{x}_0), (\underline{u}, \overline{u}))$. The trajectory Φ^{ε} preserves the south-east order [15]. The next theorem relates the embedding system with the reachable sets of system (2.7).

Theorem 6 *[15] Assume system (2.7) is mixed-monotone with respect to d. Consider $\mathcal{X}_0 = [\underline{x}, \overline{x}] \subset \mathcal{X}$ a hyperrectangle of initial states and the input functions $u_1 : [0, \infty[\rightarrow \mathcal{U}$, $u_2 : [0, \infty[\rightarrow \mathcal{U}$, satisfying $u_1(t) \leq u_2(t)$ for all $t \geq 0$, then*

$$\mathit{Reach}([\underline{x}, \overline{x}], [\underline{u}, \overline{u}])(t) \subset [\![\Phi^{e}(t, (\underline{x}, \overline{x}), (\underline{u}, \overline{u}))]\!]$$

for all $t \geq 0$.

2.7 Algebraic Geometry

In this section, two essential results in the field of algebraic geometry are presented. This content is based on [10, 52]. In a sense, algebraic geometry concerns the relationship between algebraic and geometric properties of polynomials or a set of these. The geometric part comes from the zeroes of the polynomials, and the algebraic part comes from the generating structure. It is also the background for the modern study of elliptic curves [60].

Consider k a closed field, $k[x_1, \cdots, x_n]$ is the set of polynomials in the $x_1, \cdots, x_n$ variables with coefficients in k. An affine algebraic set is the set of zeroes of a set of polynomials. When an affine algebraic set is irreducible, meaning it is not composed of the union of affine algebraic sets, it is called an affine variety. An ideal is a subset of a ring that forms a group under the addition, and it absorbs the ring under the multiplication.

Theorem 7 (Nullstellensatz) *Consider k an algebraically closed field and let $I \subset k[x_1, \cdots, x_n]$ be an ideal satisfying $V(I) = \emptyset$. Then $1 \in I$ or equivalently, $I = k[x_1, \cdots, x_n]$.*

Here, $V(I) = \emptyset$ means that the set of points that make all polynomials of the ideal equal to zero is the empty set. Then, this theorem provides a criterion for the existence of solutions of systems of polynomial equations. Similarly, the next theorem provides a criterion for the existence of points that make a system of polynomial equations non-negative.

Theorem 8 (Positivstellensatz) *[10] Let R be a real closed field. Let*

$$F = \{f_j \in R[X_1, \cdots, X_n] \ : \ j = 1, \cdots, s\},$$

$$G = \{g_k \in R[X_1, \cdots, X_n] \ : \ k = 1, \cdots, t\},$$

$$H = \{h_l \in R[X_1, \cdots, X_n] \ : \ l = 1, \cdots, u\}$$

be families of polynomials. Denote by P the cone generated by the elements of F, M the multiplicative monoid generated by the elements of G and I the ideal generated by the elements of H. Then the following properties are equivalent:

- *The set*

  $$\begin{aligned}\{x \in \mathbb{R}^n : f_j(x) \geq 0,\ j = 1, \cdots, s,\\ g_k(x) \neq 0,\ k = 1, \cdots, t,\\ h_l(x) = 0,\ l = 1, \cdots, u\}\end{aligned}$$

  is empty.

- *There exists $f \in P, g \in M$ and $h \in I$ such that $f + g^2 + h = 0$.*

Examples of these powerful theorems are provided in [52].

Chapter 3

Chen-Fliess Reachability via Interval Arithmetic

This chapter is based on [56] where an over-approximation of the output reachable set of a nonlinear control affine system (2.4) represented by a Chen-Fliess series is provided. Here, the input is assumed to lie inside a box determined by the cartesian product of one compact interval with itself. To compute this over-approximation, first, the reachable set of a single iterated integral is obtained by using interval arithmetics, specifically the power of an interval. To extend it to Chen-Fliess series, the result for each iterated integral is added up and multiplied by its corresponding weight. The advantage of this method is its closed-form, fast computation and good accuracy for short periods of time. If the time is large enough the approximation loses accuracy. Examples are provided and compared with the mixed-monotonicity approach described in Section 2.6. It is possible that the over-approximation via interval arithmetics coincides with the real reachable set but this is not guaranteed in general. Additionally, the relation between the input-output reachable set of an iterated integral and the reachable set of its state-space representation is discussed.

3.1 Interval Arithmetic

An interval is a set in $\mathbb{R}$ defined as $[a, b] = \{x \in \mathbb{R} \ : \ a \leq x \leq b\}$ for $a, b \in \mathbb{R}$. It is a box over $\mathbb{R}$ according to section 2.6. In order to shorten the notation, the box $[a, b] \times \cdots \times [a, b]$ are defined by two vectors each with the same coordinates, this is, $[\mathbf{a}, \mathbf{b}] = [(a_1, \cdots, a_n), (b_1, \cdots, b_n)] \subset \mathbb{R}^n$ with $a_i = a$ and $b_i = b$ for all $i \in \{1, \cdots, n\}$. Following [49], the product of intervals is defined.

Definition 35 *Given the intervals $I_1 = [a_1,\ b_1] \subset \mathbb{R}$ and $I_2 = [a_2,\ b_2] \subset \mathbb{R}$, the product $I_1 \cdot I_2$ is defined as the interval $\left[\underline{I}, \overline{I}\right]$, where*

$$\underline{I} = \min_{\substack{y_1 \in [a_1, b_1] \\ y_2 \in [a_2, b_2]}} y_1 y_2, \quad \overline{I} = \max_{\substack{y_1 \in [a_1, b_1] \\ y_2 \in [a_2, b_2]}} y_1 y_2.$$

Observe that by simple inspection the product of $[a_1, b_1]$ and $[a_2, b_2]$, with $a_1, a_2, b_1, b_2 \in \mathbb{R}$, is written as

$$[a_1, b_1] \cdot [a_2, b_2] = \ [\min\{a_1a_2, a_1b_2, b_1a_2, b_1b_2\},\ \max\{a_1a_2, a_1b_2, b_1a_2, b_1b_2\}].$$

In particular, when the intervals are the same $I_1 = I_2 = [a, b] \subset \mathbb{R}$, the product $[a, b] \cdot [a, b]$ is denoted as a power of intervals $[a, b]^2$. In general, the product of n times the same interval $[a, b]$ is denoted $\underbrace{[a, b] \cdots [a, b]}_{n} = [a, b]^n$.

Example 1 *Consider the intervals* $[-2, 1]$ *and* $[1, 3]$*. From Definition 35, the product* $[-2, 1] \cdot [1, 3] = [-6, 3]$*, because* $\min\{-2, -6, 1, 3\} = -6$ *and* $\max\{-2, -6, 1, 3\} = 3$.

Also, the second power of the interval $[-2,1]$ *is* $[-2,1]^2 = [-2,4]$.

Another operation used in this manuscript is the product of a real number and a set

Definition 36 *Given a set* $\mathcal{X} \subset \mathbb{R}^n$ *and a number* $\lambda \in \mathbb{R}$*, the product of* $\mathcal{X}$ *and* λ *is defined as* $\lambda\mathcal{X} = \{\lambda x \ : \ x \in \mathcal{X}\}$*.*

Example 2 *Consider the interval* $[-2,1]$ *and* $\lambda = 3$*, then* $3[-2,1] = [-6,3]$*.*

In order to distinguish between the reachable set of system (2.7) given by Definition 31 and the reachable set of a Chen-Fliess series, the next definition is provided.

3.2 Iterated Integrals over Intervals

Definition 37 *Given the alphabet* $X = \{x_0, \cdots, x_m\}$*, the formal power series* $c \in \mathbb{R}^\ell\langle\langle X\rangle\rangle$ *and the hyper-rectangle* $\mathcal{U} \subset \mathbb{R}^m$*, the reachable set of the Chen-Fliess series* $F_c[u](t)$ *taking values in the set of inputs* $\mathcal{U}$ *is the set*

$$Reach_c(\mathcal{U})(T) := \Big\{ y = F_c[u](T) \in \mathbb{R}^\ell \ : \ \textit{for some } u : [0,t] \to \mathcal{U} \Big\}.$$

Next, a simple example is provided to illustrate this definition and the idea behind the use of interval arithmetic to compute overestimations of the reachable set of a Chen-Fliess series.

3.2.1 The Idea

Example 3 *Consider the alphabet* $X = \{x_0, x_1\}$*, the formal power series* $c = x_1^2 \in \mathbb{R}\langle\langle X\rangle\rangle$ *and the interval* $\mathcal{U} = [-2,1] \subset \mathbb{R}$*. The Chen-Fliess series* $F_c[u](t)$ *is repre-*

sented by only one iterated integral $F_c[u](t) = E_{x_1^2}[u](t)$. *Since the inputs are taken in the set* $\mathcal{U} = [-2, 1]$, *then*

$$\begin{aligned} -2 \leq & \quad u(\tau) \quad \leq 1, \\ -2\tau_1 \leq & \int_0^{\tau_1} u(\tau)d\tau \leq \tau_1, \end{aligned}$$

which means that $\int_0^{\tau_1} u(\tau)d\tau \in [-2\tau_1, \tau_1]$ *and since* $\tau_1 > 0$, *then by Definition 36* $[-2\tau_1, \tau_1] = [-2, 1]\tau_1$. *On the other hand,* $u(\tau_1) \in [-2, 1]$, *then*

$$u(\tau_1) \int_0^{\tau_1} u(\tau)d\tau \in [-2, 1] \cdot [-2, 1]\tau_1$$

and

$$E_{x_1^2}[u](t) = \int_0^t u(\tau_1) \int_0^{\tau_1} u(\tau)d\tau d\tau_1 \in [-2, 1]^2 \frac{t^2}{2!}.$$

Therefore, $Reach_c(\mathcal{U})(t) \subset [-2, 1]^2 \frac{t^2}{2!}$.

Remark: The challenge to computing reachable sets of more complex Chen-Fliess series by adding up the reachable sets of the iterated integrals is that in general

$$\begin{aligned} &\min_{u \in \mathcal{U}} E_{\eta_1}[u](t) + \min_{u \in \mathcal{U}} E_{\eta_2}[u](t) \leq \min_{u \in \mathcal{U}} (E_{\eta_1}[u](t) + E_{\eta_2}[u](t)), \\ &\max_{u \in \mathcal{U}} (E_{\eta_1}[u](t) + E_{\eta_2}[u](t)) \leq \max_{u \in \mathcal{U}} E_{\eta_1}[u](t) + \max_{u \in \mathcal{U}} E_{\eta_2}[u](t), \end{aligned}$$

which means that the weighted sum of the reachable sets of the iterated integrals is not equal to the reachable set of the Chen-Fliess series necessarily.

3.2.2 Reachable Set and Iterative Integrals

To relate both reachable sets in Definition 31 and 37, notice that an arbitrary iterated integral has a dynamical system associated with it. To observe this, consider the formal power series consisting of only one word $c = \eta = x_{i_1} \cdots x_{i_n} \in X^*$. The associated Chen-Fliess series of c is the iterated integral $F_c[u](t) = E_\eta[u](t)$. Define the following set of functions

$$\begin{aligned} w_1(t) &= E_\eta[u](t), \\ &\vdots \\ w_{n-1}(t) &= E_{x_{i_{n-1}} x_{i_n}}[u](t), \\ w_n(t) &= E_{x_{i_n}}[u](t). \end{aligned} \tag{3.1}$$

By differentiating the equations above, the following state-space represented dynamical system is obtained in $\mathbb{R}^n$:

$$\begin{aligned} \dot{w}_1(t) &= u_{i_1}(t) w_2(t), \\ \dot{w}_2(t) &= u_{i_2}(t) w_3(t), \\ &\vdots \\ \dot{w}_n(t) &= u_{i_n}(t) \end{aligned} \tag{3.2}$$

with initial condition $w(0) = w_1(0) = \cdots = w_n(0) = 0$. Without loss of generality, assume that $i_n \neq 0$. Consider the set of initial states $\mathcal{W}_0 = \{(0, \cdots, 0)\} \subset \mathbb{R}^n$. According to Definition 31, for a box $\mathcal{U} \subset \mathbb{R}^n$, the reachable set of system (3.2) is $\mathrm{Reach}(\mathcal{W}_0, \mathcal{U})(t)$ and from Definition 37 the reachable set of the iterated integral

$w_1(t) = E_\eta[u](t)$ is $\text{Reach}_\eta(\mathcal{U})(t)$. Therefore,

$$\text{Reach}_\eta(\mathcal{U})(t) = \text{Proy}_{w_1}(\text{Reach}(\mathcal{W}_0, \mathcal{U})(t)).$$

The closed-form of the reachable set of an iterated integral in terms of the interval defining the input set is given next.

Lemma 2 *Consider the input function* $u : \mathbb{R} \to \mathbb{R}^m$ *with values in the box* $[\boldsymbol{a}, \boldsymbol{b}]$ *(i.e.,* $u_i(t) \in [a, b], \forall\ t \in [0, T]$ *with* $T > 0$*). For* $\eta = x_{i_1} \cdots x_{i_n} \in X^*$*, the reachable set of the iterated integral* $E_\eta[u](t)$ *is bounded by*

$$\mathit{Reach}_\eta([\boldsymbol{a}, \boldsymbol{b}])(t) \subset [a, b]^{|\eta| - |\eta|_{x_0}} \frac{t^{|\eta|}}{|\eta|!}, \forall\ t \in [0, T].$$

Proof: As shown by (3.1) and (3.2), there is a dynamical system associated to $E_\eta[u](t)$. From Theorem 5, the decomposition function associated to the embedding system of (3.2) is

$$\begin{aligned} d_n(a, b) &= a, \quad d_n(b, a) = b, \\ d_j(w_{j+1}, a, \hat{w}_{j+1}, b) &= \min_{\substack{y \in [w_{j+1}, \hat{w}_{j+1}] \\ z \in [a, b]}} zy, \ \text{ if } w_{j+1} \leq \hat{w}_{j+1} \\ d_j(\hat{w}_{j+1}, b, w_{j+1}, a) &= \max_{\substack{y \in [w_{j+1}, \hat{w}_{j+1}] \\ z \in [a, b]}} zy, \ \text{ if } \hat{w}_{j+1} \leq w_{j+1} \end{aligned}$$

for $j \in \{1, \cdots, n-1\}$. Therefore, the embedding system corresponding to $E_\eta[u](t)$ is

$$\begin{aligned} \dot{w}_1 &= d_1(w_2, a, \hat{w}_2, b), \ \cdots, \dot{w}_n = d_n(a, b), \\ \dot{\hat{w}}_1 &= d_1(\hat{w}_2, b, w_2, a), \ \cdots, \dot{\hat{w}}_n = d_n(b, a). \end{aligned} \tag{3.3}$$

According to Theorem 6, the states w_1 and $\hat{w}_1$ provide the evolution of the south-west and north-east corners of the overapproximating hyper-rectangle of the reachable set of (3.3). Given that (3.3) is also a chain of integrators, one can simply start solving for w_n and $\hat{w}_n$, and then solve sequentially for $n-1, \ldots, 1$. The solution to (3.3) is then

$$w_n = at, \quad \hat{w}_n = bt,$$

and, for any $j = 1, \ldots, n-1$,

$$w_{j-1} = \min_{\substack{y \in [w_j, \hat{w}_j] \\ z \in [a,b]}} \int_0^t zy(\tau)d\tau, \hat{w}_{j-1} = \max_{\substack{y \in [w_j, \hat{w}_j] \\ z \in [a,b]}} \int_0^t zy(\tau)d\tau.$$

Given the simple solution for w_n and $\hat{w}_n$, one can apply the change of variables $x = y/\tau^i$ in each w_{n-i} and $\hat{w}_{n-i}$ for $i \in \{1, \cdots, n-1\}$ so that the min and max are calculated over $[a, b]$. This together with the monotonicity of the integral operator gives

$$\begin{aligned} w_{n-1} &= \min_{\substack{x \in [a,b] \\ z \in [a,b]}} \int_0^t \tau zx(\tau)d\tau = \min_{\substack{x \in [a,b] \\ z \in [a,b]}} zx\frac{t^2}{2}, \\ \hat{w}_{n-1} &= \max_{\substack{x \in [a,b] \\ z \in [a,b]}} \int_0^t \tau zx(\tau)d\tau = \max_{\substack{x \in [a,b] \\ z \in [a,b]}} zx\frac{t^2}{2}. \end{aligned}$$

Continuing the recursion, it follows that

$$w_1 = \min_{\substack{x_i \in [a,b] \\ i \in \{1,\cdots,r\}}} x_1 \cdots x_r \frac{t^n}{n!},$$

$$\hat{w}_1 = \max_{\substack{x_i \in [a,b] \\ i \in \{1,\cdots,r\}}} x_1 \cdots x_r \frac{t^n}{n!},$$

where $r = |\eta| - |\eta|_{x_0}$. Finally, from Definition 35,

$$\text{Reach}_\eta([\mathbf{a}, \mathbf{b}])(t) \subset [w_1, \hat{w}_1] = [a, b]^{|\eta| - |\eta|_{x_0}} \frac{t^{|\eta|}}{|\eta|!},$$

which completes the proof. ■

3.2.3 Boxes Using Interval Arithmetics

Since the reachable set of iterated integrals with inputs taking values in a hyper-rectangle is given in terms of interval products, the following lemma provides the closed-form of the n-th power of an interval.

Lemma 3 *Given the interval $I = [a, b] \subset \mathbb{R}$, its n-th power I^n is given by*

$$I^n = \begin{cases} [a^n, b^n], & a, b > 0, n \text{ even} \\ [b^n, a^n], & a, b < 0, n \text{ even} \\ [\min\{a^{n-1}b, ab^{n-1}\},\ \max\{|a|, |b|\}^n], & a < 0, b > 0, n \text{ even} \\ [a^n, b^n], & ab > 0, n \text{ odd} \\ [\min\{a^n, ab^{n-1}\},\ \max\{a^{n-1}b, b^n\}], & a < 0, b > 0, n \text{ odd} \end{cases} \tag{3.4}$$

Proof: The lemma is proved by induction. For $n = 1$, it follows directly that $I^1 = [a,\ b]$. For $n = 2$, one has that

$$I^2 = \begin{cases} [a^2, b^2], & a, b > 0, \\ [b^2, a^2], & a, b < 0, \\ [ab, \max\{|a|, |b|\}^2], & a < 0, b > 0. \end{cases}$$

Assuming now that (3.4) holds for k odd, it follows that

$$I^k I^2 =$$

$$\begin{cases} [\min\{a^{k+2}, a^k b^2, b^k a^2, b^{k+2}\},\ \max\{a^{k+2}, a^k b^2, b^k a^2, b^{k+2}\}], & ab > 0, \\ [\min\{a^{k+1}b, a^{k+2}, a^k b^2, a^{k+1}\},\ \max\{a^{k+1}b, a^{k+2}, a^k b^2, a^{k+1}\}], & a < 0, b > 0, |a| > |b|, \\ [\min\{a^2 b^k, ab^{k+1}, b^{k+2}\},\ \max\{a^2 b^k, ab^{k+1}, b^{k+2}\}], & a < 0, b > 0, |b| > |a|. \end{cases}$$

If $ab > 0$, then

$$\min\{a^{k+2}, a^k b^2, b^k a^2, b^{k+2}\} = a^{k+2}$$

and

$$\max\{a^{k+2}, a^k b^2, b^k a^2, b^{k+2}\} = b^{k+2}.$$

If $a < 0$, $b > 0$ and $|a| > |b|$, then

$$\min\{a^{k+1}b, a^{k+2}, a^k b^2, a^{k+1}\} = a^{k+2}$$

and

$$\max\{a^{k+1}b, a^{k+2}, a^k b^2, a^{k+1}\} = a^{k+1}b.$$

If $a < 0$, $b > 0$ and $|b| > |a|$, then

$$\min\{a^2 b^k, ab^{k+1}, b^{k+2}\} = ab^{k+1}$$

and

$$\max\{a^2 b^k, ab^{k+1}, b^{k+2}\} = b^{k+2}.$$

Hence, (3.4) holds for k odd. The case for k even follows in a similar manner. ■

Observe that (3.4) can be written compactly as

$$I^n = \begin{cases} [\min\{a^n, ab^{n-1}\},\ \max\{b^n, a^{n-1}b\}],\ n \text{ odd} \\ [\min\{a^n, ab^{n-1}, a^{n-1}b, b^n\},\ \max\{a^n, b^n\}], n \text{ even}. \end{cases}$$

In the current section, the closed formula of a box formed by n-th power of an interval was provided. This is used to provide the closed formula of an overestimation of the reachable set of a single iterated integral. In the next section, the overestimation of the reachable set of a Chen-Fliess series is obtained by adding up the result for each iterated integral.

3.3 Chen-Fliess Series over Intervals

Since a Chen-Fliess series is a sum of weighted iterated integrals with coefficients in $\mathbb{R}^\ell$, the reachable set obtained in Lemma 2 of each iterated integral is used in the next theorem to provide an overapproximation of the reachable set of a Chen-Fliess series.

Theorem 9 *Consider the formal power series* $c \in \mathbb{R}_{LC}\langle\langle X \rangle\rangle$ *and* $u : \mathbb{R} \to \mathbb{R}^m$ *be a function with image in the box* $[\boldsymbol{a}, \boldsymbol{b}]$ *for all* $t > 0$*. The reachable set of the Chen-Fliess series* $F_c[u](t)$ *satisfies*

$$Reach_c([\boldsymbol{a}, \boldsymbol{b}])(t) \subset \left[F_{\underline{c}}[\mathbb{1}](t), F_{\overline{c}}[\mathbb{1}](t)\right], \;\forall t \in \mathbb{R},$$

where

$$(\underline{c}, \eta) = \min\left\{(c, \eta)[a, b]^{|\eta| - |\eta|_{x_0}}\right\}, \tag{3.5a}$$

$$(\overline{c}, \eta) = \max\left\{(c, \eta)[a, b]^{|\eta| - |\eta|_{x_0}}\right\}. \tag{3.5b}$$

Here, $\mathbb{1}$ *as the input of a Chen-Fliess series refers to the vector of* m *ones. This is,* $\mathbb{1} = (1, \cdots, 1)^T$.

Proof: *The result follows directly from adding up the reachable set of each iterated integral provided in Lemma 2. Given the minimum of a sum is not smaller than the sum of minimums and the maximum of a sum is not greater than the sum of maximums, it follows that*

$$\sum_{\eta \in X^*} \min_{u \in [\boldsymbol{a}, \boldsymbol{b}]} (c, \eta) E_\eta[u](t) \leq \min_{u \in [\boldsymbol{a}, \boldsymbol{b}]} F_c[u](t) \;\; \textit{and} \;\; \max_{u \in [\boldsymbol{a}, \boldsymbol{b}]} F_c[u](t) \leq \sum_{\eta \in X^*} \max_{u \in [\boldsymbol{a}, \boldsymbol{b}]} (c, \eta) E_\eta[u](t).$$

Then

$$F_c[u](t) \in \sum_{\eta \in X^*} (c,\eta) Reach_\eta([\boldsymbol{a},\boldsymbol{b}])(t), \forall u \in [\boldsymbol{a},\boldsymbol{b}],$$

where the product of $(c,\eta) \in \mathbb{R}$ *and the set* $Reach_\eta([\boldsymbol{a},\boldsymbol{b}])(t)$ *is as described in Definition 36. One now has that*

$$Reach_c([\boldsymbol{a},\boldsymbol{b}])(t) \subset \sum_{\eta \in X^*} (c,\eta) Reach_\eta([\boldsymbol{a},\boldsymbol{b}])(t).$$

The result follows by replacing the expression of the reachable set of each iterated integral, from Lemma 2, and noticing that

$$\begin{aligned} \min\{(c,\eta)Reach_\eta([\boldsymbol{a},\boldsymbol{b}])(t)\} &= \min\left\{(c,\eta)[a,b]^{|\eta|-|\eta|_{x_0}}\right\}E_\eta[\mathbb{1}](t), \\ \max\{(c,\eta)Reach_\eta([\boldsymbol{a},\boldsymbol{b}])(t)\} &= \max\left\{(c,\eta)[a,b]^{|\eta|-|\eta|_{x_0}}\right\}E_\eta[\mathbb{1}](t). \end{aligned}$$

■

3.3.1 The Closed-form

Next, explicit expressions of the coefficients of the defining series of $\mathrm{Reach}_c([\mathbf{a},\mathbf{b}])(t)$ are obtained.

Corollary 1 *Letting* $n = |\eta| - |\eta|_{x_0}$*, and defining the function* $f : \mathbb{R} \times \mathbb{N} \to \mathbb{R}$ *as* *i.* $a, b > 0$

$$f((c,\eta),n) = \begin{cases} (c,\eta)a^n, & (c,\eta) > 0, \\ (c,\eta)b^n, & (c,\eta) < 0 \end{cases}.$$

ii. $a, b < 0$

$$f((c,\eta),n) = \begin{cases} (c,\eta)b^n, & (c,\eta) > 0,\ n \text{ even or } (c,\eta) < 0,\ n \text{ odd} \\ (c,\eta)a^n, & (c,\eta) > 0,\ n \text{ odd or } (c,\eta) < 0,\ n \text{ even} \end{cases}.$$

iii. $a < 0, b > 0, |a| < |b|$

$$f((c,\eta),n) = \begin{cases} (c,\eta)ab^{n-1}, & (c,\eta) > 0, \\ (c,\eta)b^n, & (c,\eta) < 0, \end{cases}.$$

iv. $a < 0, b > 0, |b| < |a|$

$$f((c,\eta),n) = \begin{cases} (c,\eta)a^{n-1}b, & (c,\eta) > 0,\ n \text{ even or } (c,\eta) < 0,\ n \text{ odd} \\ (c,\eta)a^n, & (c,\eta) > 0,\ n \text{ odd or } (c,\eta) < 0,\ n \text{ even} \end{cases}.$$

then the coefficients of $\bar{c}$ *and* $\underline{c}$ *in Theorem 9 are* $(\underline{c},\eta) = f((c,\eta),n)$ *and* $(\bar{c},\eta) = -f(-(c,\eta),n)$.

Proof: *The proof follows by using Lemma 3 and taking into account that the bounds of* $Reach_c([\boldsymbol{a},\boldsymbol{b}])(t)$ *switch when multiplying by a negative number.* ∎

3.4 Numerical Simulations

Example 4 *To illustrate the proposed Chen-Fliess over-approximation, consider the following single-input single-output system*

$$\dot{x} = xu, \quad y = x, \quad x_0 = 1. \tag{3.6}$$

Assume the input u *is constrained to the interval* $\mathcal{U} = [1, 2.8]$*. Using (2.5), one can compute the coefficients of the Chen-Fliess series. Thus, one has that*

$$F_c[u] = 1 + \sum_{k=1}^{\infty} E_{x_1^k}[u](t),$$

where $(c, \eta) = 1$ *for all* $\eta \in X^*$ *which implies that* $c \in \mathbb{R}_{GC}\langle\langle X \rangle\rangle$*. This is,* $F_c[u]$ *converges for all* $t > 0$*. Also, from Definition 33, it is not difficult to see that the embedding system for (3.6) is*

$$\dot{x} = xu, \ \dot{\hat{x}} = \hat{x}\hat{u},$$

with initial set of states equal to $(x_0, \hat{x}_0) = (1, 1)$*. Solving for this embedding system (Theorem 6) provides the reachable set of (3.6) for inputs in* $\mathcal{U} = [1, 2.8]$*. On the other hand, from Theorem 9 and Corollary 1, one has that*

$$(\overline{c}, \eta) = 2.8^k \text{ and } (\underline{c}, \eta) = 1$$

for $|\eta| = k$*. Therefore,*

$$Reach_c([1, 2.8])(t) \subset [F_{\underline{c}}[\mathbb{1}](t), F_{\overline{c}}[\mathbb{1}](t)] = \left[1 + \sum_{k=1}^{\infty} \frac{t^k}{k!}\ ,\ 1 + \sum_{k=1}^{\infty} 2.8^k \frac{t^k}{k!}\right].$$

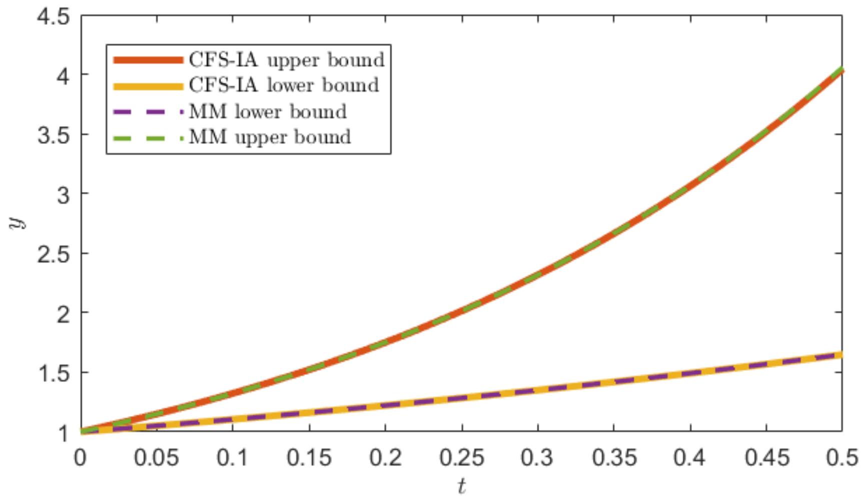


Figure 3.1: Comparison of the overestimation of the reachable set of the system in Example 4 with initial state $x_0 = 1$ *by the Chen-Fliess series interval arithmetic (CFS-IA) procedure, for an input in* $\mathcal{U} = [1, 2.8]$ *and word truncation size* $N = 3$ *and the Mixed-Monotonicity (MM) approach.*

Example 5 *Consider the following MISO Lotka-Volterra system given by*

$$\dot{x}_1 = -x_1 x_2 + x_1 u_1, \quad \dot{x}_2 = x_1 x_2 - x_2 u_2, \quad y = x_1 \tag{3.7}$$

with initial condition $x_0 = (1/6, 1/6)^\top$*. The embedding system obtained using Defini-*

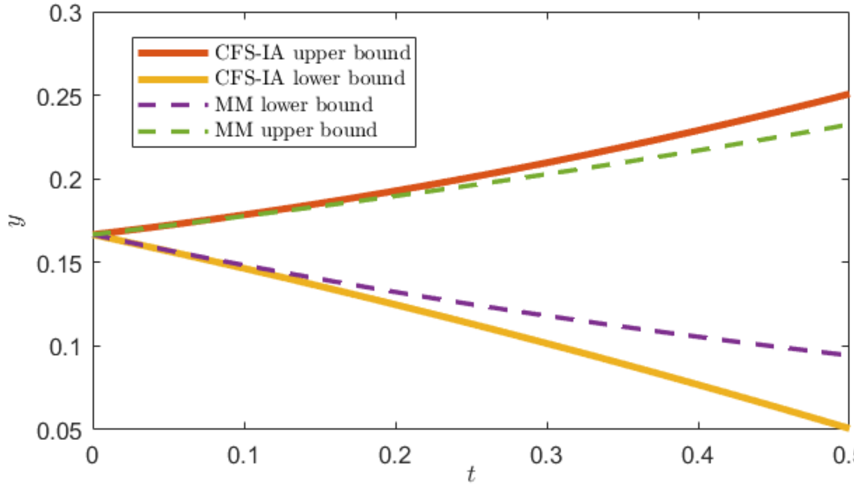


Figure 3.2: Comparison of the overestimation of the reachable set of the system in Example 5 with initial state $x_0 = (1/6, 1/6)$ by the Chen-Fliess series interval arithmetic (CFS-IA) procedure, for inputs in $\mathcal{U} = [-\boldsymbol{1}, \boldsymbol{1}]$ and word truncation size $N = 3$ and the Mixed-Monotonicity (MM) approach.

tion 33 is

$$\dot{x}_1 = -x_1\hat{x}_2 + x_1u_1,\ \ \dot{x}_2 = x_2x_1 - x_2\hat{u}_2,$$

$$\dot{\hat{x}}_1 = -\hat{x}_1x_2 + \hat{x}_1\hat{u}_1,\ \ \dot{\hat{x}}_2 = \hat{x}_2\hat{x}_1 - \hat{x}_2u_2.$$

The reachable set on the initial set $(x_{1,0}, x_{2,0}, \hat{x}_{1,0}, \hat{x}_{2,0}) = (1/6, 1/6, 1/6, 1/6)$ *is given in Figure 3.2 together with the result obtained from the interval arithmetic procedure from Theorem 9.*

Chapter 4

Input-Output Mixed Monotonicity

This chapter is based on [53] where a Chen-Fliess series as described in (2.3) is shown to have monotonic properties similar to those presented in Section 2.6. This is done by extending the property of mixed-monotonicity to Chen-Fliess series and producing an appropriate decomposition function. First, the closed-form of the Chen-Fliess series of the sum of two input functions is obtained in terms of the addend functions. For this, an *extended* Chen-Fliess series taking two input function arguments is presented. Then, a decomposition function is provided by decomposing an arbitrary input function as the difference between its positive and negative parts and lifting the function domain of the *extended* Chen-Fliess series. This decomposition function preserves the monotonicity of a partial order in the input function domain. Because of this monotonic behavior, the decomposition function is capable of providing an overestimation of the reachable set of the output of a nonlinear control affine system.

4.1 The Chen-Fliess Series of the Sum of Two Inputs

Since the procedures regarding the Chen-Fliess series with coefficients in $\mathbb{R}^\ell$ can be performed componentwise, it is assumed hereafter that $\ell = 1$ and that all inputs are defined over the time interval $[0, T]$ for some $T > 0$. To extend the Chen-Fliess series to be able to take two input functions as arguments, two alphabets are considered instead of only one.

Definition 38 *Let the alphabets $X = \{x_0, \cdots, x_m\}$, $Y = \{y_1, \cdots, y_m\}$ and $Z = X \cup Y$. A letter morphism is defined as any map $\rho : Y \mapsto X$ such that for $y_i \in Y$ one has $\rho(y_i) \in X$. This mapping is naturally extended to a word monoid homomorphism $\rho : Z^* \mapsto X^*$, where for $\eta = z_{i_1} \cdots z_{i_k}$ one has that $\rho(\eta) = \rho(z_{i_1}) \cdots \rho(z_{i_1})$. In particular, the monoid homomorphism defined for letters as $\sigma_X(y_i) = x_i$ is called a* substitution.

4.1.1 Extended Iterative Integral

The next definition extends the iterated integrals to take two inputs associated with two different alphabets.

Definition 39 *Consider the alphabets X and Y associated to the input functions $u,\ v \in L_{\mathfrak{p}}^m[0, T]$, respectively. The iterated integral of $\eta \in Z^*$ for the input (u, v) is* *given by the mapping* $\mathcal{E}_\eta : L_{\mathfrak{p}}^m[0,T] \times L_{\mathfrak{p}}^m[0,T] \to \mathcal{C}[0,T]$, *where* $\mathcal{E}_\emptyset[u,v](t) = 1$ *and*

$$\mathcal{E}_{z_i\eta}[u,v](t) := \begin{cases} \displaystyle\int_0^t u_i(\tau)\mathcal{E}_\eta[u,v](\tau)d\tau, & z_i \in X, \\ \displaystyle\int_0^t v_i(\tau)\mathcal{E}_\eta[u,v](\tau)d\tau, & z_i \in Y. \end{cases} \tag{4.1}$$

Similar to (2.2), (4.1) is linearly extended to polynomials $p \in \mathbb{R}\langle Z\rangle$ and then to series $c \in \mathbb{R}\langle\langle Z\rangle\rangle$. Hence,

$$\mathcal{F}_c[u,v](t) = \sum_{\eta \in Z^*} (c,\eta)\mathcal{E}_\eta[u,v](t) \tag{4.2}$$

is a well-defined input-output operator.

Define the *substitution language* of a word $\eta = x_{i_1}\cdots x_{i_n} \in X^*$ as the following set of words in the alphabet Z

$$I_\eta := \{z_{i_1}\cdots z_{i_n} \in Z^* : z_{i_j} \in \{x_{i_j}, y_{i_j}\},\ j = 1,\ldots,n\}.$$

Observe that $I_\eta = \operatorname{supp}((x_{i_1} + y_{i_1})\cdots(x_{i_n} + y_{i_n}))$ and that it is comprised of 2^n elements. Moreover, if $\eta_1, \eta_2 \in X^*$ are such that $\eta_1 \neq \eta_2$ then $I_{\eta_1} \neq I_{\eta_2}$. If this were not the case and $\eta_1 \neq \eta_2$ are such that $I_{\eta_1} = I_{\eta_2}$, then $\eta_1, \eta_2 \in I_{\eta_1}$. Since η_1 is the only word in X^* that belongs to I_{η_1}, then $\eta_1 = \eta_2$, which is a contradiction.

4.1.2 The Closed-Form

The following lemma provides a closed formula for the Chen-Fliess series of the sum of two inputs in terms of two alphabets which is useful for obtaining a decomposition of (2.3) for the purpose of studying its mixed-monotonicity. Recall that, from

Definition 38, $\sigma_X(\xi) = \eta$ for any $\xi \in I_\eta$.

Lemma 4 *Let X and Y be alphabets associated to $u,\ v \in L_{\mathfrak{p}}^m[t_0, t_1]$, respectively. Given $c \in \mathbb{R}\langle\langle X \rangle\rangle$, the Chen-Fliess series of $u + v$ is written as*

$$F_c[u+v](t) = \sum_{k=0}^{\infty} \sum_{\xi \in \mathbb{S}_{X^*,Y^k}} (c, \sigma_X(\xi)) \mathcal{E}_\xi[u,v](t). \tag{4.3}$$

Proof: To obtain (4.3), it is first shown that

$$E_\eta[u+v](t) = \mathcal{E}_{\mathrm{char}(I_\eta)}[u,v](t) \tag{4.4}$$

for any $\eta \in X^*$. This is proved by induction over the length of the word η. Consider $|\eta| = 1$, $\eta = x_j$ and $I_\eta = \{x_j,\ y_j\}$. By the linearity of integrals and Definition 39, it follows that

$$\begin{aligned} E_{x_j}[u+v](t) &= \int_0^t u_j(\tau) + v_j(\tau) d\tau, \\ &= \int_0^t u_j(\tau) d\tau + \int_0^t v_j(\tau) d\tau, \\ &= \mathcal{E}_{x_j}[u,v](t) + \mathcal{E}_{y_j}[u,v](t), \\ &= \mathcal{E}_{\mathrm{char}(I_{x_j})}[u,v](t). \end{aligned}$$

Now assume that (4.4) holds true for any $\eta' \in X^*$ such that $|\eta'| = k$, and compute the expression for $\eta = x_i \eta'$. That is,

$$E_\eta[u+v](t) = \int_0^t (u_i(\tau) + v_i(\tau)) E_{\eta'}[u+v](\tau) d\tau.$$

Since $|\eta'| = k$ and by the induction hypothesis, one has that

$$E_\eta[u+v](t) = \int_0^t (u_i(\tau) + v_i(\tau))\mathcal{E}_{\text{char}(I_{\eta'})}[u,v](\tau)d\tau,$$

Hence, using linearity and (2.2) over the alphabet Z, it follows that

$$\begin{aligned}E_\eta[u+v](t) &= \mathcal{E}_{x_i\text{char}(I_{\eta'})}[u,v](t) + \mathcal{E}_{y_i\text{char}(I_{\eta'})}[u,v](t) \\ &= \mathcal{E}_{\text{char}(I_\eta)}[u,v](t).\end{aligned}$$

Now, (2.3) can be expressed in terms of (4.1). That is,

$$\begin{aligned}F_c[u+v](t) &= \sum_{\eta\in X^*}(c,\eta)E_\eta[u+v](t) \\ &= \sum_{\eta\in X^*}(c,\eta)\mathcal{E}_{\text{char}(I_\eta)}[u,v](t) \\ &= \sum_{\eta\in X^*}\sum_{\xi\in I_\eta}(c,\eta)\mathcal{E}_\xi[u,v](t).\end{aligned}$$

Since $\eta = \sigma_X(\xi)$ for all $\xi \in I_\eta$ and using the inner product in (2.6), it then follows that

$$F_c[u+v](t) = \sum_{\eta\in X^*}\sum_{\xi\in I_\eta}(c,\sigma_X(\xi))\mathcal{E}_\xi[u,v](t) \tag{4.5}$$

$$= \left(\sum_{\eta\in X^*}\sum_{\xi\in I_\eta}(c,\sigma_X(\xi))\xi, \sum_{\eta\in X^*}\sum_{\xi\in I_\eta}\mathcal{E}_\xi[u,v](t)\xi\right). \tag{4.6}$$

As observed before, if $\eta_1 \neq \eta_2$, then I_{η_1} and I_{η_2} are disjoint, which gives

$$Z^* = \bigcup_{\eta \in X^*} I_\eta = \bigcup_{\eta \in X^*} \{\xi : \ \xi \in I_\eta\}.$$

and

$$\sum_{\xi \in Z^*} \xi = \sum_{\eta \in X^*} \sum_{\xi \in I_\eta} \xi. \tag{4.7}$$

Applying (4.7) in (4.6), one has that

$$F_c[u+v](t) = \sum_{\xi \in Z^*} (c, \sigma_X(\xi)) \mathcal{E}_\xi[u,v](t) \tag{4.8}$$

Notice that $Z^* = \bigcup_{k=0}^{\infty} \mathbb{S}_{X^*,Y^k}$, then (4.8) is equal to (4.3) which completes the proof.

■

When the input functions u and v in (4.2) are related to a common function (e.g., $u = g(w)$ and $v = h(w)$ for g and h arbitrary functions), one can write the extended Chen-Fliess series $\mathcal{F}_c[g(w), h(w)](t)$ as

$$\begin{aligned} \mathcal{F}_c[w](t) &= \mathcal{F}_c[g(w), h(w)](t) \\ &= \sum_{\eta \in Z^*} (c, \eta) \mathcal{E}_\eta[g(w), h(w)](t). \end{aligned}$$

In the current section, the closed form of the Chen-Fliess series of the sum of two inputs was provided. In the next section, this formula provides a decomposition function of a Chen-Fliess series in the mixed-monotonicity sense.

4.2 A Decomposition Function for Chen-Fliess Series

In the mixed-monotonicity approach, the decomposition function of a vector field is used to provide an overestimation of the reachable set. In the current section, a decomposition function for Chen-Fliess series is provided by separating the positive and negative parts. Then, a partial order in the function space is defined and used to work with the decomposition to obtain the overestimation of the reachable set of a Chen-Fliess series. When restricted to constant functions and a particular orthant, this partial order is equivalent to the partial order induced by the respective orthant cone.

4.2.1 Positive and Negative Parts of a Chen-Fliess Series

The next theorem provides a decomposition of a Chen-Fliess series in terms of non-decreasing and non-increasing parts.

Lemma 5 *Let* $u \in L_{\mathfrak{p}}^m[0,T]$ *and its corresponding positive and negative parts* $u^+(t) = \max\{u(t),0\}$ *and* $u^-(t) = \max\{-u(t),0\}$*, respectively. Then,* $F_c[u]$ *can be decomposed as*

$$F_c[u](t) = \mathcal{F}_{c^+}[u](t) - \mathcal{F}_{c^-}[u](t), \tag{4.9}$$

where

$$\mathcal{F}_{c^+}[u](t) = \sum_{k=0}^{\infty} \sum_{\eta \in X^*} \sum_{\xi \in \mathbb{S}_{\eta,Y^k}} (c^+, \xi)\mathcal{E}_\xi[u^+, u^-](t), \tag{4.10a}$$

$$\mathcal{F}_{c^-}[u](t) = \sum_{k=0}^{\infty} \sum_{\eta \in X^*} \sum_{\xi \in \mathbb{S}_{\eta,Y^k}} (c^-, \xi)\mathcal{E}_\xi[u^+, u^-](t). \tag{4.10b}$$

and $c^+, c^- \in \mathbb{R}\langle\langle Z \rangle\rangle$ *are such that*

$$(c^+, \xi) = \max\{(-1)^k (c, \sigma_X(\xi)), 0\}, \tag{4.11a}$$

$$(c^-, \xi) = -\min\{(-1)^k (c, \sigma_X(\xi)), 0\}. \tag{4.11b}$$

for any $\xi \in \mathbb{S}_{X^*,Y^k}$.

Proof: First, observe that $u = u^+ - u^-$. Then, from Lemma 4, it follows that

$$\begin{aligned} F_c[u](t) &= F_c[u^+ - u^-](t) \\ &= \sum_{k=0}^{\infty} \sum_{\eta \in X^*} \sum_{\xi \in \mathbb{S}_{\eta,Y^k}} (-1)^k (c, \sigma_X(\xi))\mathcal{E}_\xi[u^+, u^-](t). \end{aligned} \tag{4.12}$$

This summation can now be re-written using (4.11a) and (4.11b) as

$$\begin{aligned} F_c[u](t) = &\sum_{k=0}^{\infty} \sum_{\eta \in X^*} \sum_{\xi \in \mathbb{S}_{\eta,Y^k}} (c^+, \xi)\mathcal{E}_\xi[u^+, u^-](t) \\ &- \sum_{k=0}^{\infty} \sum_{\eta \in X^*} \sum_{\xi \in \mathbb{S}_{\eta,Y^k}} (c^-, \xi)\mathcal{E}_\xi[u^+, u^-](t), \end{aligned} \tag{4.13}$$

where (4.10a) and (4.10b) can be directly identified in (4.13). This completes the proof. ∎

This decomposition in terms of the positive and negative parts of the Chen-Fliess series presented in the current section defines a decomposition in the mixed-monotonicity sense, as seen later. A decomposition needs a partial order to overestimate the reachable set of a Chen-Fliess series in a box. In the next section, the partial order is defined.

4.2.2 Partial Order over the Set of Functions

The following partial order is useful for establishing monotonicity properties of decomposition functions of Chen-Fliess series.

Definition 40 *Let $u_1 : \mathbb{R} \to \mathbb{R}^m$ and $u_2 : \mathbb{R} \to \mathbb{R}^m$. These functions are ordered $u_1 \preceq u_2$ if and only if $u_1^+ \leq u_2^+$ and $u_1^- \leq u_2^-$, where $\leq$ is the standard order of real numbers (componentwise).*

Example 6 *Consider the function $u_1(t) = \sin(t)$ and $u_2(t) = 0.5\sin(t)$. The positive and negative parts are then $u_2^+(t) \leq u_1^+(t)$ and $u_2^-(t) \leq u_1^-(t)$. Therefore $u_2 \preceq u_1$.*

The next definition extends the notion of mixed-monotonicity to Chen-Fliess series according to the partial order in Definition 40.

Definition 41 *A Chen-Fliess series $F_c[u](t)$ is Input-Output Mixed-Monotone (IOMM) if there exists a decomposition function*

$$d[u, \hat{u}](t) : L_{\mathfrak{p}}^m[0, T] \times L_{\mathfrak{p}}^m[0, T] \to C([0, T])$$

that satisfies the following:

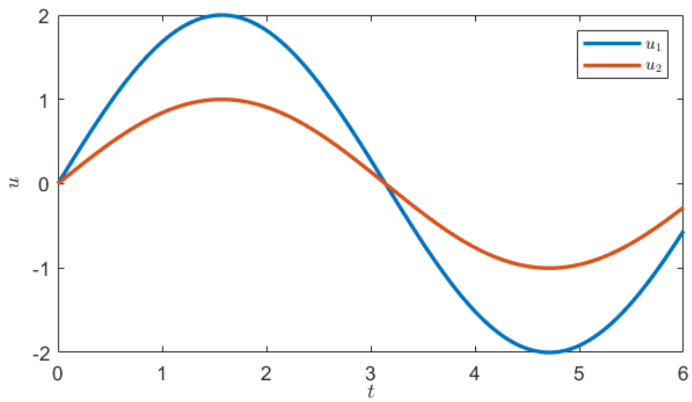


Figure 4.1: The graph shows that $u_2^+ \leq u_1^+$ and $u_2^- \leq u_1^-$, therefore $u_1 \preceq u_2$.

i. $d[u,u](t) = F_c[u](t)$,

ii. $d[u,\hat{u}](t)$ *is non-decreasing in* u,

iii. $d[u,\hat{u}](t)$ *is non-increasing in* $\hat{u}$,

where the monotonicity of the arguments is in the sense of the partial order $\preceq$ *in Definition 40.*

The partial order acts on the argument of the decomposition function of the Chen-Fliess series and later it is seen that by restricting the domain of the input the partial order is preserved for Chen-Fliess series. The decomposition function is provided in the next section.

4.2.3 The Decomposition Function

The next result provides a closed form of a decomposition function of a Chen-Fliess series that is used to obtain an overestimation of the reachable set of a system's output.

Theorem 10 *Let $c \in \mathbb{R}_{LC}\langle\langle X\rangle\rangle$ and $u \in B_{\mathfrak{p}}^{m}(R)[0,T]$. Given the Chen-Fliess series $F_c[u](t)$, the decomposition function*

$$d[u,\hat{u}](t) := \mathcal{F}_{c^+}[u](t) - \mathcal{F}_{c^-}[\hat{u}](t) \tag{4.14}$$

satisfies Definition 41, and therefore $F_c[u](t)$ is IOMM.

Proof: Notice first that since

$$|(c^+,\xi)| = \max\{|(c,\sigma_X(\xi))|,0\},$$

then $|(c^+,\xi)| = \max\{|(c,\sigma_X(\xi))|,0\} \leq KM^{|\xi|}|\xi|, \forall \xi \in Z^*$. In the same manner $|(c^-,\xi)| \leq \min\{|(c,\sigma_X(\xi))|,0\}$ and $|(c^-,\xi)| \leq KM^{|\xi|}|\xi|, \forall \xi \in Z^*$ for K, M associated with c. Therefore $c^+, c^- \in \mathbb{R}_{LC}\langle\langle Z\rangle\rangle$ and $\mathcal{F}_{c^+}[u](t)$ and $\mathcal{F}_{c^-}[u](t)$ are well-defined maps. The theorem is now proved by checking directly the properties in Definition 41. That is, condition i. holds from (4.9) in Theorem 5, where

$$d[u,\hat{u}](t)\,\Big|_{\hat{u}=u} = F_c[u](t).$$

By fixing $\hat{u}$, condition ii. is satisfied since the coefficients of $\mathcal{F}_{c^+}[u](t)$ are non-negative, and noticing that $0 \leq \mathcal{E}_\xi[u_1^+,u_1^-] \leq \mathcal{E}_\xi[u_2^+,u_2^-]$ when $u_1 \preceq u_2$ for any $\xi \in X^*$. Similarly, by fixing u, condition iii. holds since the coefficients of $\mathcal{F}_{c^-}[u](t)$ are non-negative. Hence, $F_c[u](t)$ is IOMM.

■

A Chen-Fliess series can have several decomposition functions and the one given in (4.14) is not unique (as is the case for the mixed-monotonicity property). In general

(4.14) is not the tightest but it is applicable to any Chen-Fliess series. The next corollary deals with the ordering of the decomposition function (4.14) as a consequence of the south-east order originating from $\preceq$.

Corollary 2 *Let* $c \in \mathbb{R}\langle\langle X\rangle\rangle$ *and* $u \in B_{\mathfrak{p}}^m(R)[0,T]$. *Given the Chen-Fliess series* $F_c[u](t)$ *and its decomposition* $d[u,\hat{u}]$, *if* $(u_1,\hat{u}_1) \preceq_{SE} (u_2,\hat{u}_2)$, *then* $d[u_1,\hat{u}_1] \leq d[u_2,\hat{u}_2]$.

Proof: *From the SE order definition, one has that* $u_1 \preceq u_2$ *and* $\hat{u}_2 \preceq \hat{u}_1$. *Now, from the monotonicity of the arguments in the decomposition function given in Theorem 10, one has that* $d[u_1,\hat{u}_1] \leq d[u_2,\hat{u}_1] \leq d[u_2,\hat{u}_2]$. *This completes the proof.* ■

In the next section, the partial order and the decomposition function are used together to provide an overestimation of the reachable set of a Chen-Fliess series.

4.3 Overestimation of Reachable Sets

Next, the points in the box $\mathcal{U} \subset \mathbb{R}^m$ are grouped in subsets of $\mathcal{U}$ such that each subset has a maximum element according to $\preceq$. For example, for the interval $[-1,1] \subset \mathbb{R}$, the points $\hat{u} = 1$ and $u = -1$ are not ordered as $u^+ \leq \hat{u}^+$, but $\hat{u}^- \leq u^-$ then $u \npreceq \hat{u}$ nor $\hat{u} \npreceq u$. On the other hand, by grouping the elements in two subsets as $[-1,1] = [-1,0] \cup [0,1]$, any two elements in each subset are ordered in the same subset. Notice the farther from the origin the greater. To see this, take $\hat{u} = -1$ and $u = -0.5$, then $u \preceq \hat{u}$. In general, for an orthant $K_\nu = \{x \in \mathbb{R}^m : 0 \leq (-1)^{\nu_i} x_i\}$ where $\nu = (\nu_1, \cdots, \nu_m)$ with $\nu_i \in \{0,1\}$, the partial order $\preceq$ behaves as the partial order induced by the cone orthant $\leq_{K_\nu}$. The next theorem and corollary show that (4.14) can be used to construct an over-approximation of $\text{Reach}_c(\mathcal{U})(t)$.

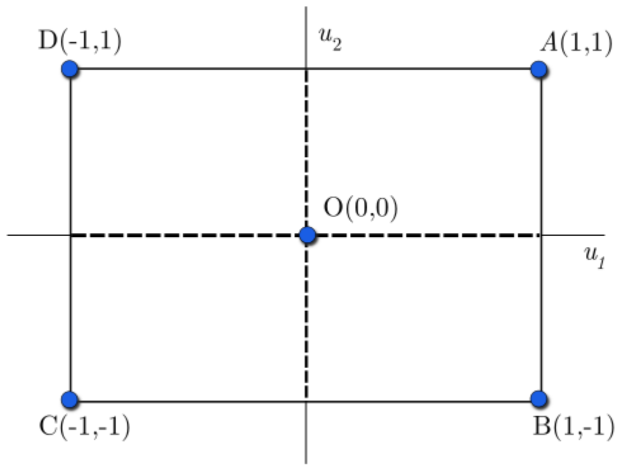


Figure 4.2: The box $[(-1,1),(1,1)]$ defined by the component-wise partial order $\leq$ is partitioned in the box $[(0,0),(1,1)],[(0,0),(1,-1)],[(0,0),(-1,-1)],[(0,0),(-1,1)]$ defined in terms of the partial order $\preceq$.

Theorem 11 *Consider the Chen-Fliess series $F_c[v](t)$ with $v \in L_{\mathfrak{p}}^m[0,T]$ taking values in the box $\mathcal{U}_\nu := [u_\nu, \hat{u}_\nu] \subset K_\nu$ for some fixed ν with partial order $\preceq$, then*

$$Reach_c(\mathcal{U}_\nu)(t) \subset \Big[d[u_\nu, \hat{u}_\nu](t), d[\hat{u}_\nu, u_\nu](t)\Big].$$

Proof: First, one has $u_\nu \preceq v(t) \preceq \hat{u}_\nu$, which implies $(u_\nu, \hat{u}_\nu) \preceq_{SE} (v(t), v(t)) \preceq_{SE} (\hat{u}_\nu, u_\nu)$ for all t. Then, from Corollary 2, it follows that

$$d[u_\nu, \hat{u}_\nu](t) \leq F_c[v](t) \leq d[\hat{u}_\nu, u_\nu](t)$$

which completes the proof. ■

Note that any box $\mathcal{U} = [u, \hat{u}] \subset \mathbb{R}^m$ can be written as $\mathcal{U} = \bigcup_{\nu \in J} \Big(\mathcal{U} \cap K_\nu\Big)$, where $J = \{(\nu_1, \ldots, \nu_m) : \nu_j \in \{0,1\}, j = 0, \ldots m\}$. Define each part of $\mathcal{U}$ in K_ν as

$[u_\nu, \hat{u}_\nu] = [u, \hat{u}] \cap K_\nu$, where $u_\nu \preceq \hat{u}_\nu$ for $u_\nu, \hat{u}_\nu \in K_\nu$.

Corollary 3 *Let $F_c[v](t)$ be a Chen-Fliess series with $v \in L_\mathfrak{p}^m[0,T]$ taking values in the box $\mathcal{U} = [u, \hat{u}] \subset \mathbb{R}^m$, it then follows that*

$$Reach_c(\mathcal{U})(t) \subset \bigcup_{\nu \in J} \Big[d[u_\nu, \hat{u}_\nu](t), d[\hat{u}_\nu, u_\nu](t) \Big],$$

where $[u_\nu, \hat{u}_\nu] = \mathcal{U} \cap K_\nu$ for all $\nu \in J$.

Proof: The proof follows directly from Theorem 11 and the fact that $\mathcal{U} = \bigcup_{\nu \in J}[u_\nu, \hat{u}_\nu]$.

■

In this chapter, a decomposition function of the Chen-Fliess series in the mixed-monotonicity sense is provided. This decomposition was obtained using the closed form of the Chen-Fliess series of the sum of two inputs. This representation allows the separation of the Chen-Fliess series into its positive and negative parts, then the domain is lifted to obtain the decomposition function. A partial order is defined that preserves the order of the decomposition function. This is used to provide an overestimation of the reachable set of a Chen-Fliess series by restricting the input domain to the orthants of the real coordinate domain and applying the decomposition in each orthant, and finally adding up each part.

Chapter 5

Chen-Fliess Calculus and Minimum Bounding Box

The current chapter is based entirely on [57]. Previously, in Chapter 4, an overestimation of the reachable set of the output of non-linear affine systems was provided by extending the concepts of mixed-monotonicity to Chen-Fliess series. This overestimating box is not the minimum bounding box of the reachable set. In the present section, the minimum bounding box is computed by optimizing the Chen-Fliess series of the system, this is, finding the minimum and maximum of $F_c[u]$ for all u taking values in the box $\mathcal{U}$. The closed form of the Fréchet and Gâteaux derivatives are obtained for this purpose. In general, this optimization problem is non-convex with respect to the input function u, and the intersection of the border of $\mathrm{Reach}_c(\mathcal{U})$ and the minimum bounding box is non-empty as seen in Figure 1.2 whenever the output set is compact.

If the optimal points are interior points u^*, then they satisfy

$$DF_c[u^*][h](t) = 0, \forall h \in B_{\mathfrak{p}}^m(R)[0,T],$$

where $DF_c[u^*][.](t)$ represents the *Fréchet derivative* of $F_c[u^*](t)$. To obtain a numerical solution, the Gâteaux derivative along with the *Gradient Descent* is used. This recursion is set for some initial condition u_0 that has the form

$$u_{i+1} = u_i - \varepsilon \nabla F_c[u_i](t), \tag{5.1}$$

where ε is the *learning* parameter and $\nabla F_c[u_i](t)$ is an appropriate gradient with respect to u of the Chen-Fliess series $F_c[u]$ for some generating series $c \in \mathbb{R}^{\ell}_{LC}\langle\langle X \rangle\rangle$. The section will first define an appropriate gradient of $F_c[u]$ to be used in (5.1) and then show that such recursion is well-posed.

In the following sections, the closed-forms of the tools from analysis are developed to solve the optimization problems.

5.1 Derivatives of Chen-Fliess series

To perform derivative-based optimization, first, the closed form of the derivative of the Chen-Fliess series needs to be obtained. Since the input domain of the Chen-Fliess series lies in a Banach space, the involved derivative is the *Fréchet derivative*, a functional map that assigns the input perturbation measure to each input perturbation direction. By assuming a particular direction, the *Gâteaux derivative* is obtained. It is proved that algebraically, these two have the same closed form. The derivatives must satisfy the next definitions.

Definition 42 *Given* $c \in \mathbb{R}\langle\langle X \rangle\rangle$ *and the input functions* $u \in L_{\mathfrak{p}}^{m}[0,t]$*, the Chen-Fliess operator is Fréchet differentiable at* $u \in B_{\mathfrak{p}}^{m}(R)[0,t]$ *if and only if there exists* $DF_c[u][.](t) : B_{\mathfrak{p}}^{m}(R)[0,t] \to \mathbb{R}$ *such that the following limit is satisfied for all* $u+h \in B_{\mathfrak{p}}^{m}(R)[0,t]$*:*

$$\lim_{h\to 0} \frac{1}{||h||_p}\Big(F_c[u+h](t) - F_c[u](t) - DF_c[u][h](t)\Big) = 0.$$

The concept of the *Gâteaux derivative* in [25] is extended to Chen-Fliess series in the next definition.

Definition 43 *Given* $c \in \mathbb{R}\langle\langle X \rangle\rangle$ *and the input functions* $u,\ v \in L_{\mathfrak{p}}^{m}[0,t]$*, the Chen-Fliess operator is Gâteaux differentiable at* u *in the direction of* v *if and only if there exists* $\frac{\partial}{\partial v}F_c[u](t) \in \mathbb{R}$ *such that the following limit is satisfied:*

$$\lim_{\varepsilon\to 0} \frac{1}{\varepsilon}\Big(F_c[u+\varepsilon v](t) - F_c[u](t) - \frac{\partial}{\partial v}F_c[u](t)\varepsilon\Big) = 0.$$

In the next sections, the closed forms of the derivatives are provided.

5.1.1 The Fréchet Derivative

Based on the formula of the Chen-Fliess series of the sum of two inputs in Lemma 4, the closed form of the Fréchet derivative is provided next.

Theorem 12 *[57] Let* X *and* Y *be alphabets associated with* $u, h \in B_{\mathfrak{p}}^{m}(R)[0,T]$*,* *respectively. The Chen-Fliess series is Fréchet differentiable if and only if*

$$\lim_{h\to 0}\frac{1}{||h||_p}\left(\sum_{k=2}^{\infty}\sum_{\eta\in X^*}\sum_{\xi\in\mathbb{S}_{\eta,Y^k}}(c,\sigma_X(\xi))\mathcal{E}_\xi[u,h](t)\right)=0,$$

and its Fréchet derivative is expressed as

$$DF_c[u][h](t)=\sum_{\eta\in X^*}\sum_{\xi\in\mathbb{S}_{\eta,Y}}(c,\sigma_X(\xi))\mathcal{E}_\xi[u,h](t),$$

whenever $c\in\mathbb{R}_{LC}\langle\langle X\rangle\rangle$.

Proof: The proof is done by a direct application of Lemma 4 and Definition 42. Consider $\delta>0$ and h such that $||h||_p<\delta$, from (4.3), it follows that

$$F_c[u+h](t)=\sum_{k=0}^{\infty}\sum_{\eta\in X^*}\sum_{\xi\in\mathbb{S}_{\eta,Y^k}}(c,\sigma_X(\xi))\mathcal{E}_\xi[u,h](t).$$

For $k=0$, one has that

$$F_c[u](t)=\sum_{\eta\in X^*}\sum_{\xi\in\mathbb{S}_{\eta,Y^0}}(c,\sigma_X(\xi))\mathcal{E}_\xi[u,h](t). \tag{5.2}$$

Note here that $\mathcal{E}_\xi[u,h]=E_\xi[u]$ since $\xi\in X^*$, which is why the left-hand side of (5.2) does not depend on h. Then, it follows that

$$F_c[u+h](t)-F_c[u](t)-\sum_{\eta\in X^*}\sum_{\xi\in\mathbb{S}_{\eta,Y}}(c,\sigma_X(\xi))\mathcal{E}_\xi[u,h](t)=$$
$$\sum_{k=2}^{\infty}\sum_{\eta\in X^*}\sum_{\xi\in\mathbb{S}_{\eta,Y^k}}(c,\sigma_X(\xi))\mathcal{E}_\xi[u,h](t).$$

Multiplying by $1/||h||_p$ and taking the limit of h to 0 gives the desired result. Finally, observe that the generating series of $DF_c[u][h](t)$ inherits the local convergent bounds of the original series c. Therefore, for $c \in \mathbb{R}^{\ell}_{LC}\langle\langle X\rangle\rangle$, the Fréchet derivative $DF_c[u][h](t)$ converges, which completes the proof. ■

The closed form of the input perturbation of the Chen-Fliess series in a particular direction is obtained next.

5.1.2 The Gâteaux Derivative

The Gâteaux derivative is obtained by assuming a particular direction in the Fréchet derivative closed formula. As shown next, algebraically, both derivatives are the same.

Corollary 4 *[54, 57] Let X and Y be alphabets associated with u, $v \in L^m_{\mathfrak{p}}[t_0, t_1]$, respectively. The Chen-Fliess series is Gâteaux differentiable in the direction of v if and only if*

$$\lim_{\varepsilon \to 0} \sum_{k=2}^{\infty} \sum_{\eta \in X^*} \sum_{\xi \in \mathbb{S}_{\eta, Y^k}} (c, \sigma_X(\xi)) \mathcal{E}_{\xi}[u, v](t)\, \varepsilon^k \;=\; 0, \tag{5.3}$$

and its Gâteaux derivative is expressed as

$$\frac{\partial}{\partial v} F_c[u](t) = \sum_{\eta \in X^*} \sum_{\xi \in \mathbb{S}_{\eta, Y}} (c, \sigma_X(\xi)) \mathcal{E}_{\xi}[u, v](t),$$

whenever $c \in \mathbb{R}_{LC}\langle\langle X\rangle\rangle$.

Proof: The proof follows directly from Theorem 12 by taking the limit in the direction of $h = \varepsilon v$ when ε tends to zero. ■

Some extra operations and notation are needed before presenting some examples about computing the Gâteaux derivative of $F_c[u](t)$. Let X and Y be alphabets as in Definition 38. For $\eta = x_{i_1} \cdots x_{i_k} \in X^k$, the set of all words formed by the substitution of r letters in η with letters in Y is denoted by

$$I_\eta^r = \{\xi \in (X \cup Y)^k : \sigma_X(\xi) = \eta,\ |\xi|_Y = r\}, \tag{5.4}$$

where σ_X is a substitution homomorphism transforming any letter in Y of ξ into its corresponding letter in X. Furthermore, one can see from (5.4) that

$$\bigcup_{r+s=k} \mathbb{S}_{X_\eta^r, Y_\eta^s} = \bigcup_{r=0}^{k} I_\eta^r.$$

Example 7 *Let $u, v \in B_{\mathfrak{p}}^m(R)[0,t]$ be associated with the alphabets X and Y, respectively. Consider the series c comprised of just one word $c = \eta = x_{i_1} \cdots x_{i_k} \in X^*$ and let the substitution homomorphism σ_Y such that $\sigma_Y(x_i) = y_i$ for $i = 1, \ldots, m$. The corresponding Chen-Fliess series for input u is $F_c[u](t) = E_\eta[u](t)$. In this example, the objective is to obtain the Gâteaux derivative of $F_c[u](t)$ showing that it satisfies (5.3). From Lemma 4 and (5.4), the variation between $E_\eta[u + \varepsilon v](t)$ and $E_\eta[u](t)$ is expressed as*

$$\frac{1}{\varepsilon}\left(E_\eta[u + \varepsilon v](t) - E_\eta[u](t)\right) = \sum_{r=1}^{k} \sum_{\xi \in I_\eta^r} \mathcal{E}_\xi[u, v](t)\, \varepsilon^{r-1}.$$

To establish (5.3), observe that for every $\xi \in I_\eta$ one has that

$$|\mathcal{E}_\xi[u, v](t)| \leq \frac{R^{|\xi|}}{|\xi|!}$$

where $R = \max\{||u_{[0,t]}||_p, ||v_{[0,t]}||_p, t\}$ *[30]. Then, assuming* $\varepsilon < 1$ *and*

$$M = \max\left\{\frac{R^{|\xi|}}{|\xi|!} : \ \xi \in I_\eta^r, \ 2 \leq r \leq k\right\},$$

the sum in (5.3) is bounded as

$$\left|\sum_{r=2}^{k} \sum_{\xi \in I_\eta^r} \mathcal{E}_\xi[u,v](t)\varepsilon^{r-1}\right| \leq (2^k - (1+k))M\varepsilon.$$

It is clear now that the limit of the sum of higher order terms when ε *goes to zero is*

$$\lim_{\varepsilon \to 0} \sum_{r=2}^{k} \sum_{\xi \in I_\eta^r} \mathcal{E}_\xi[u,v](t)\varepsilon^{r-1} = 0.$$

Therefore, the Gâteaux derivative of $F_c[u]$ *is*

$$\frac{\partial}{\partial v} E_\eta[u](t) = \sum_{\xi \in I_\eta^1} \mathcal{E}_\xi[u,v](t)$$

as stated by Corollary 4.

The next example considers computing the Fréchet derivative of the Chen-Fliess series corresponding to a linear state space system.

Example 8 *Consider the system*

$$\begin{aligned} \dot{x} &= Ax + Bu, \ x(0) = x_0 \\ y &= Cx, \end{aligned} \tag{5.5}$$

and the functions $u, v \in B_{\mathfrak{p}}(R)[0,t]$*. The Chen-Fliess series is computed using (2.5),* *and is given by*

$$F_c[u](t) = \sum_{k=0}^{\infty} CA^k x_0 \frac{t^k}{k!} + \sum_{k=0}^{\infty} CA^k B\ E_{x_0^k x_1}[u](t).$$

Note the first term on the right-hand side corresponds to the natural response, and the second term is the forced response. This representation is in agreement with what a Volterra operator gives for a linear system with analytic Kernels. To compute the Fréchet derivative, consider $\delta > 0$ *and* h *such that* $||h||_p < \delta$*. The series is perturbed as*

$$F_c[u+h](t) = \sum_{k=0}^{\infty} CA^k x_0 \frac{t^k}{k!} + \sum_{k=0}^{\infty} CA^k B\ \mathcal{E}_{x_0^k x_1}[u,h](t) + \sum_{k=0}^{\infty} CA^k B\ \mathcal{E}_{x_0^k y_1}[u,h](t).$$

Since there are no higher order terms, then the condition in Theorem 12 is satisfied, and the Fréchet derivative is

$$DF_c[u][h](t) = \sum_{k=0}^{\infty} CA^k B\ \mathcal{E}_{x_0^k y_1}[u,h](t).$$

Example 9 *Consider the scalar bilinear system*

$$\dot{x} = xu,\ \ y = x,\ \ x_0 = 1. \tag{5.6}$$

$u \in B_{\mathfrak{p}}(R)[0,t]$*. It can be easily checked that the output of the system is*

$$y(u(t)) = \exp\left(\int_0^t u(\tau)d\tau\right).$$

Starting from the Gâteaux derivative of the Chen-Fliess series as given in Corollary 4, one has that

$$\begin{aligned}
\frac{\partial}{\partial v} F_c[u](t) &= \sum_{k=0}^{\infty} \sum_{\xi \in \mathbb{S}_{x_1^k, y_1}} \mathcal{E}[u,v](t) \\
&= \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} (F_c[u+\varepsilon v](t) - F_c[u](t)) \\
&= \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \sum_{k=0}^{\infty} E_{x_1^k}[u+\varepsilon v](t) - E_{x_1^k}[u](t) \\
&= \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \sum_{k=0}^{\infty} \frac{1}{k!} \left[k! E_{x_1^k}[u+\varepsilon v](t) - k! E_{x_1^k}[u](t) \right] \\
&= \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \sum_{k=0}^{\infty} \frac{1}{k!} \left[E_{x_1^{\sqcup\sqcup k}}[u+\varepsilon v](t) - E_{x_1^{\sqcup\sqcup k}}[u](t) \right] \\
&= \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \sum_{k=0}^{\infty} \frac{1}{k!} \left[E_{x_1}[u+\varepsilon v](t)^k - E_{x_1}[u](t)^k \right].
\end{aligned}$$

The last expression is equal to

$$\begin{aligned}
&\lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \sum_{k=0}^{\infty} \frac{1}{k!} \left[\left(\int_0^t u(\tau) + \varepsilon v(\tau) d\tau \right)^k - \left(\int_0^t u(\tau) d\tau \right)^k \right] \\
&= \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \exp\left(\int_0^t u(\tau) + \varepsilon v(\tau) d\tau \right) - \exp\left(\int_0^t u(\tau) d\tau \right) \\
&= \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} (y(u(t) + \varepsilon v(t)) - y(u(t))) \\
&= \frac{dy}{dv}.
\end{aligned}$$

In the following section, the Gâteaux derivative is used to obtain the gradient.

5.1.3 The Gradient of Chen-Fliess series

The Gâteaux derivative in Corollary 4 is now used in (5.1) for the purpose of obtaining the input signal that produces the reachable sets of a Chen-Fliess series characterized by the generating series $c \in \mathbb{R}_{LC}\langle\langle X \rangle\rangle$. As a reminder, the objective is to find the minimum bounding box of the reachable set of a Chen-Fliess series such that,

$$\mathrm{Reach}_c\left(\mathcal{U}\right)(t) \subset [\underline{F}(t), \overline{F}(t)],$$

where

$$\underline{F}(t) = \min_{u \in \mathcal{U}} F_c[u](t) \quad \text{and} \quad \overline{F}(t) = \max_{u \in \mathcal{U}} F_c[u](t),$$

and $\mathcal{U}$ is a box in $\mathbb{R}^m$. Hereafter, the existence of the Gâteaux derivative in Corollary 4 is assumed.

In the following paragraphs, the gradient of a Chen-Fliess series is obtained. It is used along with a Gradient Descent algorithm to provide a solution to the optimization of a Chen-Fliess series on the box $\mathcal{U}$.

The following result is useful in the implementation of line-search optimization methods.

Corollary 5 *[54,57] Let the elementary functions $e_i : [0,T] \to \mathbb{R}^m$, such that $e_1(t) = (1, 0, \cdots, 0)^\top, \ldots, e_m(t) = (0, 0, \cdots, 1)^\top$ for all $t \in [0,T]$. The Gâteaux derivative of*

$F_c[u](t)$ in the direction of u_i is

$$\frac{\partial}{\partial u_i} F_c[u](t) = \sum_{\eta \in X^*} \sum_{\xi \in \mathbb{S}_{\eta, y_i}} (c, \sigma_X(\xi)) \mathcal{E}_\xi[u, e_i](t).$$

Example 10 *Consider $\eta = x_0 x_i \in X^2$ and the associated Chen-Fliess series $F_\eta[u](t) = E_{x_0 x_i}[u](t)$, the Gâteaux derivative in the direction of v is*

$$\frac{\partial}{\partial v} F_c[u](t) = \mathcal{E}_{x_0 y_i}[u, v](t).$$

Example 11 *Consider $\eta = x_1 x_2 \in X^2$ and the associated Chen-Fliess series $F_\eta[u](t) = E_{x_1 x_2}[u](t)$, the Gâteaux derivative in the direction of v is*

$$\frac{\partial}{\partial v} F_c[u](t) = \mathcal{E}_{y_1 x_2}[u, v](t) + \mathcal{E}_{x_1 y_2}[u, v](t).$$

The gradient of a Chen-Fliess series is therefore naturally defined as $\nabla F_c : B_{\mathfrak{p}}^m(R)[t_0, t_1] \to B_{\mathfrak{q}}^m(R)[t_0, t_1]$ such that

$$\nabla F_c[u](t) = \left(\frac{\partial}{\partial u_1} F_c[u](t), \cdots, \frac{\partial}{\partial u_m} F_c[u](t) \right)^T. \tag{5.7}$$

The next lemma provides the Gâteaux derivative of a Chen-Fliess series in an arbitrary constant direction v in terms of (5.7).

Lemma 6 *[54, 57] Consider the constant vector $v = (v_1, \cdots, v_m) \in \mathbb{R}^m$, $u \in L_{\mathfrak{p}}^m[0, t]$ and the Chen-Fliess series $F_c[u](t)$, the Gâteaux derivative and the gradient are related* *by*

$$\frac{\partial}{\partial v}F_c[u](t) = v^T\nabla F_c[u](t).$$

Proof: The proof follows directly from Corollary 4 and $\mathbb{S}_{\eta,Y} = \bigcup_{i=1}^{m}\mathbb{S}_{\eta,y_i}$. That is,

$$\begin{aligned}\frac{\partial}{\partial v}F_c[u](t) &= \sum_{\eta\in X^*}\sum_{\xi\in\mathbb{S}_{\eta,Y}}(c,\sigma_X(\xi))\mathcal{E}_\xi[u,v](t),\\ &= \sum_{i=1}^{m}v_i\left(\sum_{\eta\in X^*}\sum_{\xi\in\mathbb{S}_{\eta,y_i}}(c,\sigma_X(\xi))\mathcal{E}_\xi[u,e_i](t)\right),\\ &= v^T\nabla F_c[u](t).\end{aligned}$$

■

Example 12 *Consider the linear system (5.5) once again with $u \in L_{\mathfrak{p}}[0,t]$. The gradient of $F_c[u]$ is*

$$\begin{aligned}\nabla F_c[u](t) &= \sum_{k=0}^{\infty}CA^kB\mathcal{E}_{x_0^k y_1}[u,e_1](t),\\ &= \sum_{k=0}^{\infty}CA^kBE_{x_0^{k+1}}[u](t),\\ &= \sum_{k=0}^{\infty}CA^kB\frac{t^{k+1}}{(k+1)!}.\end{aligned}$$

Note that by integrating (5.5), the output is

$$y(t) = C\exp(-At)x_0 + \int_0^t C\exp A(t-\tau)Bu(\tau)d\tau.$$

Taking the derivative with respect to u gives

$$\frac{dy}{du} = \int_0^t C \exp A(t-\tau)B d\tau,$$

which coincides with the expression obtained using (5.7). This is,

$$\frac{dy}{du} = \nabla F_c[u](t).$$

In the next section, the approximation of the Chen-Fliess series using derivatives is addressed. A useful tool to provide an algebraic proof of the mean value theorem is presented.

5.2 First-Order Approximation of Chen-Fliess Series

In the current section, the input perturbation of the Chen-Fliess series is approximated and a tool to proof the mean value theorem is provided. From Lemma 6 and assuming the conditions of Corollary 4, it is easy to see that

$$F_c[u+\varepsilon v] = F_c[u] + v^T \nabla F_c[u](t)\varepsilon + \sum_{k=2}^{\infty} \sum_{\eta \in X^*} \sum_{\xi \in \mathbb{S}_{\eta, Y^k}} (c, \sigma_X(\xi))\mathcal{E}_\xi[u,v](t)\varepsilon^k. \quad (5.8)$$

As the limit of the higher order terms (rightmost term in (5.8)) is zero, then, for a small $\varepsilon > 0$, it follows that

$$F_c[u+\varepsilon v] \approx F_c[u] + v^T \nabla F_c[u](t)\varepsilon.$$

The following result is a tool to provide an algebraic proof of the mean value theorem.

Lemma 7 *[57] Let $r \in \mathbb{R}$, $c \in \mathbb{R}^{\ell}\langle\langle X \rangle\rangle$, and X and Y be alphabets associated to $u \in L_{\mathfrak{p}}^{m}[t_0, t_1]$ and $h \in B_{\mathfrak{p}}^{m}(R)[t_0, t_1]$, respectively. It follows that*

$$DF_c[u + rh][h](t) = \sum_{k=1}^{\infty} \sum_{\xi \in \mathbb{S}_{X^*,Y^k}} kr^{k-1}(c, \sigma_X(\xi))\mathcal{E}_\xi[u, h](t).$$

Proof: Let $\xi = x_{i_1} \cdots y_{i_j} \cdots x_{i_n} \in \mathbb{S}_{X^{n-1},Y}$ such that

$$J_\xi = \{z_1 \cdots z_j \cdots z_n \in (X \cup Y)^n : z_j = y_{i_j}, z_r \in \{x_{i_r}, y_{i_r}\} \forall r \neq j\}.$$

First it is proved that if $\xi \in \mathbb{S}_{X^*,Y}$ then

$$\mathcal{E}_\xi[u + rh, h](t) = \sum_{\zeta \in J_\xi} r^{|\zeta|_Y - 1}\mathcal{E}_\zeta[u, h](t). \tag{5.9}$$

The proof follows by induction on the length of the word. Consider $\xi \in \mathbb{S}_{X^*,Y}$ with $|\xi| = 1$, $\xi = y_j$, then $J_\xi = \{y_j\}$, then

$$\begin{aligned}\mathcal{E}_\xi[u + rh, h](t) &= \int_0^t h_j(\tau)d\tau \\ &= \sum_{\zeta \in J_\xi} r^{|\zeta|_Y - 1}\mathcal{E}_\zeta[u, h](t).\end{aligned}$$

Now assume that (5.9) holds true for any $\xi' \in X^*, Y$ such that $|\xi'| = k$. Computing the expression for $\xi = x_i\xi'$ gives

$$\mathcal{E}_\xi[u+rh, h](t) = \int_0^t (u_i(\tau) + rh_i(\tau))\mathcal{E}_{\xi'}[u + rh, h](\tau)d\tau.$$

Since $|\xi'| = k$ and by the induction hypothesis, one has that

$$\mathcal{E}_\xi[u + rh, h](t) = \int_0^t (u_i(\tau) + rh_i(\tau)) \sum_{\zeta \in J_{\xi'}} r^{|\zeta|_Y - 1} \mathcal{E}_\zeta[u, h](\tau) d\tau.$$

Using linearity and the iterated integral in (4.1) over $(X \cup Y)^*$, it follows that

$$\begin{aligned}
\mathcal{E}_\xi[u + rh, h](t) &= \sum_{\zeta \in J_{\xi'}} r^{|x_i\zeta|_Y - 1} \mathcal{E}_{x_i\zeta}[u, h](\tau) + r^{|y_i\zeta|_Y - 1} \mathcal{E}_{y_i\zeta}[u, h](\tau) d\tau \\
&= \sum_{\zeta \in J_\xi} r^{|\zeta|_Y - 1} \mathcal{E}_\zeta[u, h](\tau) d\tau.
\end{aligned}$$

The Fréchet derivative is now expressed in terms of (5.9) as

$$\begin{aligned}
DF_c[u + rh][h](t) &= \sum_{\xi \in \mathbb{S}_{X^*,Y}} (c, \sigma_X(\xi)) \mathcal{E}_\xi[u + rh, h](t), \\
&= \sum_{\xi \in \mathbb{S}_{X^*,Y}} \sum_{\zeta \in J_\xi} r^{|\zeta|_Y - 1} (c, \sigma_X(\zeta)) \mathcal{E}_\zeta[u, h](t).
\end{aligned}$$

Now it is showed that for each $\xi \in \mathbb{S}_{X^*,Y}$, the elements of $\zeta \in J_\xi$ repeat $|\zeta|_Y$ times in the series. Assume $\xi \in \mathbb{S}_{X^*,Y^k}$ such that $\xi = x_{i_1} \cdots y_{j_1} \cdots x_{i_{m-1}} \cdots y_{j_k} \cdots x_{i_m}$. Consider the word $\xi_{y_{j_r}}$ formed from ξ after substituting all letters in Y except for y_{j_r} with $\sigma_X(y_{j_1}) = x_{j_1} \cdots \sigma_X(y_{j_k}) = x_{j_k}$. This is, $\xi_{y_{j_r}} = x_{i_1} \cdots x_{j_1} \cdots x_{i_{m-1}} \cdots y_{j_r} \cdots x_{j_k} \cdots x_{i_m}$. Then by definition, $\xi \in J_{\xi_{j_r}}$ for all $r \in \{1, \cdots k\}$. Note that these are the only sets formed from elements of $\mathbb{S}_{X^*,Y}$. Therefore, $\xi \in \mathbb{S}_{X^*,Y^k}$ appears k times in $\bigcup_{\xi \in \mathbb{S}_{X^*,Y}} J_\xi$, which implies that

$$DF_c[u + rh][h](t) = \sum_{k=1}^{\infty} \sum_{\xi \in \mathbb{S}_{X^*,Y^k}} k r^{k-1} (c, \sigma_X(\xi)) \mathcal{E}_\xi[u, h](t).$$

This completes the proof. ■

In the next section, Lemma 7 is used to prove the mean value theorem for Chen-Fliess series.

5.2.1 The Mean Value Theorem

The local monotonicity of the Chen-Fliess series is expressed in terms of the sign of the Fréchet derivative. This is done by proving the mean value theorem for Chen-Fliess series. The next result is an alternative proof of the mean value theorem by an algebraic avenue using Lemma 4 instead of the classical proof from the book using the chain rule. This proof forces us to compute the closed form of the Fréchet derivative of the sum of two input functions which helps obtain the closed form of higher derivatives of the Chen-Fliess series, in the next chapter.

Theorem 13 *[57] Consider the open convex set $\mathcal{U} \subset L_{\mathfrak{p}}^m[0,t]$, $u \in \mathcal{U}$ and $c \in \mathbb{R}_{LC}\langle\langle X\rangle\rangle$, $\delta > 0$ and $h \in B_{\mathfrak{p}}^m(R)[0,t]$ such that $||h||_{\mathfrak{p}} < \delta$ and $u+h \in \mathcal{U}$. Then there exists $\varepsilon_0 \in (0,1)$ such that*

$$F_c[u+h](t) = F_c[u](t) + DF_c[u+\varepsilon_0 h][h](t).$$

Proof: The theorem is proved by an application of Rolle's theorem [9] and a continuity argument. Basically, any continuous function that is zero when evaluated at the two extreme points of an interval $[0,1]$ must have a point $\varepsilon_0 \in (0,1)$ where its derivative is zero. Define the function $\phi : \mathbb{R} \to \mathbb{R}$ as

$$\phi(\gamma) = \int_0^\gamma DF_c[u+rh][h](t)dr - (F_c[u+h](t) - F_c[u](t))\gamma. \tag{5.10}$$

Applying Lemmas 6 and 7 to the term inside the integral in (5.10) gives

$$DF_c[u+rh][h](t) = DF_c[u][h](t) + \sum_{k=2}^{\infty} \sum_{\xi \in \mathbb{S}_{X^*,Y^k}} kr^{k-1}(c, \sigma_X(\xi))\mathcal{E}_\xi[u,v](t).$$

Integrating with respect to r, it follows that

$$\int_0^\gamma DF_c[u+rh][h](t)dr = DF_c[u][h](t)\gamma + \sum_{k=2}^{\infty} \sum_{\xi \in \mathbb{S}_{X^*,Y^k}} (c, \sigma_X(\xi))\mathcal{E}_\xi[u,v](t)\gamma^k. \quad (5.11)$$

Using equation (5.8), the second term in the right hand side of (5.10) can also be written as

$$(F_c[u+h](t) - F_c[u](t))\gamma = DF_c[u][h](t)\gamma + \sum_{k=2}^{\infty} \sum_{\xi \in \mathbb{S}_{X^*,Y^k}} (c, \sigma_X(\xi))\mathcal{E}_\xi[u,h](t)\gamma. \quad (5.12)$$

The fact that $\phi(1) = 0$ follows from using (5.11), (5.12) and making $\gamma = 1$ in (5.10). Also, it is easy to see that $\phi(0) = 0$. Thus, by the continuity of $F_c[u]$, Rolle's Theorem guarantees the existence of $\varepsilon_0 \in (0,1)$ such that $\phi'(\varepsilon_0) = 0$. This implies that

$$DF_c[u+\varepsilon_0 h][h](t) - (F_c[u+h](t) - F_c[u](t)) = 0.$$

Solving for $F_c[u+h](t)$ completes the proof. ■

The procedure of the proof can be used to provide an approximation by means of the gradient of a Chen-Fliess series.

Corollary 6 *[57] Consider the constant vector $v \in \mathbb{R}^m$, the function $u \in B_{\mathfrak{p}}^m(R)[0,t]$*

and $c \in \mathbb{R}_{LC}\langle\langle X \rangle\rangle$. *Then there exists* $\varepsilon_0 \in (0, \varepsilon)$ *such that*

$$F_c[u + \varepsilon v](t) = F_c[u](t) + v^T \nabla F_c[u + \varepsilon_0 v](t)\varepsilon.$$

Proof: From Theorem 13 and the fact that

$$DF_c[u + rv][v](t) = \frac{\partial}{\partial v} F_c[u + rv](t),$$

consider the function $\phi : \mathbb{R} \to \mathbb{R}$ over interval $[0, \varepsilon]$ given by

$$\phi(\gamma) = \int_0^\gamma v^T \nabla F_c[u + rv](t)\varepsilon dr - (F_c[u + \varepsilon v](t) - F_c[u](t))\gamma. \tag{5.13}$$

The result follows by applying Rolle's Theorem to (5.13). ■

Corollary 6 reveals the fact that if $v^T \nabla F_c[u](t) < 0$, then there exists a neighborhood of u for which the Chen-Fliess series $F_c[u](t)$ decreases in the direccion of v. More explicitly, taking $\bar{\varepsilon}$ small enough such that $u + \bar{\varepsilon} v$ is still inside this neighborhood of u, from Corollary 6, it follows that there exists an $\bar{\varepsilon}_0 \in (0, \bar{\varepsilon})$ such that $F_c[u + \bar{\varepsilon} v] = F_c[u] + v^T \nabla F_c[u + \bar{\varepsilon}_0 v](t)\varepsilon$. As $v^T \nabla F_c[u + \bar{\varepsilon}_0 v](t) < 0$, then $F_c[u + \bar{\varepsilon} v] < F_c[u]$.

In the next section, the use of gradient descent algorithm is outlined for Chen-Fliess series.

5.3 The Gradient Descent Algorithm

In the following paragraphs, the optimization is performed for each coordinate of the output separately. This is,

$$\min_{u \in \mathcal{U}} F_{c_i}[u](t)$$

The direction of the greatest decrease in equation (5.8) is $v = -\nabla F_c[u](t)/||\nabla F_c[u](t)||$ which is obtained by solving

$$\begin{aligned} &\min v^T \nabla F_c[u](t) \\ &\text{s.t.} \quad ||v|| \leq 1. \end{aligned}$$

The optimal value is then obtained continuing in such direction with an appropriate choice of ε. Finding an input u such that the gradient is zero reduces to the search of a fixed-point of the function $\Phi : L_{\mathfrak{p}}^m[t_0, t_1] \to L_{\mathfrak{p}}^m[t_0, t_1]$ such that

$$\Phi[u] = u - \varepsilon \nabla F_c[u](t).$$

Furthermore, if Φ is a contraction, then the sequence

$$u_{i+1} = u_i - \varepsilon \nabla F_c[u_i](t) \tag{5.14}$$

converges to such fixed point. Based on this recursion, a gradient descent algorithm on Chen-Fliess series can be formulated as follows:

Algorithm 1 Gradient Descent

Input: N_{GD}, u_0, ε, v, $\mathcal{U}$

Initialization : u_0

for $i = 1$ to N_{GD} **do**

  $u_{i+1} = u_i - \varepsilon \nabla F_c[u_i](t)$,

  $u_{i+1} \leftarrow \text{sat}_{\mathcal{U}}(u_{i+1})$

end for

return $F_c[u_{N_{GD}}](t)$

Here $\mathcal{U}$ is a box defined by its lower and upper limits given, respectively, by $\underline{u} \in \mathbb{R}^m$ and $\overline{u} \in \mathbb{R}^m$, and the function $\text{sat}_{\mathcal{U}}$ is defined componentwise as

$$\text{sat}_{\mathcal{U}}(u) = \begin{cases} \overline{u}, & u > \overline{u}, \\ u, & u \in \mathcal{U}, \\ \underline{u} & u < \underline{u}. \end{cases}$$

Algorithm 1 gives $\underline{F}(t)$ and $\overline{F}(t)$, which gives the minimum bounding box.

5.4 Independence of the Optimization Order

In this section, it is proved that the optimal input function of the Chen-Fliess series in a time interval is equal to the sum of the optimal input functions of any partition of the convergent time interval.

Theorem 14 *Consider* $c \in \mathbb{R}_{LC}\langle\langle X \rangle\rangle$, $\mathcal{U} \subset B_{\mathfrak{p}}^m(R)[0,t]$ *and a partition* $\{t_k\}_{k=1}^N$ *of* *the interval* $[0, t]$*, then*

$$\min_{\mathcal{U}} F_c[u](t) = \sum_{k=1}^{N-1} \min_{\mathcal{U}_i} F_c[u](t_i, t_{i+1})$$

where $\mathcal{U}_i \subset B_{\mathfrak{p}}^m(R)[t_i, t_{i+1}]$*.*

Proof: *Notice that, in general, for* $u \in \mathcal{U}$*,*

$$\sum_{k=1}^{N-1} \min_{\mathcal{U}_i} F_c[u](t_i, t_{i+1}) \leq F_c[u](t)$$

then

$$\sum_{k=1}^{N-1} \min_{\mathcal{U}_i} F_c[u](t_i, t_{i+1}) \leq \min_{\mathcal{U}} F_c[u](t). \tag{5.15}$$

Now consider the $u^*(t) := u_1^*(t_1, t_2)\# \cdots \# u_N^*(t_{N-1}, t_N)$ *where each function* $u_i(t_i, t_{i+1})^* = \arg\min_{\mathcal{U}} F_c[u](t_i, t_{i+1})$ *and # is the operator that concatenates paths. To prove that the equality holds in (5.15), a function* $u \in \mathcal{U}$ *has to be found to satisfy the equality. The candidate is* $u^*(t)$*. Notice that*

$$\sum_{k=1}^{N-1} \min_{\mathcal{U}_i} F_c[u](t_i, t_{i+1}) = F_c[u^*](t).$$

since $u^*(t) \in \mathcal{U}$*, then the theorem is proved.*

■

This result reduces the optimization of Chen-Fliess series over the convergence time interval to the optimization of Chen-Fliess series over smaller intervals. This is useful to approximate the optimal input function by optimizing over the set of constant functions under the appropriate conditions.

In the next section, examples of the computation of the minimum bounding box are provided.

5.5 Numerical Simulations

This section presents two examples illustrating how IOMM and the gradient descent are used to compute overestimations of the reachable sets of dynamical systems. The results are compared to the overestimating sets using mixed-monotonicity. The first example considers the single input single output bilinear system seen in Example 9. The second example then considers the dynamics of a multiple input multiple output Lotka-Volterra system. In both examples, the formalism for the optimization of Chen-Fliess series via the gradient descent algorithm provides the minimum bounding box of the corresponding reachable sets.

Example 13 *Consider the bilinear state space system in example 9. This system was first presented in [20] in the context of interconnection of systems. Assume the input u is constrained to the interval $u \in [-1, 1]$. From (2.5), the Chen-Fliess series of the system is*

$$F_c[u] = 1 + \sum_{k=1}^{\infty} E_{x_1^k}[u](t), \tag{5.16}$$

where $(c, \eta) = 1$ for all $\eta \in X^*$. Note also that $c \in \mathbb{R}_{GC}\langle\langle X \rangle\rangle$, and thus the output is well-defined for all times.

For the IOMM approach, the coefficients of the decomposition function are ob-

tained from (4.11).

$$(c^+,\xi) = \begin{cases} 1, & |\xi|_{y_1} \ \textit{even} \\ 0, & |\xi|_{y_1} \ \textit{odd} \end{cases},$$

$$(c^-,\xi) = \begin{cases} 0, & |\xi|_{y_1} \ \textit{even} \\ 1, & |\xi|_{y_1} \ \textit{odd} \end{cases}.$$

From (4.10), the decomposition function is given by $d[u,\hat{u}](t) = \mathcal{F}_{c^+}[u](t) - \mathcal{F}_{c^-}[u](t)$*, where*

$$\mathcal{F}_{c^+}[u](t) = 1 + \sum_{k\ \textit{even}} \sum_{r=0}^{\infty} \sum_{\xi \in \mathbb{S}_{x_1^r, y_1^k}} \mathcal{E}_{\xi}[u^+,u^-](t),$$

$$\mathcal{F}_{c^-}[u](t) = \sum_{k\ \textit{odd}} \sum_{r=0}^{\infty} \sum_{\xi \in \mathbb{S}_{x_1^r, y_1^k}} \mathcal{E}_{\xi}[u^+,u^-](t).$$

From Corollary 3, the interval $[-1,1]$ *in terms of the component-wise partial order* $\leq$ *in section 7 is expressed as the union of* $[0,1]$ *and* $[0,-1]$ *in terms of the partial order* $\preceq$ *in Definition 40. Then, the reachable set satisfies the following inclusion*

$$\textit{Reach}_c([-1,1])(t) \subset \Big[d[0,1](t), d[1,0](t)\Big] \cup \Big[d[0,-1](t), d[-1,0](t)\Big],$$

which implies that

$$\textit{Reach}_c([-1,1])(t) \subset \Big[\min\{d[0,1](t), d[0,-1](t)\}, \max\{d[1,0](t), d[-1,0](t)\}\Big].$$

This is depicted in Fig. 5.1, where clearly the magenta and cyan lines lower and upper *bound the reachable sets of (5.6). As expected, the boundaries created by the IOMM overapproximations are conservative.*

On the other hand, the gradient descent algorithm requires the gradient of (5.16). From Corollary 4, the Gâteaux derivative of (5.16) is

$$\frac{\partial}{\partial v} F_c[u] = \sum_{k=0}^{\infty} \sum_{\xi \in \mathbb{S}_{x_1^k, y_1}} \mathcal{E}_\xi[u,v](t).$$

This expression is used in Algorithm 1 to compute the input that produces the maximum and minimum values of $F_c[u](t)$ *over time. One finds the maximum by flipping the sign of the increment in the gradient descent recursion. Fig. 5.1 shows the result of the algorithm. For comparison purposes and according to Definition 33 for the mixed-monotonicity methodology, the embedding system for (5.6) is found to be*

$$\dot{x} = xu, \ \dot{\hat{x}} = \hat{x}\hat{u} \tag{5.17}$$

Selecting as the initial set of states equal to $(x_0, \hat{x}_0) = (1, 1)$ *in order to match the conditions for the IOMM and gradient descent methods. From Theorem 6, the reachable set of (5.6) for inputs in* $\mathcal{U} = [-1, 1]$ *is the solution to the embedding system (5.17). Fig. 5.1 shows such solutions in relation to the ones obtained from the IOMM and gradient descent methods. The mixed-monotonicity and the Chen-Fliess series gradient descent approaches coincide for a step size of* $\varepsilon = 0.1$, $N_{GD} = 100$. *A truncation length of* $N = 5$ *for the Chen-Fliess series was used, which gave the same minimum bounding box as the mixed-monotonicity approach.*

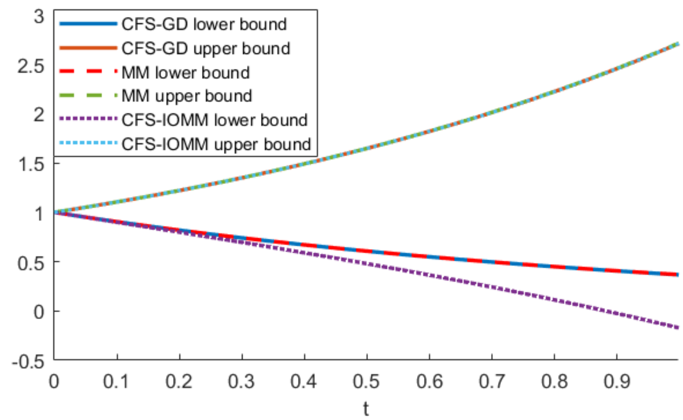


Figure 5.1: Estimation of the reachable set of the system in Example 13 with initial state $x_0 = 1$ and inputs in $\mathcal{U} = [-1, 1]$ by three approaches: mixed-monotonicity (MM), IOMM with word truncation $N = 5$, and the optimization of the Chen-Fliess series with the gradient descent algorithm (CFS-GD) for $N_{GD} = 100$ iterations, step of $\varepsilon = 0.1$, initial value of $u_0 = 0$ and same word truncation as in the IOMM method (CFS-IOMM).

Example 14 *Consider the following MIMO Lotka-Volterra system given by*

$$\dot{x}_1 = -x_1 x_2 + x_1 u_1, \tag{5.18a}$$

$$\dot{x}_2 = x_1 x_2 - x_2 u_2, \tag{5.18b}$$

$$y = x \tag{5.18c}$$

with initial condition $x_0 = (1/6, 1/6)^\top$. The Chen-Fliess series representing the out-

puts y_1 and y_2 of the Lotka-Volterra systems are given by

$$\begin{aligned}
F_{c_1}[u](t) =& 0.1667 - 0.0278E_{x_0}[u](t) + 0.1667E_{x_1}[u](t) + \\
& - 0.0278E_{x_0x_1}[u](t) - 0.0278E_{x_1x_0}[u](t) + \\
& + 0.1667E_{x_1x_1}[u](t) + 0.0278E_{x_2x_0}[u](t) + \\
& + 0.0015E_{x_0x_0x_0}[u](t) + \cdots \\
F_{c_2}[u](t) =& 0.1667 + 0.0278E_{x_0}[u](t) - 0.1667E_{x_2}[u](t) + \\
& - 0.0278E_{x_0x_2}[u](t) + 0.0278E_{x_1x_0}[u](t) + \\
& - 0.0278E_{x_2x_0}[u] + 0.1667E_{x_2x_2}[u](t) + \\
& - 0.0015E_{x_0x_0x_0}[u](t) + \cdots
\end{aligned}$$

From corollary (4), the Gâteaux derivatives are the following:

$$\begin{aligned}
\frac{\partial}{\partial v}F_{c_1}[u] =& 0.1667\mathcal{E}_{y_1}[u,v](t) - 0.0278\mathcal{E}_{x_0y_1}[u,v](t) + \\
& - 0.0278\mathcal{E}_{y_1x_0}[u,v](t) + 0.1667\mathcal{E}_{y_1x_1}[u,v](t) + \\
& + 0.1667\mathcal{E}_{x_1y_1}[u,v](t)(t) + 0.0278\mathcal{E}_{y_2x_0}[u,v](t) + \\
& - 0.0278\mathcal{E}_{x_0y_1x_1}[u,v](t)\cdots, \\
\frac{\partial}{\partial v}F_{c_2}[u] =& - 0.1667\mathcal{E}_{y_2}[u,v](t) - 0.0278\mathcal{E}_{x_0y_2}[u,v](t) + \\
& + 0.0278\mathcal{E}_{y_1x_0}[u,v](t) - 0.0278\mathcal{E}_{y_2x_0}[u,v](t) + \\
& + 0.1667\mathcal{E}_{x_2y_2}[u,v](t) + 0.1667\mathcal{E}_{y_2x_2}[u,v](t) + \\
& + 0.0278\mathcal{E}_{x_0y_2x_2}[u,v](t)\cdots.
\end{aligned}$$

According to the mixed-monotonicity method and Theorem 5, the decomposition func-

tion of (5.18) is

$$d_1(x, u, \hat{x}, \hat{u}) = -x_1\hat{x}_2 + x_1u_1$$

$$d_2(x, u, \hat{x}, \hat{u}) = x_2x_1 - x_2\hat{u}_2.$$

Thus, from Definition 33, it follows that the embedding system has the form

$$\dot{x}_1 = d_1(x, u, \hat{x}, \hat{u}), \;\; \dot{x}_2 = d_2(x, u, \hat{x}, \hat{u}),$$

$$\dot{\hat{x}}_1 = d_1(\hat{x}, \hat{u}, x, u), \;\; \dot{\hat{x}}_2 = d_2(\hat{x}, \hat{u}, x, u).$$

The mixed-monotonicity overestimation of the reachable sets using the initial set

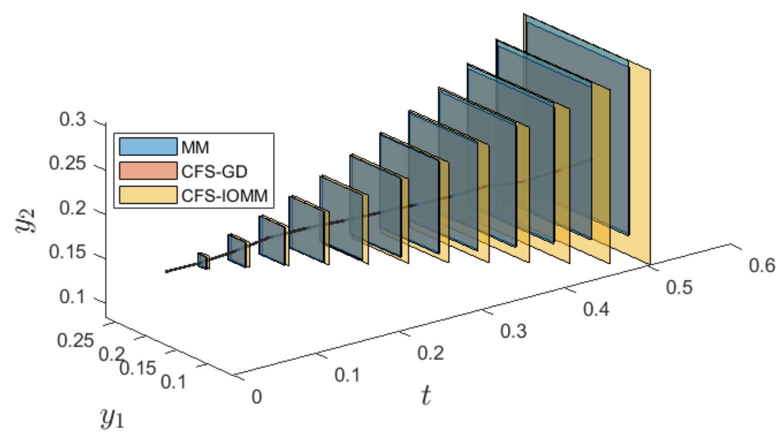


Figure 5.2: Estimation of the reachable set of the system in Example 14 with inputs satisfying $-1 \leq u_1(t) \leq 1$, $-1 \leq u_2(t) \leq 1$. The three approaches shown are mixed-monotonicity (MM); gradient descent (GD) with $N_{GD} = 100$ iterations, $\varepsilon = (0.1, 1)$, $u_0 = (0, 0)$, and truncation length $N = 5$; and IOMM with the same truncation as the gradient descent method.

$(x_{1,0}, x_{2,0}, \hat{x}_{1,0}, \hat{x}_{2,0}) = (1/6, 1/6, 1/6, 1/6)$ is given in Fig. 5.2. For the IOMM approach, the input box $[(-1,-1),(1,1)]$ defined in terms of the coordinate-wise partial order $\leq$ was decomposed as the union of boxes $[(0,0),(1,1)] \cup [(0,0),(-1,1)] \cup [(0,0),(-1,-1)] \cup [(0,0),(1,-1)]$ defined in terms of the partial order $\preceq$. Then

$$Reach_{c_i}([(-1,-1),(1,1)])(t) \subset [\underline{L}_i, \overline{L}_i], \text{ for } i \in \{1,2\}$$

where the bounds of the intervals are given in terms of the decomposition function (4.11). Thus,

$$\begin{aligned}\underline{L}_i = \min\{&d_{c_i}[(0,0),(1,1)](t), d_{c_i}[(0,0),(-1,1)](t),\\ &d_{c_i}[(0,0),(-1,-1)](t), d_{c_i}[(0,0),(1,-1)](t)\},\\ \overline{L}_i = \max\{&d_{c_i}[(1,1),(0,0)](t), d_{c_i}[(-1,1),(0,0)](t),\\ &d_{c_i}[(-1,-1),(0,0)](t), d_{c_i}[(1,-1),(0,0)](t)\},\end{aligned}$$

and from Lemma 5, the Chen-Fliess series decomposition functions are

$$\begin{aligned}d_{c_1}[u,\hat{u}] &= \mathcal{F}_{c_1^+}[u](t) - \mathcal{F}_{c_1^-}[\hat{u}](t)\\ d_{c_2}[u,\hat{u}] &= \mathcal{F}_{c_2^+}[u](t) - \mathcal{F}_{c_2^-}[\hat{u}](t)\end{aligned}$$

with

$$
\begin{aligned}
\mathcal{F}_{c_1^+}[u](t) = {} & 0.1667 + 0.1667\mathcal{E}_{x_1}[u^+, u^-](t) + \\
& + 0.0278\mathcal{E}_{x_0y_1}[u^+, u^-](t) + 0.1667\mathcal{E}_{x_1x_1}[u^+, u^-](t) + \\
& + 0.0278\mathcal{E}_{x_2x_0}[u^+, u^-](t) + 0.0278\mathcal{E}_{y_1x_0}[u^+, u^-](t) + \\
& + 0.1667\mathcal{E}_{y_1y_1}[u^+, u^-](t) + \cdots, \\
\mathcal{F}_{c_1^-}[u](t) = {} & 0.0278\mathcal{E}_{x_0}[u^+, u^-](t) + 0.1667\mathcal{E}_{y_1}[u^+, u^-](t) + \\
& + 0.0278\mathcal{E}_{x_0x_1}[u^+, u^-](t) + 0.0278\mathcal{E}_{x_1x_0}[u^+, u^-](t) + \\
& + 0.1667\mathcal{E}_{x_1y_1}[u^+, u^-](t) + 0.1667\mathcal{E}_{y_1x_1}[u^+, u^-](t) + \\
& + 0.0278\mathcal{E}_{y_2x_0}[u^+, u^-](t) + \cdots,
\end{aligned}
$$

$$
\begin{aligned}
\mathcal{F}_{c_2^+}[u](t) = {} & 0.1667 + 0.0278\mathcal{E}_{x_0}[u^+, u^-](t) + \\
& + 1.667\mathcal{E}_{y_2}[u^+, u^-](t) + 0.0278\mathcal{E}_{x_0y_2}[u^+, u^-](t) + \\
& + 0.0278\mathcal{E}_{x_1x_0}[u^+, u^-](t) + 0.1667\mathcal{E}_{x_2y_2}[u^+, u^-](t) + \\
& + 0.0278\mathcal{E}_{y_2x_0}[u^+, u^-](t) + \cdots, \\
\mathcal{F}_{c_2^-}[u](t) = {} & 1.667\mathcal{E}_{x_2}[u^+, u^-](t) + 0.0278\mathcal{E}_{x_0x_2}[u^+, u^-](t) + \\
& + 0.0278\mathcal{E}_{x_2x_0}[u^+, u^-](t) + 0.1667\mathcal{E}_{x_2y_2}[u^+, u^-](t) + \\
& + 0.1667\mathcal{E}_{x_2y_2}[u^+, u^-](t) + 0.0278\mathcal{E}_{y_1x_0}[u^+, u^-](t) + \\
& + 0.1667\mathcal{E}_{y_2x_2}[u^+, u^-](t) + \cdots.
\end{aligned}
$$

Fig. 5.2 shows an overlaying of overestimations of the reachable sets of (5.18) obtained using mixed-monotonicity, IOMM, and gradient descent of Chen-Fliess series

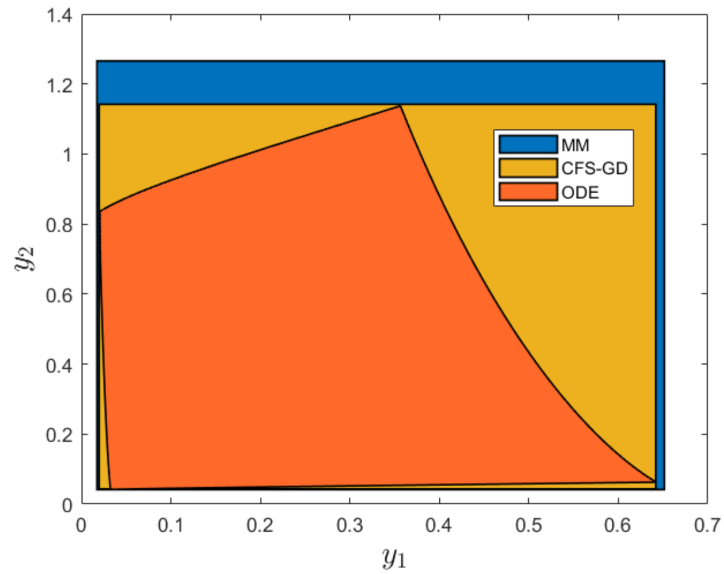


Figure 5.3: Estimation of the reachable set of the system in Example 14 for $t = 1.5s$ with initial state $x_0 = (1/6, 1/6)$ and inputs satisfying $-1 \leq u_1(t) \leq 1$, $-1 \leq u_2(t) \leq 1$. The three approaches shown are mixed-monotonicity (MM), gradient descent (CFS-GD), and the brute force computation of the output reachable set directly from solving the corresponding ODE. For the gradient descent method $N_{GD} = 10000$ iterations were used, $\varepsilon = (0.01, 0.04)$, $u_0 = (0, 0)$, and the truncation length was $N = 8$.

up to $t = 0.5s$. It can be seen that the three approaches are very closed to each other for small time horizons, then they start to diverge from each other as time passes. In Fig. 5.3, the true reachable set of system (5.18) for $t = 1.5s$ along with the gradient descent of Chen-Fliess series and the mixed-monotonicity approach are presented. The truncation length of $N = 8$ was selected due to the negligible error between the solution of (5.18) using standard numerical ODE solvers and the truncated Chen-Fliess representation at $t = 1.5$. It can be clearly observed that the gradient descent of Chen-Fliess series provides the minimum bounding box of the reachable set while the mixed-monotonicity approach is strictly larger than the minimum bounding box despite being tight as in Definition 34.

In the current chapter, the closed form of the derivatives of Chen-Fliess series were provided. These are the Fréchet, the Gâteaux, and the gradient. Also, an algebraic proof of the mean value theorem was given. The gradient descent was used to obtain the minimum bounding box of the reachable set of a Chen-Fliess series. Finally, the independence of the order of optimization within a time interval partition was proved.

Chapter 6

Calculus Over Power Series

This chapter is based on [55, 58]. The goal is to introduce an algebraic framework for describing the derivatives of a Chen-Fliess series introduced in Chapter 5 and also the higher order derivatives. For this, a derivation on the monoid is defined which helps provide a derivative rule for Chen-Fliess series. With this, the second order derivative is used together with the trust region optimization algorithm to provide the minimum bounding box of a reachable set. Hereafter, it is assumed without loss of generality that $\ell = 1$ since all the following formulations can be applied componentwise.

6.1 Differential Monoids

Motivated by the description of *differential fields* in [16], a differential algebraic structure based on a monoid structure is presented next. Consider the monoid $(X^*, \odot, \emptyset)$ with an alphabet $X = \{x_0, x_1, \cdots, x_m\}$, associate a differential alphabet to X by defining the set of letters $\delta X = \{\delta x_1, \cdots, \delta x_m\}$, and set $Z = X \cup \delta X$.

6.1.1 Derivation

The next definition satisfies the Leibniz rule of derivation.

Definition 44 *[55, 58] Let $\eta \in Z^*$ such that $|\eta|_X = n_1 \geq 1$ and $|\eta|_{\delta X} = n_2$ and consider the language*

$$L_\eta := \{\xi \in \mathbb{S}_{X^{n_1-1},\delta X^{n_2+1}} \ s.t. \ \sigma_X(\xi) = \sigma_X(\eta)\}. \tag{6.1}$$

The derivative *of η is $\delta(\eta) := char(L_\eta) \in \mathbb{R}\langle Z\rangle$. When $n_1 = 0$, L_η is empty and $\delta(\eta) := 0$.*

Alternatively, this derivation can be defined in a simpler way as

Definition 45 *[19] Let $X = \{x_0, \cdots, x_m\}$ and define the language $\delta X = \{\delta x_1, \cdots, \delta x_m\}$ and $Z = X \cup \delta X$. Consider the mapping $\delta : Z \to \{\delta X, 0\}$, where $\delta(x_i) = \delta x_i$ for $i = 1, 2, \cdots, m$ and zero otherwise. Extend the definition of δ to Z^* by letting it act as a derivation with respect to the concatenation. Equivalently,*

$$\delta(\eta) = \delta(x_i)\eta' + x_i\delta(\eta'), \tag{6.2}$$

where $\eta = x_i\eta' \in Z^*$.

The derivation can be extended, by linearity, to polynomials $p = \sum_{i=1}^{n}(p, \eta_i)\eta_i \in \mathbb{R}\langle Z\rangle$. That is, $\delta(p) := \sum_{i=1}^{n}(p, \eta_i)\delta(\eta_i)$. This operation is included next in a monoid structure to provide the underlying differential algebraic structure for computing derivatives of Chen-Fliess series.

Definition 46 *Given the monoid* $(X^*, \odot, \emptyset)$*, a* differential monoid *is defined as the tuple* $(Z^*, \odot, \emptyset, \delta)$ *where* $Z = X \cup \delta X$.

6.1.2 Combinatorial Properties

This algebraic structure is used in the rest of the document. It is expected that δ operating on words will satisfy properties related to the traditional derivative operation.

Example 15 *Let* $\eta = x_0 x_1 \in X^2$. *Note that* $\xi = x_0 \delta x_1$ *is the only element in* $\mathbb{S}_{X,\delta X}$ *such that* $\sigma_X(\xi) = \sigma_X(\eta)$. *Then* $\delta(x_0 x_1) = x_0 \delta x_1$. *Hence,* x_0 *behaves as a constant with respect to* δ.

Example 16 *Let* $\eta = x_1 x_2 \in X^2$. *One can easily find that* $L_\eta = \{\delta x_1 x_2, x_1 \delta x_2\}$. *Thus,* $\delta(x_1 x_2) = char(L_\eta) = \delta x_1 x_2 + x_1 \delta x_2$*, which matches Leibniz's derivative rule.*

These examples can be generalized into the properties shown in the next lemma.

Lemma 8 *The derivative operator in Definition 44 satisfies the following properties:*

i. $\delta(\eta) = \sum_{j=1}^{n} x_{i_1} \cdots x_{i_{j-1}} \delta x_{i_j} x_{i_{j+1}} \cdots x_{i_n}, \ \forall \eta \in X^n$,

ii. $\delta^2(\eta) = 0$, *for* $|\eta|_X = 0$ *or* 1,

iii. $\delta(\eta \sqcup\!\sqcup\, \xi) = \delta(\eta) \sqcup\!\sqcup\, \xi + \eta \sqcup\!\sqcup\, \delta(\xi), \ \eta, \xi \in Z^*$,

iv. $\delta(x_{i_1}^{n_1} \sqcup\!\sqcup \cdots \sqcup\!\sqcup\, x_{i_k}^{n_k}) = \sum_{j=1}^{k} x_{i_1}^{n_1} \sqcup\!\sqcup \cdots x_{i_j}^{n_j - 1} \cdots \sqcup\!\sqcup\, x_{i_k}^{n_k} \sqcup\!\sqcup\, \delta x_{i_j}$

where $\{x_{i_1}, \ldots, x_{i_k}\} \subseteq X$.

Proof: Property i is shown directly from the definition of $\delta(\eta)$ for $\eta = x_{i_1} \cdots x_{i_n} \in X^n$. Observe that

$$L_\eta = \{x_{i_1} \cdots x_{i_{j-1}} \; \delta x_{i_j} \; x_{i_{j+1}} \; \cdots x_{i_n} \text{ for } j = 1, \ldots, n\}.$$

Hence, the result follows since $\delta(\eta) = \mathrm{char}(L_\eta)$. Property ii is checked for $|\eta|_X = 0$ and 1. The case for $|\eta|_X = 0$ follows from Definition 44. For $|\eta|_X = 1$, note that $\delta(\eta) = \delta x_{i_1} \cdots \delta x_{i_n}$ since $\delta x_{i_1} \cdots \delta x_{i_n} \in \mathbb{S}_{X^0,\delta(X)^n}$ is the only element such that $\sigma_X(\delta x_{i_1} \cdots \delta x_{i_n}) = \eta$. By Definition 44, it follows that $\delta(\delta(\eta)) = 0$, which completes the proof. Property iii is proved by induction on the $k = |\eta| + |\xi|$. For $n = 0, 1$, the result holds true by Definition 44. Assume property iii holds for $k-1$ and consider $\eta = \xi_i \eta'$, $\xi = x_k \xi' \in Z^*$ and $x_i, x_j \in X$. From (13) and property i

$$\begin{aligned}\delta(\eta \sqcup\!\sqcup\, \xi) &= \delta(x_i(\eta' \sqcup\!\sqcup\, \xi) + x_j(\eta \sqcup\!\sqcup\, \xi')) \\ &= \delta(x_i)(\eta' \sqcup\!\sqcup\, \xi) + x_j \delta(\eta' \sqcup\!\sqcup\, \xi) + \delta(x_j)(\eta \sqcup\!\sqcup\, \xi') + x_j \delta(\eta \sqcup\!\sqcup\, \xi').\end{aligned}$$

Using property i and the induction hypothesis, it follows

$$\begin{aligned}\delta(\eta \sqcup\!\sqcup\, \xi) &= \delta x_i(\eta' \sqcup\!\sqcup\, \xi) + x_i(\delta(\eta') \sqcup\!\sqcup\, \xi) + x_i(\eta' \sqcup\!\sqcup\, \delta(\xi)) + \delta x_j(\eta \sqcup\!\sqcup\, \xi') \\ &\quad + x_j(\delta(\eta) \sqcup\!\sqcup\, \xi') + x_j(\eta \sqcup\!\sqcup\, \delta(\xi')) \\ &= \delta x_i(\eta' \sqcup\!\sqcup\, \xi) + x_i(\delta(\eta') \sqcup\!\sqcup\, \xi) + x_i(\eta' \sqcup\!\sqcup\, (\delta x_j \xi' + x_j \delta(\xi'))) \\ &\quad + \delta x_j(\eta \sqcup\!\sqcup\, \xi') + x_j(\eta \sqcup\!\sqcup\, \delta(\xi')) + x_j((\delta x_i \eta' + x_i \delta(\eta')) \sqcup\!\sqcup\, \eta').\end{aligned}$$

From the linearity of the shuffle product, the terms are rearranged as follows

$$\begin{aligned}\delta(\eta \sqcup\!\sqcup \xi) &= (\delta x_i \eta') \sqcup\!\sqcup \xi + \eta \sqcup\!\sqcup (\delta x_j \xi') + x_i \delta(\eta') \sqcup\!\sqcup \xi + \eta \sqcup\!\sqcup (x_j \delta(\xi')) \\ &= \delta(\eta) \sqcup\!\sqcup \xi + \eta \sqcup\!\sqcup \delta(\xi),\end{aligned}$$

which completes the proof. The last property is also proved by induction on the number of letters k. For $k = 1$, $\eta = x_{i_1}^{n_1}$ and from property i, $\delta(x_{i_1}^{n_1}) = x_{i_1}^{n_1-1} \sqcup\!\sqcup \delta x_{i_1}$. Assume the induction hypothesis holds for $k = r$. The result is proved for $k = r + 1$. Notice from iii that

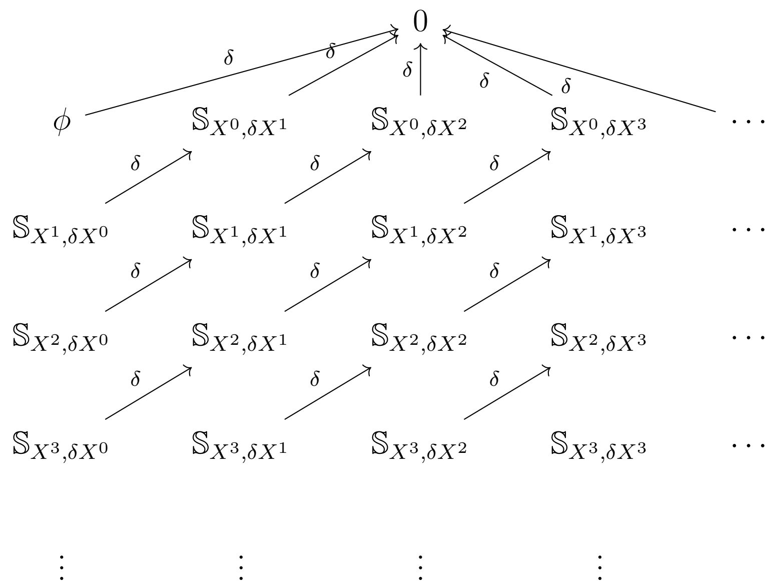
$$\delta(x_{i_1}^{n_1} \sqcup\!\sqcup \cdots \sqcup\!\sqcup x_{i_k}^{n_{r+1}}) = \delta(x_{i_1}^{n_1} \sqcup\!\sqcup \cdots \sqcup\!\sqcup x_{i_k}^{n_r}) \sqcup\!\sqcup x_{i_{r+1}}^{n_{r+1}} + x_{i_1}^{n_1} \sqcup\!\sqcup \cdots \sqcup\!\sqcup x_{i_k}^{n_r} \sqcup\!\sqcup \delta(x_{i_{r+1}}^{n_{r+1}}).$$

Using the induction hypothesis for $k = r$ and the proved case for $k = 1$ gives

$$\begin{aligned}\delta(x_{i_1}^{n_1} \sqcup\!\sqcup \cdots \sqcup\!\sqcup x_{i_k}^{n_{r+1}}) &= \left(\sum_{j=1}^{r} x_{i_1}^{n_1} \sqcup\!\sqcup \cdots \sqcup\!\sqcup x_{i_j}^{n_j-1} \sqcup\!\sqcup \cdots \sqcup\!\sqcup x_{i_r}^{n_r} \sqcup\!\sqcup \delta x_{i_j}\right) \sqcup\!\sqcup x_{i_{r+1}}^{n_{r+1}} \\ &\quad + x_{i_1}^{n_1} \sqcup\!\sqcup \cdots \sqcup\!\sqcup x_{i_k}^{n_r} \sqcup\!\sqcup x_{i_{r+1}}^{n_{r+1}-1} \sqcup\!\sqcup \delta x_{i_{r+1}} \\ &= \sum_{j=1}^{r} x_{i_1}^{n_1} \sqcup\!\sqcup \cdots \sqcup\!\sqcup x_{i_j}^{n_j-1} \sqcup\!\sqcup \cdots \sqcup\!\sqcup x_{i_r}^{n_r} \sqcup\!\sqcup x_{i_{r+1}}^{n_{r+1}} \sqcup\!\sqcup \delta x_{i_j} \\ &\quad + x_{i_1}^{n_1} \sqcup\!\sqcup \cdots \sqcup\!\sqcup x_{i_k}^{n_r} \sqcup\!\sqcup x_{i_{r+1}}^{n_{r+1}-1} \sqcup\!\sqcup \delta x_{i_{r+1}} \\ &= \sum_{j=1}^{r+1} x_{i_1}^{n_1} \sqcup\!\sqcup \cdots \sqcup\!\sqcup x_{i_j}^{n_j-1} \sqcup\!\sqcup \cdots \sqcup\!\sqcup x_{i_r}^{n_r} \sqcup\!\sqcup x_{i_{r+1}}^{n_{r+1}} \sqcup\!\sqcup \delta x_{i_j},\end{aligned}$$

which completes the proof. ■

The derivation satisfies the following diagram:



It should be noticed in Lemma 8 that property i constitutes Leibniz rule in the context of formal power series and that the proof of property iii has also appeared in [19]. The next definition extends (6.1) to multiple applications of the derivative operation δ.

Definition 47 *Let $\eta \in Z^*$ with $|\eta|_X = n_1 \geq 1$ and $|\eta|_{\delta X} = n_2$. The language to describe k applications of δ is defined as*

$$L_\eta^k := \{\xi \in \mathbb{S}_{X^{n_1-k},\delta X^{n_2+k}} \ s.t.\ \sigma_X(\xi) = \sigma_X(\eta)\}.$$

Example 17 *Compute $\delta^2(\eta)$ and $\delta^3(\eta)$ for $\eta = x_{i_1}x_{i_2}x_{i_3}$. Obtaining $\delta(\eta)$ is trivial* *using Lemma 8. Applying δ twice to η gives*

$$\delta^2(x_{i_1}x_{i_2}x_{i_3}) = 2!(\delta x_{i_1}\delta x_{i_2}x_{i_3} + x_{i_1}\delta x_{i_2}\delta x_{i_3} + \delta x_{i_1}x_{i_2}\delta x_{i_3}).$$

Applying δ once more produces

$$\delta^3(x_{i_1}x_{i_2}x_{i_3}) = 3!\delta x_{i_1}\delta x_{i_2}\delta x_{i_3}.$$

Observe that the application of δ twice to a word with no letters in the differential alphabet δX produced $2!$ copies of every word in L_η^2, and a third iteration produced $3!$ copies of each element in L_η^3. This is generalized in the following lemma.

Lemma 9 *Given $\eta \in X^n$ it follows that*

$$\delta^k(\eta) = k!\ char(L_\eta^k). \tag{6.3}$$

If $k > n$, then $\delta^k(\eta) = 0$.

Proof: The proof is done by induction on k. The case for $k = 1$ holds true from Definition 44. Assume the induction hypothesis for $k = r$ and solve the case for $r+1$. Taking the derivative and from its linearity, one has that $\delta^{r+1}(\eta) = r!\delta(\text{char}(L_\eta^r))$. Next, the elements of L_η^{r+1} are counted in the polynomial $D := \delta(\text{char}(L_\eta^r))$. Without loss of generality consider $\xi \in L_\eta^r$ such that $\xi = \delta x_{i_1}\delta x_{i_2}\cdots\delta x_{i_r}x_{i_{r+1}}\cdots x_{i_n}$. From Lemma 8, $\delta(\xi) = \sum_{j=r+1}^n \delta x_{i_1}\delta x_{i_2}\cdots\delta x_{i_r}x_{i_{r+1}}\cdots\delta x_{i_j}\cdots x_{i_n}$. Each element in $\text{supp}(\delta(\xi)) \subset L_\eta^{r+1}$ repeats $r+1$ times in D. To see this, consider the element $\zeta = \delta x_{i_1}\delta x_{i_2}\cdots\delta x_{i_r}\delta x_{i_{r+1}}x_{i_{r+2}}\cdots x_{i_{r+n}}$ in $\text{supp}(\delta(\xi))$. Next, it is shown that ζ appears in the derivative of other r elements different from ξ in L_η^r. Take $\xi_s \in L_\eta^r$ for

$s \in \{1, \cdots, r\}$ where

$$\xi_s = \delta x_{i_1} \cdots \delta x_{i_{s-1}} x_{i_s} \delta x_{i_{s+1}} \cdots \delta x_{i_{r+1}} x_{i_{r+2}} \cdots x_{i_n}.$$

By the Leibniz rule in property i of Lemma 8, $\zeta \in \mathrm{supp}(\delta(\xi_s))$ for $s \in \{1, \cdots, r\}$. These along with ξ are the $r+1$ elements, which completes the proof. ■

The following lemma will be helpful in Section 6.3 for characterizing the Gâteaux derivative of a Chen-Fliess series.

Lemma 10 *The k-th derivative of $char(X^*)$ satisfies*

$$\delta^k(char(X^*)) = k!char(\mathbb{S}_{X^*,\delta X^k}). \tag{6.4}$$

Proof: The proof is performed by induction on k. Consider $k = 1$ and $\eta = x_{i_1} \cdots x_{i_n} \in X^n$ for $n \in \mathbb{N}$. It is clear that $\mathrm{char}(X^n) = \sum_{\eta \in X^n} \eta$. From properties i and iii in Lemma 8, one can rewrite $\delta(\mathrm{char}(X^n))$ as

$$\begin{aligned}
\delta\left(\sum_{\eta \in X^n} \eta\right) &= \delta\left(\sum_{n_0+\cdots n_m=n} x_0^{n_0} \sqcup\!\sqcup \cdots \sqcup\!\sqcup x_m^{n_m}\right) \\
&= \sum_{l=1}^{m} \sum_{n_0+\cdots n_m=n-1} x_0^{n_0} \sqcup\!\sqcup \cdots \sqcup\!\sqcup x_m^{n_m} \sqcup\!\sqcup \delta x_l \\
&= \sum_{l=1}^{m} \mathrm{char}(X^{n-1}) \sqcup\!\sqcup \delta x_l \\
&= \mathrm{char}(X^{n-1}) \sqcup\!\sqcup \delta X \\
&= \mathrm{char}\left(\mathbb{S}_{X^{n-1},\delta X}\right),
\end{aligned}$$

which is (6.5) for $k = 1$. Assume now $k > 1$ and that the induction hypothesis holds true for any integer lesser than k. One has that

$$\begin{aligned}\delta^k\left(\mathrm{char}(X^n)\right) &= \delta\left(\delta^{k-1}\left(\mathrm{char}(X^n)\right)\right)\\ &= \delta\left((k-1)!\ \mathrm{char}\left(\mathbb{S}_{X^{n-k+1},\delta X^{k-1}}\right)\right)\\ &= (k-1)!\ \delta\left(\mathrm{char}(X^{n-k+1}) ⧢ \delta X^{k-1}\right)\\ &= (k-1)!\ \delta\left(\mathrm{char}(X^{n-k+1})\right) ⧢ \delta X^{k-1}\\ &= (k-1)!\ \mathrm{char}(X^{n-k}) ⧢ \delta X ⧢ \delta X^{k-1}.\end{aligned}$$

Since $z_i^k ⧢ z_i^{n-k} = \binom{n}{k} z_i^n$ for any $z_i \in Z$ and

$$\delta X^{k-1} = \sum_{n_1+\cdots+n_m=k-1} \delta x_1^{n_1} ⧢ \cdots ⧢ \delta x_m^{n_m},$$

then $\delta X ⧢ \delta X^{k-1} = k\ \delta X^k$. Hence,

$$\delta^k(\mathrm{char}(X^n)) = k!\mathrm{char}(\mathbb{S}_{X^{n-k},\delta X^k}). \tag{6.5}$$

Finally, the linearity of δ provides (6.4), which completes the proof. ■

An identity for the k-th application of the mapping δ to formal power series is provided in the next lemma.

Lemma 11 *The k-th derivative of $c \in \mathbb{R}\langle\langle X\rangle\rangle$ satisfies*

$$\delta^k(c) = k! \sum_{\xi\in\mathbb{S}_{X^*,\delta X^k}} (c, \sigma_X(\xi))\xi. \tag{6.6}$$

Proof: By the linearity of the derivation and from Lemma 9, it follows

$$\begin{aligned}\delta^k(c) &= \sum_{\eta \in X^*} (c,\eta)\delta^k(\eta) \\ &= k! \sum_{\eta \in X^*} (c,\eta)\mathrm{char}(L^k_\eta) \\ &= k! \sum_{\eta \in X^*} \sum_{\xi \in L^k_\eta} (c, \sigma_X(\xi))\xi \\ &= k! \sum_{\xi \in \mathbb{S}_{X^*,\delta X^k}} (c, \sigma_X(\xi))\xi,\end{aligned}$$

where the last equation comes from the fact that $L^k_{\eta_1} \cap L^k_{\eta_2} = \emptyset$ for $\eta_1 \neq \eta_2$ and $\bigcup_{\eta \in X^*} L^k_\eta = \mathbb{S}_{X^*,\delta X^k}$, which concludes the proof. ■

Example 18 *Consider the word $x_1\delta x_2 x_3 \delta x_4 x_5$ in the set $\mathbb{S}_{X^*,\delta X^2}$. Taking the derivative operation three times gives*

$$\delta^3(x_1\delta x_2 x_3\delta x_4 x_5) = 3!\delta x_1 \delta x_2 \delta x_3 \delta x_4 \delta x_5.$$

The word $\delta x_1 x_2 \delta x_3 x_4 x_5 \in \mathbb{S}_{X^*,\delta X^2}$, which is different from $x_1\delta x_2 x_3\delta x_4 x_5$, also satisfies

$$\delta^3(\delta x_1 x_2 \delta x_3 x_4 x_5) = 3!\delta x_1 \delta x_2 \delta x_3 \delta x_4 \delta x_5.$$

It is easy to see that there are $\binom{5}{2}$ different words ξ in $\mathbb{S}_{X^*,\delta X^2}$ such that $\sigma_X(\xi) = x_1x_2x_3x_4x_5$ and they all satisfy $\delta^3(\xi) = 3!\delta x_1 \delta x_2 \delta x_3 \delta x_4 \delta x_5$. Adding all of these words *it follows that*

$$\frac{1}{3!}\delta^3\Big(\delta x_1\delta x_2x_3x_4x_5+\delta x_1x_2\delta x_3x_4x_5+\delta x_1x_2x_3\delta x_4x_5+\delta x_1x_2x_3x_4\delta x_5$$
$$+x_1\delta x_2\delta x_3x_4x_5+x_1\delta x_2x_3\delta x_4x_5+x_1\delta x_2x_3x_4x_5+x_1x_2\delta x_3\delta x_4x_5$$
$$+x_1x_2\delta x_3x_4\delta x_5+x_1x_2x_3\delta x_4\delta x_5\Big)$$
$$=\binom{5}{2}\delta x_1\delta x_2\delta x_3\delta x_4\delta x_5.$$

Since for power series, all these words will have the same coefficient $(c, x_1x_2x_3x_4x_5)$, *then this behavior extends to power series by the linearity of the derivative.*

The next lemma will be used in Chapter 7 to present a proof of the mean value theorem for Chen-Fliess series by algebraic means and provide a second-order approximation for a Chen-Fliess series.

Lemma 12 *Let* $(Z^*, \odot, \emptyset, \delta)$ *be a differential monoid. For* $k, r \in \mathbb{N}$, *it follows that*

$$\frac{1}{k!}\delta^k\left(char\left(\mathbb{S}_{X^*,\delta X^r}\right)\right)=\binom{r+k}{r}char\Big(\mathbb{S}_{X^*,\delta X^{r+k}}\Big) \tag{6.7}$$

and, for $c \in \mathbb{R}\langle\langle X\rangle\rangle$, *one has that*

$$\sum_{\xi\in\mathbb{S}_{X^*,\delta X^r}}\frac{1}{k!}(c,\sigma_X(\xi))\delta^k(\xi)=\binom{r+k}{r}\sum_{\xi\in\mathbb{S}_{X^*,\delta X^{r+k}}}(c,\sigma_X(\xi))\xi. \tag{6.8}$$

Proof: The proof is done by double induction on r and k. The case for $r=0$ and $k\in\mathbb{N}$ is proved in Lemma 10. The case for $k=0$ and $r\in\mathbb{N}$ is trivial. Assume that the result is satisfied for an arbitrary $r=p$ and $k=q$. First, the result is proved for

$k = q + 1$ and $r = p$. That is,

$$\delta \left(\frac{1}{q!} \delta^q \left(\text{char } \mathbb{S}_{X^*, \delta X^p} \right) \right) = \binom{p+q}{q} \delta \left(\text{char} \left(\mathbb{S}_{X^*, \delta X^{p+q}} \right) \right).$$

From Lemma 10,

$$\begin{aligned} \frac{1}{q!} \delta^{q+1} \left(\text{char } \mathbb{S}_{X^*, \delta X^p} \right) &= \binom{p+q}{q} (p+q+1) \left(\text{char} \left(\mathbb{S}_{X^*, \delta X^{p+q+1}} \right) \right) \\ &= \frac{(p+q+1)!}{p! q!} \left(\text{char} \left(\mathbb{S}_{X^*, \delta X^{p+q+1}} \right) \right). \end{aligned}$$

Thus, dividing both sides by $(q+1)$ gives the result for $q+1$. Now the result is proved for $r = p + 1$ and $k = q$. From Lemma 10, one has that

$$\text{char}(\mathbb{S}_{X^*, \delta X^{p+1}}) = \frac{1}{(p+1)!} \delta^{p+1} (\text{char}(X^*)).$$

Taking the derivative q times gives

$$\delta^q \left(\text{char}(\mathbb{S}_{X^*, \delta X^{p+1}}) \right) = \frac{1}{(p+1)!} \delta^{p+q+1} (\text{char}(X^*)). \tag{6.9}$$

Again, from Lemma 10, the right-hand side is expressed as

$$\delta^{p+q+1} (\text{char}(X^*)) = (p+q+1)! \text{char}(\mathbb{S}_{X^*, \delta X^{p+q+1}}). \tag{6.10}$$

Replacing (6.10) in (6.9), it follows that

$$\delta^q \left(\text{char}(\mathbb{S}_{X^*, \delta X^{p+1}}) \right) = \frac{(p+q+1)!}{(p+1)!} \delta^{p+q+1} \text{char}(\mathbb{S}_{X^*, \delta X^{p+q+1}}).$$

Thus, (6.7) follows by dividing both sides by $q!$. ∎

6.2 Chen-Fliess Series over Differential Languages

In this section, a Chen-Fliess series is characterized in terms of a differential monoid. Hereafter, all statements assume the underlying differential monoid $(Z, \odot, \emptyset, \delta)$, where X and δX are alphabets associated with inputs $u, v \in B_{\mathfrak{p}}^m(R)[0,t]$, and $Z = X \cup \delta X$.

The characterization of the Chen-Fliess series of the sum of two inputs in terms of the derivation of words is given next.

Lemma 13 *Given $c \in \mathbb{R}\langle\langle X \rangle\rangle$, the Chen-Fliess series of the sum of u and v is written as*

$$F_c[u+v](t) = \sum_{k=0}^{\infty} \sum_{\xi \in \delta^k(X^*)} \frac{1}{k!}(c, \sigma_X(\xi))\mathcal{E}_\xi[u,v](t). \tag{6.11}$$

Proof: *The proof follows from Lemma 4 by identifying the alphabet Y associated with the function v with δX since both are sets of symbols and by using the inner product* *in (2.6). That is,*

$$\begin{aligned}
F_c[u+v](t) &= \sum_{k=0}^{\infty} \sum_{\xi\in\mathbb{S}_{X^*,\delta X^k}} (c,\sigma_X(\xi))\mathcal{E}_\xi[u,v](t) \\
&= \sum_{k=0}^{\infty} \left(\sum_{\xi\in\mathbb{S}_{X^*,\delta X^k}} (c,\sigma_X(\xi))\xi \ , \sum_{\xi\in\mathbb{S}_{X^*,\delta X^k}} \mathcal{E}_\xi[u,v](t)\xi \right) \\
&= \sum_{k=0}^{\infty} \left(\sum_{\eta\in X^*} (c,\eta)\frac{1}{k!}\delta^k(\eta), \sum_{\eta\in X^*} \mathcal{E}_\xi[u,v](t)\frac{1}{k!}\delta^k(\eta) \right) \\
&= \sum_{k=0}^{\infty} \sum_{\xi\in\delta^k(X^*)} \frac{1}{k!}(c,\sigma_X(\xi))\mathcal{E}_\xi[u,v](t),
\end{aligned}$$

where the third equation comes from Lemma 11. ■

Notice that from Lemma 13 if the exponential of the derivative of $c \in \mathbb{R}^\ell\langle\langle X\rangle\rangle$ is defined as

$$e^{\delta(c)} = \sum_{k=0}^{\infty} \frac{1}{k!}\delta^k(c)$$

then Chen-Fliess series of the sum of two inputs $u, v \in L_\mathfrak{p}^m[0,t]$ is expressed as

$$F_c[u+v](t) = \mathcal{F}_{e^{\delta(c)}}[u,v](t).$$

6.2.1 Link Between Analysis and Algebra

Consider set $\mathscr{F} := \{F_c : c \in \mathbb{R}_{LC}\langle\langle X\rangle\rangle\}$ as in [40], and define the sets $\mathscr{F}_\delta := \{F_{\delta(c)} : c \in \mathbb{R}_{LC}\langle\langle Z\rangle\rangle\}$ and $\mathscr{F}_{\delta^2} := \{F_{\delta^2(c)} : c \in \mathbb{R}_{LC}\langle\langle Z\rangle\rangle\}$. The next theorem establishes the link between analysis and algebra by relating the Gâteaux derivative of a Chen-Fliess series to the derivation of a differential monoid.

Theorem 15 *Given $c \in \mathbb{R}\langle\langle X \rangle\rangle$, if*

$$\lim_{\varepsilon \to 0} \sum_{s=2}^{\infty} \sum_{\xi \in \mathbb{S}_{X^*, \delta X^\tau}} \frac{1}{s!} (c, \sigma_X(\xi)) \mathcal{E}_{\delta^s(\xi)}[u,v](t) \varepsilon^{s-1} = 0, \tag{6.12}$$

for $1 \leq \tau \leq k-1$, then the k-th order Gâteaux derivative of $F_c[u](t)$ in the direction of v is written as

$$\frac{\partial^k}{\partial v^k} F_c[u](t) = k! \sum_{\xi \in \mathbb{S}_{X^*, \delta X^k}} (c, \sigma_X(\xi)) \mathcal{E}_{\xi}[u,v](t).$$

Furthermore, the derivation δ and the Gâteaux derivative satisfy the following commutative diagram

$$\begin{array}{ccccc}
\mathscr{F} & \xrightarrow{\frac{\partial}{\partial v}} & \mathscr{F}_{\delta} & \xrightarrow{\frac{\partial}{\partial v}} & \mathscr{F}_{\delta^2} \cdots \\
\uparrow & & \uparrow & & \uparrow \cdots \\
\mathbb{R}_{LC}\langle\langle X \rangle\rangle & \xrightarrow{\delta} & \mathbb{R}_{LC}\langle\langle Z \rangle\rangle & \xrightarrow{\delta} & \mathbb{R}_{LC}\langle\langle Z \rangle\rangle \cdots
\end{array}$$

Proof: The proof follows by induction on k. The case for $k = 1$ is proved directly from Definition 43 and Corollary 4 by identifying the alphabet Y associated with function v with the alphabet δX. Assume the induction hypothesis holds true for $k = r$, the case for $k = r+1$ will be constructed from Definition 43. Applying Lemma

13 to the term $\mathcal{E}_\xi[u+\varepsilon v, v](t)$, it follows that

$$\frac{\partial^r}{\partial v^r} F_c[u+\varepsilon v](t) = r! \sum_{\xi \in \mathbb{S}_{X^*,\delta X^r}} (c, \sigma_X(\xi)) \mathcal{E}_\xi[u+\varepsilon v, v](t)$$
$$= r! \sum_{s=0}^{\infty} \sum_{\xi \in \mathbb{S}_{X^*,\delta X^r}} \frac{1}{s!} (c, \sigma_X(\xi)) \mathcal{E}_{\delta^s(\xi)}[u, v](t) \varepsilon^s. \tag{6.13}$$

Notice that the term for $s=0$ in the double sum on the right side of (6.13) is equal to

$$\frac{\partial^r}{\partial v^r} F_c[u](t) = r! \sum_{\xi \in \mathbb{S}_{X^*,\delta X^r}} (c, \sigma_X(\xi)) \mathcal{E}_\xi[u, v](t).$$

Then, moving the $s=0$ and $s=1$ terms in (6.13) to the left side of the equal sign and dividing by ε, it follows that

$$\frac{1}{\varepsilon}\left(\frac{\partial^r}{\partial v^r} F_c[u+\varepsilon v](t) - \frac{\partial^r}{\partial v^r} F_c[u](t) - r! \sum_{\xi \in \mathbb{S}_{X^*,\delta X^r}} (c, \sigma_X(\xi)) \mathcal{E}_{\delta(\xi)}[u, v](t) \varepsilon \right)$$
$$= r! \sum_{s=2}^{\infty} \sum_{\xi \in \mathbb{S}_{X^*,\delta X^r}} \frac{1}{s!} (c, \sigma_X(\xi)) \mathcal{E}_{\delta^s(\xi)}[u, v](t) \varepsilon^{s-1}.$$

Using (6.12) and the limit when ε tends to zero gives

$$\frac{\partial^{r+1}}{\partial v^{r+1}} F_c[u](t) = r! \sum_{\xi \in \mathbb{S}_{X^*,\delta X^r}} (c, \sigma_X(\xi)) \mathcal{E}_{\delta(\xi)}[u, v](t). \tag{6.14}$$

Applying Lemma 12 with $k=1$ to (6.14) provides

$$\frac{\partial^{r+1}}{\partial v^{r+1}} F_c[u](t) = (r+1)! \sum_{\xi \in \mathbb{S}_{X^*,\delta X^{r+1}}} (c, \sigma_X(\xi)) \mathcal{E}_\xi[u, v](t). \tag{6.15}$$

Hence, applying Lemma 11 in (6.15) gives the generating series resulting from $\delta^k(c)$. That is,

$$\frac{\partial^{k+1}}{\partial v^{k+1}} F_c[u](t) = F_{\delta^{k+1}(c)}[u](t),$$

which shows that the commutative diagram between the Gâteaux derivative and the derivation δ holds. ■

In the next section, the derivatives of the second order of a Chen-Fliess series are characterized using the derivation.

6.3 Second Order Derivatives of Chen-Fliess series

6.3.1 Partial Derivation

Define first the restriction of δ to a single letter $x_i \in X$. That is, let $\delta_{x_i} : Z \to Z$ such that $\delta_{x_i}(x_j) = \delta x_i$ for $x_j = x_i$, $\delta_{x_i}(x_j) = 0$ for $x_j \neq x_i$, and $\delta_{x_i}(\delta x_j) = \delta(x_0) = \delta(\emptyset) = 0$ for any i, j.

Definition 48 *Let $Z_{\delta_{x_i}} := Z \setminus \{\delta x_i\}$ be the alphabet where δx_i has been removed from Z, $\eta \in Z^*$ such that $|\eta|_{Z_{\delta_{x_i}}} = n_1 \geq 1$ and $|\eta|_{\delta x_i} = n_2$ and consider the language*

$$L_{\delta_{x_i}(\eta)} := \{\xi \in \mathbb{S}_{{Z_{x_i}}^{n_1-1}, \delta x_i^{n_2+1}} \ s.t. \ \sigma_X(\xi) = \sigma_X(\eta)\}.$$

The derivative of η *relative to* x_i *is*

$$\delta_{x_i}(\eta) := char(L_{\delta_{x_i}(\eta)}) \in \mathbb{R}\langle Z\rangle.$$

When $|\eta|_{x_i} = 0$*,* $L_{\delta_{x_i}(\eta)}$ *is empty and* $\delta_{x_i}(\eta) := 0$*.*

Example 19 *Consider the alphabet* $X = \{x_0, x_1, x_2\}$*,* $\eta = x_0x_1x_2x_1 \in X$ *and compute* $\delta_{x_1}(\eta)$*. Since* $Z = \{x_0, x_1, x_2, \delta x_1, \delta x_2\}$*,* $Z_{\delta_{x_i}} = \{x_0, x_1, x_2, \delta x_2\}$ *and* $L_{\delta_{x_1}(\eta)} = \{x_0\delta x_1x_2x_1, x_0x_1x_2\delta x_1\}$*, then* $\delta_{x_1}(x_0x_1x_2x_1) = x_0\delta x_1x_2x_1 + x_0x_1x_2\delta x_1$*. Similarly,* $\delta_{x_2}(\eta) = x_0x_1\delta x_2x_1$*.*

The following two lemmas characterize the Gâteaux derivative of a Chen-Fliess series with respect to the canonical directions given by $e_i : [0, T] \to \mathbb{R}^m$, such that $e_1(t) = (1, 0, \cdots, 0)^\top, \ldots, e_m(t) = (0, 0, \cdots, 1)^\top$.

Lemma 14 *Consider* $c \in \mathbb{R}_{LC}\langle\langle X\rangle\rangle$*, the Gâteaux derivative in the i-th canonical direction satisfies*

$$\frac{\partial}{\partial u_i} F_c[u](t) = F_{\delta_{x_i}(c)}[u](t).$$

Proof: Similar to Theorem 15, the proof follows by identifying the alphabet Y with δX which associates y_i with δx_i and the application of Corollary 5. ■

Lemma 15 *Consider the derivative operators* δ_{x_i} *and* δ_{x_j} *for* $x_i, x_j \in X$*. It then follows that*

$$\sum_{\xi \in \mathbb{S}_{X^*,\delta x_i}} (c, \sigma_X(\xi))\delta_{x_j}(\xi) = \sum_{\xi \in \mathbb{S}_{X^*,\mathrm{supp}(\delta x_i \sqcup\!\sqcup\, \delta x_j)}} (c, \sigma_X(\xi))\xi. \tag{6.16}$$

Proof: The proof follows the same steps as that of Lemma 11 but taking the δ_{x_j} derivative instead of δ and the fact that $L_{\delta_{x_j}(\xi_1)} \cap L_{\delta_{x_j}(\xi_2)} = \emptyset$ for $\xi_1, \xi_2 \in \mathbb{S}_{X^*,\delta x_i}$ and $\xi_1 \neq \xi_2$, and $\bigcup_{\xi \in \mathbb{S}_{X^*,\delta x_i}} L_{\delta_{x_j}(\xi)} = \mathbb{S}_{X^*,\mathrm{supp}(x_i \sqcup\!\sqcup\, x_j)}$. ■

6.3.2 Second-Order Partial Derivation

The next Lemma shows that the second-order canonical derivatives of a Chen-Fliess series are expressed in terms of the derivative of words.

Lemma 16 *Let $c \in \mathbb{R}_{LC}\langle\langle X \rangle\rangle$ and $u \in B_{\mathfrak{p}}^m(R)[0,T]$, if*

$$\begin{aligned} &\lim_{\varepsilon \to 0} \sum_{k=2}^{\infty} \sum_{\xi \in \mathbb{S}_{X^*,\delta x_i}} \frac{1}{k!}(c, \sigma_X(\xi)) \mathcal{E}_{\delta^k_{x_j}(\xi)}[u, e_{i,j}](t) \varepsilon^{k-1} = 0, \ \ \textit{and} \\ &\lim_{\varepsilon \to 0} \sum_{k=2}^{\infty} \sum_{\xi \in \mathbb{S}_{X^*,\delta x_j}} \frac{1}{k!}(c, \sigma_X(\xi)) \mathcal{E}_{\delta^k_{x_i}(\xi)}[u, e_{i,j}](t) \varepsilon^{k-1} = 0 \end{aligned} \tag{6.17}$$

then

$$\frac{\partial^2}{\partial u_j \partial u_i} F_c[u](t) = \sum_{\xi \in \mathbb{S}_{X^*,\mathrm{supp}(\delta x_i \,\sqcup\!\sqcup\, \delta x_j)}} (c, \sigma_X(\xi)) \mathcal{E}_\xi[u, e_{i,j}](t), \tag{6.18}$$

where $e_{i,j}(t) = (0, \cdots, \underbrace{1}_{i-th}, 0, \cdots, \underbrace{1}_{j-th}, \cdots, 0)$.

Proof: The proof is similar to that of Theorem 15, but taking instead the Gâteaux derivative in the canonical directions. That is,

$$\begin{aligned} \frac{\partial}{\partial u_i} F_c[u + \varepsilon e_j](t) &= \sum_{\xi \in \mathbb{S}_{X^*,\delta x_i}} (c, \sigma_X(\xi)) \mathcal{E}_\xi[u + \varepsilon e_j, e_i](t) \\ &= \sum_{k=0}^{\infty} \sum_{\xi \in \mathbb{S}_{X^*,\delta x_i}} \frac{1}{k!}(c, \sigma_X(\xi)) \mathcal{E}_{\delta^k_{x_j}(\xi)}[u, e_{i,j}](t) \varepsilon^k. \end{aligned}$$

By taking the $k=0$ and $k=1$ terms to the left of the equal sign and dividing by ε, one obtains

$$\frac{1}{\varepsilon}\left(\frac{\partial}{\partial u_i}F_c[u+\varepsilon e_j](t)-\frac{\partial}{\partial u_i}F_c[u](t)-\sum_{\xi\in\mathbb{S}_{X^*,\delta x_i}}(c,\sigma_X(\xi))\mathcal{E}_{\delta_{x_j}(\xi)}[u,e_{i,j}](t)\varepsilon\right)$$
$$=\sum_{k=2}^{\infty}\sum_{\xi\in\mathbb{S}_{X^*,\delta x_i}}\frac{1}{k!}(c,\sigma_X(\xi))\mathcal{E}_{\delta^k_{x_j}(\xi)}[u,e_{i,j}](t)\varepsilon^{k-1}.$$

Thus, from (6.17), it follows directly that

$$\frac{\partial^2}{\partial u_j\partial u_i}F_c[u](t)=\sum_{\xi\in\mathbb{S}_{X^*,\delta x_i}}(c,\sigma_X(\xi))\mathcal{E}_{\delta_{x_j}(\xi)}[u,e_{i,j}](t).$$

Finally, (6.18) is obtained from Lemma 15. ■

Observe that when the second derivatives exist and the condition of Lemma 16 holds, then they satisfy the Schwarz Theorem for the symmetry of second order differentiation [9], i.e.,

$$\frac{\partial^2}{\partial u_j\partial u_i}F_c[u](t)=\frac{\partial^2}{\partial u_i\partial u_j}F_c[u](t).$$

6.3.3 The Hessian

Grouping all the second-order derivatives of a Chen-Fliess series in a matrix arrangement where its components are indexed with respect to all canonical directions gives then a symmetric matrix. This is presented in the next definition.

Definition 49 *Let $c\in\mathbb{R}_{LC}\langle\langle X\rangle\rangle$ and $u\in B^m_{\mathfrak{p}}(R)[0,T]$. The Hessian of $F_c[u](t)$ is* *given by*

$$\nabla^2 F_c[u](t) = \begin{bmatrix} 2\frac{\partial^2}{\partial u_1^2}F_c[u](t) & \cdots & \frac{\partial^2}{\partial u_1 \partial u_m}F_c[u](t) \\ \vdots & \ddots & \vdots \\ \frac{\partial^2}{\partial u_m \partial u_1}F_c[u](t) & \cdots & 2\frac{\partial^2}{\partial u_m^2}F_c[u](t) \end{bmatrix}.$$

The next lemma shows the expression for the Hessian matrix with respect to a constant direction. $v = (v_1, \cdots, v_m)^T \in \mathbb{R}^m$.

Lemma 17 *For* $c \in \mathbb{R}_{LC}\langle\langle X \rangle\rangle$, $u \in L_{\mathfrak{p}}^m[0,T]$ *and* $v = (v_1, \cdots, v_m)^T \in \mathbb{R}^m$, *the second order Gâteaux derivative and the Hessian matrix of Chen-Fliess series' are related as*

$$\frac{\partial^2}{\partial v^2}F_c[u](t) = v^T \nabla^2 F_c[u](t) v.$$

Proof: Define $I_m = \{1, \cdots, m\}$. For $k = 2$ in Theorem 15, one has that

$$\begin{aligned} \frac{\partial^2}{\partial v^2}F_c[u](t) &= 2 \sum_{\xi \in \mathbb{S}_{X^*, \delta X^2}} (c, \sigma_X(\xi))\mathcal{E}_\xi[u, v](t) \\ &= 2 \sum_{i \in I_m} \sum_{\xi \in \mathbb{S}_{X^*, \delta x_i^2}} v_i^2 (c, \sigma_X(\xi))\mathcal{E}_\xi[u, e_{i,j}](t) \\ &\quad + \sum_{\substack{(i,j) \in I_m^2 \\ i \neq j}} \sum_{\xi \in \mathbb{S}_{X^*, \{\delta x_i \delta x_j, \delta x_j \delta x_i\}}} v_i v_j (c, \sigma_X(\xi))\mathcal{E}_\xi[u, e_{i,j}](t) \\ &= 2 \sum_{i \in I_m} v_i^2 \frac{\partial^2}{\partial u_i^2}F_c[u](t) + \sum_{\substack{(i,j) \in I_m^2; \\ i \neq j}} v_i v_j \frac{\partial^2}{\partial u_j \partial u_i}F_c[u](t) \\ &= v^T \nabla^2 F_c[u](t) v, \end{aligned}$$

which completes the proof. ■

In what follows, the Gâteaux derivative of the output y of a system in the direction of the input function v at time t is denoted $D_v[y](t)$ in contrast to the Gâteaux derivative of the Chen-Fliess series, $F_c[u](t)$, denoted $\frac{\partial}{\partial v}F_c[u](t)$. The next example shows that computing the Hessian of a Chen-Fliess series using the differential monoid structure coincides with the analytic Hessian computation of the corresponding nonlinear state space system.

Example 20 *Consider the bilinear system*

$$\dot{x} = xu,\ y = x,\ x(0) = 1 \tag{6.19}$$

with input $u \in L_{\mathfrak{p}}[0,t]$*. Its power series is* $c = \sum_{n\geq 0} x_1^n \in \mathbb{R}_{GC}\langle\langle X\rangle\rangle$*. Since the number of inputs is* $m = 1$ *and from Lemma 17, the Hessian of the Chen-Fliess series of (6.19) is obtained by calculating the second-order Gâteaux derivative in the direction of* $u_1 = 1$*. That is,*

$$\nabla^2 F_c[u](t) = 2! \sum_{\xi \in \mathbb{S}_{X^*,\delta x_1^2}} \mathcal{E}_\xi[u, e_1](t) \tag{6.20}$$

$$= 2! \sum_{\xi \in \mathbb{S}_{X^*,x_0^2}} E_\xi[u](t). \tag{6.21}$$

On the other hand, since the output of (6.19) is

$$y(t) = \exp\left(\int_0^t u(\tau)d\tau\right),$$

one can compute the derivative in the direction of v *analytically as*

$$\begin{aligned} D_v[y](t) = & \lim_{\varepsilon\to 0}\frac{1}{\varepsilon}(y(u+\varepsilon v)-y(u)) \\ &= \lim_{\varepsilon\to 0}\frac{1}{\varepsilon}\left(\exp\left(\int_0^t u(\tau)+\varepsilon v(\tau)d\tau\right)-\exp\left(\int_0^t u(\tau)d\tau\right)\right) \\ &= \lim_{\varepsilon\to 0}\frac{1}{\varepsilon}\left(\exp\left(\int_0^t u(\tau)d\tau\right)\left(\exp\left(\int_0^t \varepsilon v(\tau)d\tau\right)-1\right)\right) \\ &= \exp\left(\int_0^t u(\tau)d\tau\right)\left(\lim_{\varepsilon\to 0}\frac{1}{\varepsilon}\left(\sum_{k=1}^{\infty}\frac{\left(\varepsilon\int_0^t v(\tau)d\tau\right)^k}{k!}\right)\right) \\ &= \exp\left(\int_0^t u(\tau)d\tau\right)\int_0^t v(\tau)d\tau. \end{aligned}$$

Using the same procedure, it follows that

$$D^2_{v^2}[y](t) = \exp\left(\int_0^t u(\tau)d\tau\right)\left(\int_0^t v(\tau)d\tau\right)^2.$$

Expanding the exponential and re-writing in terms of the shuffle product, the second-order Gâteaux derivative is

$$\begin{aligned} D^2_{v^2}[y](t) &= \sum_{k=0}^{\infty}\frac{\left(\int_0^t u(\tau)d\tau\right)^k}{k!}\left(\int_0^t v(\tau)d\tau\right)^2 \\ &= \sum_{k=0}^{\infty}\frac{E_{x_1^{\sqcup\!\sqcup k}}[u](t)}{k!}\left(\mathcal{E}_{\delta x_1^{\sqcup\!\sqcup 2}}[u,v](t)\right). \end{aligned}$$

Notice that $x_1^{\sqcup\!\sqcup\, k} = k!x^k$ *and* $\delta x_1^{\sqcup\!\sqcup\, 2} = 2!\delta x_1$*, then*

$$\begin{aligned} D^2_{v^2}[y](t) &= 2\sum_{k=0}^{\infty} E_{x_1^k}[u](t)\mathcal{E}_{\delta x_1^2}[u,v](t) \\ &= 2\sum_{k=0}^{\infty} \mathcal{E}_{x_1^k \sqcup\!\sqcup\, \delta x_1^2}[u,v](t) \\ &= 2! \sum_{\xi \in \mathbb{S}_{X^*,\delta x_1^2}} \mathcal{E}_\xi[u,v](t). \end{aligned}$$

This agrees with (6.20) when δx_1 *is associated to* $v = 1$*.*

Example 21 *Consider the linear system*

$$\dot{x} = Ax + Bu, \;\; y = x. \tag{6.22}$$

with input $u \in L_{\mathfrak{p}}[0,t]$*. The output of (6.22) is*

$$y = e^{At}x_0 + \int_0^t e^{A(t-\tau)}Bu(\tau)d\tau.$$

Computing the derivative analytically gives

$$\begin{aligned} D_v[y](t) &= \lim_{\varepsilon\to 0} \frac{1}{\varepsilon}(y(u+\varepsilon v) - y(u)) \\ &= \int_0^t e^{A(t-\tau)}Bv(\tau)d\tau. \end{aligned}$$

The second-order derivative follows similarly

$$\begin{aligned} D^2_{v^2}[y](t) = & \lim_{\varepsilon\to 0}\frac{1}{\varepsilon}\left(\frac{dy}{dv}(u+\varepsilon v)-\frac{dy}{dv}(u)\right) \\ = & \lim_{\varepsilon\to 0}\frac{1}{\varepsilon}\left(\int_0^t e^{A(t-\tau)}Bv(\tau)d\tau-\int_0^t e^{A(t-\tau)}Bv(\tau)d\tau\right) \\ = & \, 0. \end{aligned} \tag{6.23}$$

On the other hand, from Lemma 17 the second-order Gâteaux derivative is

$$\frac{\partial^2}{\partial v^2}F_c[u](t) = 2!\sum_{\xi\in\mathbb{S}_{X^*,\delta x_1^2}}(c,\sigma_X(\xi))\mathcal{E}[u,v](t).$$

Observe that for all $\xi \in \mathbb{S}_{X^*,\delta x_1^2}$*, then* $\sigma_X(\xi) = \eta \in \mathbb{S}_{X^*,x_1^2}$ *and* $(c,\sigma_X(\xi)) = (c,\eta)$*. For the linear system and from (2.5), for words* η *containing two* x_1 *letters, the Lie derivative* $L_\eta x = 0$*, then* $(c,\eta) = 0$*. Therefore* $\frac{\partial^2}{\partial v^2}F_c[u](t) = 0$*. This implies that the Hessian is* $\nabla^2 F_c[u](t) = 0$*, which is expected from a linear system and coincides with (6.23).*

6.3.4 Approximation of Chen-Fliess Series

Here it is shown that the Chen-Fliess series with a small perturbation in its input can be written in terms of its gradient and Hessian. This perturbation together with the second-order mean value theorem for a Chen-Fliess series is essential to ensure the convergence of the Newton and trust regions methods to be presented in Chapter 7. The underlying setting for the following lemmas, theorems, and corollaries remain the same except that the input v related to the alphabet δX is a constant vector $v \in \mathbb{R}^m$.

Lemma 18 *For* $c \in \mathbb{R}_{LC}\langle\langle X\rangle\rangle$*,* $u \in L_{\mathfrak{p}}^m[0,T]$*,* $v = (v_1,\cdots,v_m)^T \in \mathbb{R}^m$ *and* $\varepsilon > 0$*,* *one has that*

$$F_c[u+\varepsilon v](t) = F_c[u](t) + v^T \nabla F_c[u](t)\varepsilon + \frac{1}{2} v^T \nabla^2 F_c[u](t) v \varepsilon^2 + \sum_{k=3}^{\infty} \sum_{\xi \in \mathbb{S}_{X^*,\delta X^k}} (c, \sigma_X(\xi)) \mathcal{E}_\xi[u,v](t)\varepsilon^k.$$

Proof: The proof is by construction and follows directly from the application of Lemmas 13 and 17. ■

Prior to presenting the second-order mean value theorem the next lemma is needed.

Lemma 19 *Let $\rho \in \mathbb{R}$, $c \in \mathbb{R}\langle\langle X \rangle\rangle$, $u \in L_{\mathfrak{p}}^m[0,t]$, and $v \in \mathbb{R}^m$. It follows that*

$$\frac{1}{2} v^T \nabla^2 F_c[u+\rho v](t) v = \sum_{k=2}^{\infty} \sum_{\xi \in \mathbb{S}_{X^*,\delta X^k}} \binom{k}{2} \rho^{k-2} (c, \sigma_X(\xi)) \mathcal{E}_\xi[u,v](t). \tag{6.24}$$

Proof: Applying Lemma 12 for $r=2$ and adding up the terms in k, it follows that

$$\sum_{k=0}^{\infty} \sum_{\xi \in \mathbb{S}_{X^*,\delta X^2}} \frac{1}{k!} (c, \sigma_X(\xi)) \delta^k(\xi) = \sum_{k=0}^{\infty} \sum_{\xi \in \mathbb{S}_{X^*,\delta X^{2+k}}} \binom{k+2}{2} (c, \sigma_X(\xi)) \xi. \tag{6.25}$$

Similar to (6.13), the left side of the equation is the power series of the second derivative evaluated at $u+\rho v$

$$\frac{\partial^2}{\partial v^2} F_c[u+\rho v](t) = \sum_{k=0}^{\infty} \sum_{\xi \in \mathbb{S}_{X^*,\delta X^2}} \frac{1}{k!} (c, \sigma_X(\xi)) \mathcal{E}_{\delta^k(\xi)}[u,v](t).$$

This expression can be rewritten using Lemma 17 in terms of the Hessian as

$$\frac{1}{2}v^T\nabla^2 F_c[u+\rho v](t)v = \sum_{k=0}^{\infty}\sum_{\xi\in\mathbb{S}_{X^*,\delta X^2}}\frac{1}{k!}(c,\sigma_X(\xi))\mathcal{E}_{\delta^k(\xi)}[u,v](t).$$

where the input associated to $\delta^k(\xi)$ is now ρv. Then the CFS of the power series on the right side of (6.25) is

$$\sum_{k=0}^{\infty}\sum_{\xi\in\mathbb{S}_{X^*,\delta X^{2+k}}}\binom{k+2}{2}\rho^k(c,\sigma_X(\xi))\mathcal{E}_{\xi}[u,v](t).$$

Thus, from (6.25) substituting $k+2$ with k, one can obtain (6.24), which completes the proof. ■

The next theorem gives the second-order mean value theorem for a CFS which is proved algebraically by the developed tools instead of the standard chain rule.

Theorem 16 *Let* $c\in\mathbb{R}_{LC}\langle\langle X\rangle\rangle$ *and* $\varepsilon>0$. *Then there exists* $\varepsilon_0\in(0,\varepsilon)$ *such that*

$$F_c[u+\varepsilon v] = F_c[u] + v^T\nabla F_c[u](t)\varepsilon + \frac{1}{\varepsilon_0}\int_0^{\varepsilon_0}\frac{1}{2}v^T\nabla^2F_c[u+rv](t)v\varepsilon^2 dr. \tag{6.26}$$

Proof: The theorem is proved by an application of Rolle's theorem [9] and the continuity of the Chen-Fliess series [17]. Any continuous function that is zero when evaluated at the two extreme points of an interval $[0,\varepsilon]$ must have a point $\varepsilon_0\in(0,\varepsilon)$ where its derivative is zero. Define the function $\phi:\mathbb{R}\to\mathbb{R}$ such that

$$\begin{aligned}\phi(\gamma) = &\int_0^{\gamma}\int_0^{\theta}\frac{1}{2}v^T\nabla^2F_c[u+rv](t)v\varepsilon^2 dr d\theta\\ &-\frac{1}{2}\gamma^2(F_c[u+\varepsilon v](t)-F_c[u](t)-v^T\nabla F_c[u](t)\varepsilon).\end{aligned}\tag{6.27}$$

Applying Lemmas 17 and 19 and by direct integration with respect to r, it follows that

$$\int_0^\gamma \int_0^\theta \frac{1}{2} v^T \nabla^2 F_c[u+rv](t) v \varepsilon^2 dr d\theta = \frac{1}{4} v^T \nabla^2 F_c[u](t) v \varepsilon^2 \gamma^2 + \\ + \sum_{k=3}^{\infty} \sum_{\xi \in \mathbb{S}_{X^*,\delta X^k}} \frac{1}{2} (c, \sigma_X(\xi)) \mathcal{E}_\xi[u,v](t) \varepsilon^2 \gamma^k. \tag{6.28}$$

Using Lemma 18, the term $\frac{1}{2}\gamma^2(F_c[u+\varepsilon v](t) - F_c[u](t) - v^T \nabla F_c[u](t)\varepsilon)$ is equal to the right hand side of (6.28). Thus, if $\gamma = \varepsilon$ in (6.27) then $\phi(\varepsilon) = 0$. Also, it is easy to see that $\phi(0) = 0$. Thus, by the continuity of $F_c[u]$, Rolle's Theorem guarantees the existence of $\varepsilon_0 \in (0, \varepsilon)$ such that the derivative of ϕ at ε_0 is zero. That is,

$$\phi'(\varepsilon_0) = \int_0^{\varepsilon_0} \frac{1}{2} v^T \nabla^2 F_c[u+rv](t) v \varepsilon^2 dr - (F_c[u+\varepsilon v](t) - F_c[u](t) - v^T \nabla F_c[u](t)\varepsilon)\varepsilon_0 \\ = 0.$$

Hence, solving for $F_c[u+\varepsilon v]$ completes the proof. ■

The next corollary follows form Theorem 16 and gives a condition for the existence of an input producing a local minimum in a Chen-Fliess series. Define a ball centered at an input u^* with radius R as $B_{\mathfrak{p}}^m(u^*, R)[0,T] := \{u \in L_{\mathfrak{p}}^m[0,T] : \|u - u^*\|_{\mathfrak{p}} \leq R\}$

Corollary 7 *Let $c \in \mathbb{R}_{LC}\langle\langle X \rangle\rangle$ and $u^* \in L_{\mathfrak{p}}^m[0,t]$ such that $v^T \nabla F_c[u^*](t) = 0$. If there exists a neighborhood $B_{\mathfrak{p}}^m(u^*, R)[0,T]$ of u^* in which*

$$v^T \nabla^2 F_c[u^* + rv](t)\ v > 0,$$

for all $r \in \mathbb{R}$ such that $u^* + rv \in B_{\mathfrak{p}}^m(u^*, R)[0,T]$, then u^* produces a local minimum in the direction v.

Proof: From Theorem 16, u^* satisfying $v^T \nabla F_c[u^*](t) = 0$ and $u^* + \varepsilon v \in B_{\mathfrak{p}}^m(u^*, R)[0, T]$ give

$$F_c[u^* + \varepsilon v] = F_c[u^*] + \frac{1}{\varepsilon_0}\int_0^{\varepsilon_0} \frac{1}{2} v^T \nabla^2 F_c[u^* + rv](t) v \varepsilon^2 dr$$

with $u^* + rv \in B_{\mathfrak{p}}^m(u^*, R)[0, T], \forall r \in (0, \varepsilon)$. Hence, it follows that $F_c[u^* + rv] > F_c[u^*]$ in the direction of v, which implies that u^* produces a local minimum $F_c[u^*](t)$ for $t \in [0, T]$. ■

Chapter 7

Minimum Bounding Box via Second-Order Optimization

The problem of computing the minimum bounding box of reachable sets in an input-output context as described in Definition 37 corresponds to finding the minimum and maximum of $F_c[u](t)$ for all u taking values in the hyper-rectangle $\mathcal{U}$. In general, this problem is non-convex. The goal of this section is to find the minimum and maximum of $F_c[u](t)$ for all $u \in \mathcal{U}$ in a systematic manner for any system that can be represented as a Chen-Fliess series. One way of solving this is by extending *Newton's* method for a Chen-Fliess series given an initial condition u_0. The algorithm for a Chen-Fliess series has the form

$$u_{i+1} = u_i - \nabla^2 F_c[u_i](t)^{-1} \nabla F_c[u_i](t)^T, \tag{7.1}$$

where $\nabla F_c[u_i](t)$ and $\nabla^2 F_c[u_i](t)$ are the gradient and the Hessian of $F_c[u_i](t)$ for the generating series $c \in \mathbb{R}_{LC}\langle\langle X\rangle\rangle$. The section focuses on showing that a recursion

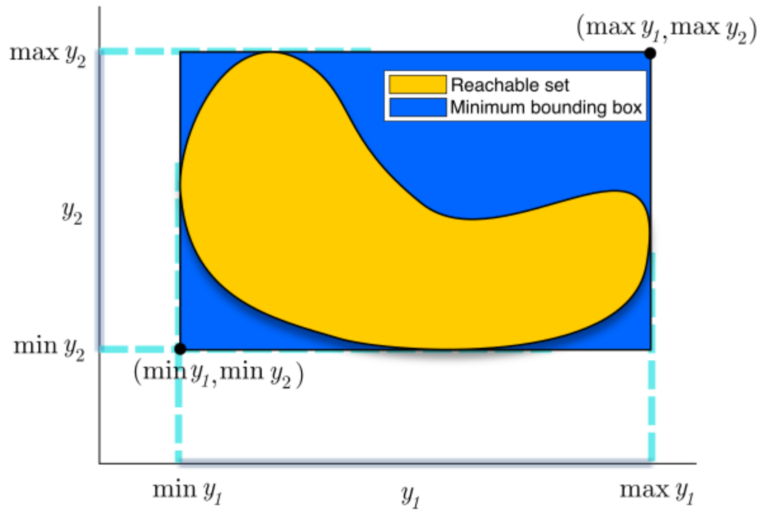


Figure 7.1: Output reachable set of a control affine system with a 2 dimensional output and its minimum bounding box (MBB) in terms of its maximum and minimum outputs.

based on (7.1) is well-posed. Fig. 7.1 outlines the idea for computing the minimum bounding box of a reachable set for a Chen-Fliess series by noticing that for a system with ℓ outputs the points $(\min y_1, \cdots, \min y_\ell)$ and $(\max y_1, \cdots, \max y_\ell)$ explicitly define the minimum bounding box of output reachable set.

7.1 Minimum Bounding Box via Newton

The Hessian in Theorem 16 can now be used to obtain the input signal that produces the MBB of the reachable sets of a CFS characterized by the generating series $c \in \mathbb{R}_{LC}\langle\langle X \rangle\rangle$. As a reminder, the objective is to find

$$\min_{u \in \mathcal{U}} F_c[u](t) \quad \text{and} \quad \max_{u \in \mathcal{U}} F_c[u](t),$$

where $\mathcal{U}$ is a hyper-rectangle in $\mathbb{R}^m$. Hereafter, the Hessian in Definition 49 is assumed to exist.

Theorem 17 *Consider a constant vector* $v \in \mathbb{R}^m$, $u \in L_{\mathfrak{p}}^m[0,t]$, $c \in \mathbb{R}_{LC}\langle\langle X \rangle\rangle$ *and the positive definite Hessian* $\nabla^2 F_c[u](t) > 0$. *The decreasing direction* v *for the input* u *is given by*

$$v = -\nabla^2 F_c[u](t)^{-1} \nabla F_c[u](t)^T.$$

Proof: From Lemma 18, $F_c[u+v](t)$ is approximated by

$$F_c[u](t) + v^T \nabla F_c[u](t) + \frac{1}{2} v^T \nabla^2 F_c[u](t) v,$$

which is a quadratic expression in terms of v with a positive quadratic coefficient. Then, the minimum is obtained by taking the derivative with respect to v and equating it to zero. That is,

$$\nabla F_c[u](t)^T + \nabla^2 F_c[u](t) v = 0. \tag{7.2}$$

Thus, the direction is obtained solving for v in (7.2). ■

Theorem 17 implies that if $\nabla^2 F_c[u](t) > 0$, then the sequence of inputs

$$u_{i+1} = u_i - \nabla^2 F_c[u_i](t)^{-1} \nabla F_c[u_i](t)^T$$

provides a decreasing sequence $F_c[u_i](t)$. Note that this recursion coincides with the standard Newton's iteration. Similar to the gradient projection method in [51], to satisfy the input constraints at each iteration, a projection into the feasible regions is applied. Given that the feasible set is a box, such projection is equivalent to a saturation function. That is, given the box $\mathcal{U} = [\underline{u}, \overline{u}]$, at each iteration step the new input is obtained after applying the function $\text{sat}_{\mathcal{U}}(u_i) = \underline{u}$ if $u_i < \underline{u}$, $\text{sat}_{\mathcal{U}}(u_i) = \overline{u}$ if $u_i > \overline{u}$, and $\text{sat}_{\mathcal{U}}(u_i) = u_i$ otherwise. Thus, Newton's method for a Chen-Fliess series is given in Algorithm 2.

Algorithm 2 Newton's method

Input: $R, u_0, \mathcal{U}$

Initialization : u_0

for $i = 1$ to R **do**

  $u_{i+1} = u_i - \nabla^2 F_c[u_i](t)^{-1} \nabla F_c[u_i](t)^T$,

  $u_{i+1} \leftarrow \text{sat}_{\mathcal{U}}(u_{i+1})$

end for

return $F_c[u_R](t)$

7.2 Minimum Bounding Box via Trust Regions

The underlying assumption in Newton's method is that the Hessian is positive definite. When this is not the case, the trust regions' method is an alternative to find local minima [51]. Here the objective is to adapt such methodology for the case of a Chen-Fliess series. Specifically, the *Cauchy point* optimization method is used in the present work. For simplicity, set $g_i = \nabla F_c[u_i](t)$ and $B_i = \nabla^2 F_c[u_i](t)$. First, the optimization problem is restricted to a region of fixed size where decreasing is ensured. That is, the minimization problem becomes

$$\min_{||v||\leq\Delta} F_c[u_i](t) + v^T g_i,$$

whose solution is $v = -\frac{\Delta}{||g_i||} g_i$. Then, the second step consists in optimizing the step τ in the direction of decreasing by solving

$$\min_{||v||\leq\Delta} F_c[u_i](t) + \tau v^T g_i + \frac{\tau^2}{2} v^T B_i v.$$

The solution to this problem is $\tau_i = 1$ if $g_i^T B_i g_i \leq 0$ and $\tau_i = \min(||g_i||^3/(\Delta g_i^T B_i g_i), 1)$ otherwise. Thus, the *trust regions*' method for a Chen-Fliess series is given in Algorithm 3.

Algorithm 3 Trust regions' method

Input: R, $u_0, \mathcal{U}$

$\quad$ *Initialization* : u_0

for $i = 1$ to R **do**

$\quad g_i \leftarrow \nabla F_c[u_i](t),$

$\quad B_i \leftarrow \nabla^2 F_c[u_i](t),$

$\quad v_i \leftarrow -\frac{\Delta}{||g_i||} g_i,$

$\quad$ **if** $g_i^T B_i g_i \leq 0$ **then**

$\quad\quad \tau_i = 1,$

$\quad$ **else**

$\quad\quad \tau_i = \min(||g_i||^3/(\Delta_i g_i^T B_i g_i), 1),$

$\quad$ **end if**

$\quad v_i \leftarrow \tau_i v_i,$

$\quad u_{i+1} = u_i + v_i,$

$\quad u_{i+1} \leftarrow \text{sat}_{\mathcal{U}}(u_{i+1})$

end for

return $F_c[u_R](t)$

7.3 Numerical Simulations

Example 22 *Consider the system in Example 20. The reachable set of the system with input set* $\mathcal{U} := \{u \in \mathbb{R} : -1 \leq u \leq 1\}$ *is provided in Fig. 7.2 together with the outcome of Algorithm 2 applied to the Chen-Fliess series corresponding to (6.19). Fig. 7.2 shows that Algorithm 2 approximates the reachable set up to* $t = 1$ *very*

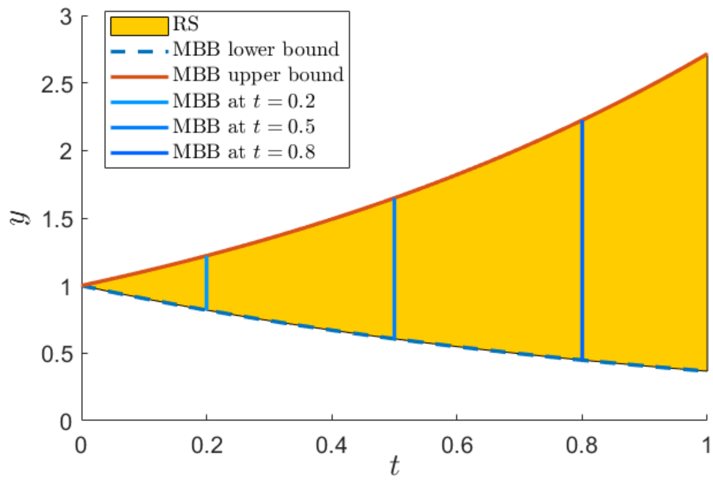


Figure 7.2: Estimation of the minimum bounding box (MBB) of the reachable sets in Example 20 with $x(0) = 1$ using Algorithm 2, $u_0 = 0$, $\mathcal{U} = \{u : -1 \leq u \leq 1\}$, and Chen-Fliess series truncation $N = 3$.

well. Also, it is observed that the number of iterations for Newton's method is faster ($N_N \approx 10$) than that of the gradient descent method presented in [54] ($N_{GD} \approx 1000$).

Example 23 *Consider the bi-steerable car in Fig. 7.3 described by the set of equations*

$$\dot{x}_1 = \cos(x_3 + x_4)u_1,$$

$$\dot{x}_2 = \sin(x_3 + x_4)u_1,$$

$$\dot{x}_3 = \frac{\sin((1-k)\alpha)}{(L\cos(k\alpha))},$$

$$\dot{x}_4 = u_2$$

with output $y = (x_1,\ x_2)^T$, $k = -0.7$, $\alpha = \pi/8$, $L = 1$, $x_0 = (0, 0, 0.1, 0.2)$, and u_1 and u_2 the inputs to the system. The outputs of the system as Chen-Fliess series' are $y_1(t) = F_{c_1}[u](t)$ and $y_2(t) = F_{c_2}[u](t)$, where the coefficients are computed using

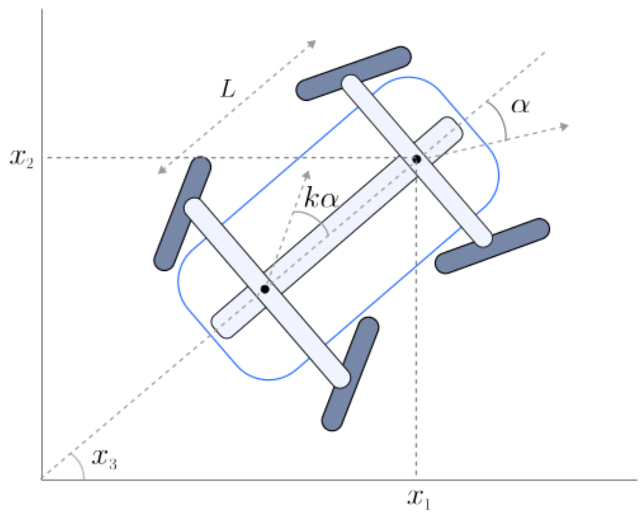


Figure 7.3: Bi-steerable car.

(2.5). Thus,

$$\begin{aligned}c_1 =& 0.95x_1 - 0.19x_1x_1 - 0.29x_1x_2 - 0.39x_1x_1x_1 + \\ & - 0.61x_1x_1x_2 - 0.61x_1x_2x_1 - 0.95x_1x_2x_2 + \cdots \\ c_2 =& 0.29x_1 + 0.61x_1x_1 + 0.95x_1x_2 - 0.12x_1x_1x_1 \\ & - 0.19x_1x_1x_2 - 0.19x_1x_2x_1 - 0.29x_1x_2x_2 + \cdots\end{aligned}$$

From Lemma 14 and Theorem 15, the derivatives $(\delta_{x_1}(c_1), \delta_{x_2}(c_1))$ *and* $(\delta_{x_1}(c_2), \delta_{x_2}(c_2))$ *determine the generating series of gradient of* $F_{c_1}[u](t)$ *and* $F_{c_2}[u](t)$*, respectively. From Lemma 11, these are*

$$\begin{aligned}\delta_{x_1}(c_1) =& 0.95\delta x_1 - 0.19\delta x_1x_1 - 0.19x_1\delta x_1 \\ & - 0.29\delta x_1x_2 - 0.39\delta x_1x_1x_1 + \cdots ,\end{aligned}$$

$$
\begin{aligned}
\delta_{x_2}(c_1) = & -0.29x_1\delta x_2 - 0.61x_1x_1\delta x_2 - 0.61x_1\delta x_2x_1 \\
& - 0.95x_1\delta x_2x_2 - 0.95x_1x_2\delta x_2 + \cdots ,
\end{aligned}
$$

$$
\begin{aligned}
\delta_{x_1}(c_2) = & 0.29\delta x_1 + 0.61\delta x_1x_1 + 0.61x_1\delta x_1 \\
& + 0.95\delta x_1x_2 - 0.12\delta x_1x_1x_1 + \cdots ,
\end{aligned}
$$

$$
\begin{aligned}
\delta_{x_2}(c_2) = & 0.95x_1\delta x_2 - 0.19x_1x_1\delta x_2 - 0.19x_1\delta x_2x_1 \\
& - 0.29x_1\delta x_2x_2 - 0.29x_1x_2\delta x_2 + \cdots .
\end{aligned}
$$

Using Lemma 16, the second-order derivatives are

$$
\begin{aligned}
\delta_{x_1x_1}(c_1) = & -0.38\delta x_1\delta x_1 - 0.78\delta x_1\delta x_1x_1 \\
& - 0.78\delta x_1x_1\delta x_1 - 0.78x_1\delta x_1\delta x_1 + \cdots ,
\end{aligned}
$$

$$
\begin{aligned}
\delta_{x_1x_2}(c_1) = & -0.29\delta x_1\delta x_2 - 0.61\delta x_1x_1\delta x_2 \\
& - 0.61x_1\delta x_1\delta x_2 - 0.61\delta x_1\delta x_2x_1 + \cdots ,
\end{aligned}
$$

$$
\begin{aligned}
\delta_{x_2x_2}(c_1) = & -1.90x_1\delta x_2\delta x_2 + 0.38x_1x_1\delta x_2\delta x_2 \\
& + 0.38x_1\delta x_2x_1\delta x_2 + 0.38x_1\delta x_2\delta x_2x_1 + \cdots ,
\end{aligned}
$$

$$
\begin{aligned}
\delta_{x_1x_1}(c_2) = &\,1.22\delta x_1\delta x_1 - 0.24\delta x_1\delta x_1 x_1 \\
&- 0.24\delta x_1 x_1\delta x_1 - 0.24 x_1\delta x_1\delta x_1 + \cdots ,
\end{aligned}
$$

$$
\begin{aligned}
\delta_{x_1x_2}(c_2) = &\,0.95\delta x_1\delta x_2 - 0.19\delta x_1 x_1\delta x_2 \\
&- 0.19 x_1\delta x_1\delta x_2 - 0.19\delta x_1\delta x_2 x_1 + \cdots ,
\end{aligned}
$$

$$
\begin{aligned}
\delta_{x_2x_2}(c_2) = &\; -0.58 x_1\delta x_2\delta x_2 - 1.22 x_1 x_1\delta x_2\delta x_2 \\
&- 1.22 x_1\delta x_2 x_1\delta x_2 - 1.22 x_1\delta x_2\delta x_2 x_1 + \cdots .
\end{aligned}
$$

According to Lemma 17, these are the power series that determine the Hessian of the Chen-Fliess series. Fig. 7.4 shows the result of applying Algorithm 3 to compute the minimum bounding box of the reachable set at different points in time. It is clear from the plots at $t = 0.5$*,* 1 *and* 1.5 *seconds that the computed over-approximations are indeed the minimum bounding box of the true reachable sets. Furhermore, Fig. 7.5 compares the trust regions method against the gradient descent method for the computation of minimum bounding boxes of the system in Example 23. The gradient descent method in [53] produced the black dashed box in Fig. 7.5 with* 10 *iterations whereas the trust regions method converged to the true minimum bounding box with the same number of iterations. To match the true minimum bounding box, the gradient descent method needed approximately* 100 *iterations.*

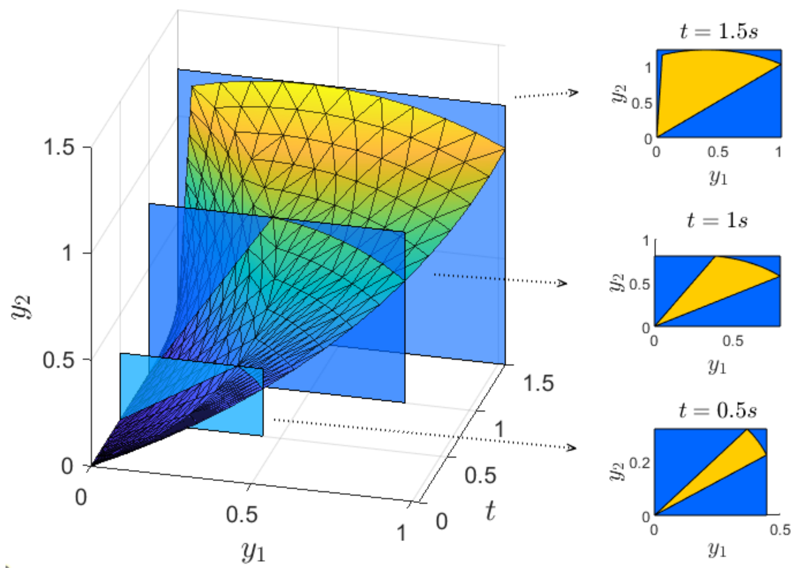


Figure 7.4: Reachable sets and minimum bounding boxes in Example 23 for $\mathcal{U} = \{(u_1, u_2) : 0 \leq u_1 \leq 1,\ 0 \leq u_2 \leq 1\}$ and truncation $N = 8$.

Example 24 *Consider the Lotka-Volterra system described by the set of equations*

$$\dot{x}_1 = -x_1 x_2 + x_1 u_1,$$

$$\dot{x}_2 = x_1 x_2 - x_2 u_2,$$

with output $y = (x_1,\ x_2)^T$, initial condition $x_0 = (1/3, 2/3)^\top$ and inputs u_1 and u_2. Similarly to the previous example, the outputs of the system are described as Chen-Fliess series by $y_1(t) = F_{c_1}[u](t)$ and $y_2(t) = F_{c_2}[u](t)$. The corresponding coefficients are computed from (2.5). Thus, one has that

$$c_1 = 0.33 - 0.22x_0 + 0.33x_1 + 0.07x_0x_0 - 0.22x_0x_1 + 0.22x_0x_2 - 0.22x_1x_0 + 0.33x_1x_1 + \cdots,$$

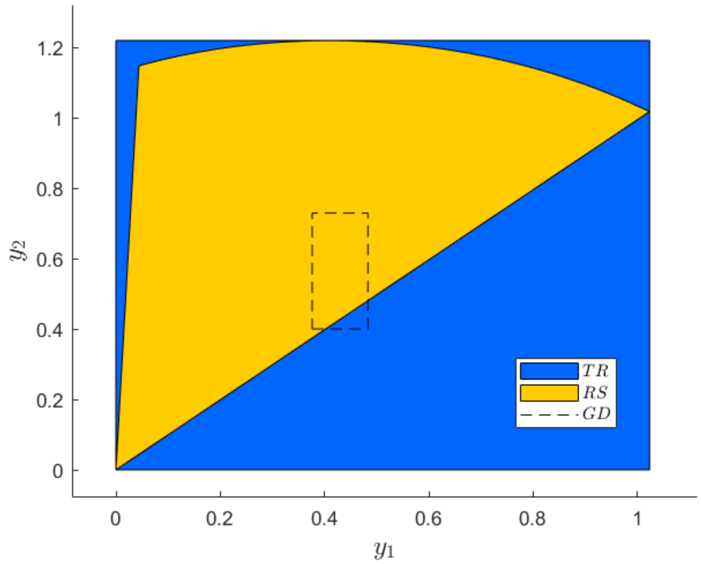


Figure 7.5: Minimum bounding box and reachable sets (RS) in Example 23 at $t = 1.5s$ with $\mathcal{U} = \{(u_1, u_2) \; : \; 0 \le u_1 \le 1, \; 0 \le u_2 \le 1\}$ and truncation $N = 8$. The trust regions method (TR) needed 10 iterations to converge to the minimum bounding box. The gradient descent method (GD) in [53] with 10 iterations and a step size of 0.01 gives the black dashed box. Both methods were initialized with $(u_1, u_2) = (0.5, 0.5)$.

$$
\begin{aligned}
c_2 = \; & 0.66 + 0.22x_0 - 0.66x_2 - 0.07x_0x_0 + 0.22x_0x_1 \\
& - 0.22x_0x_2 - 0.22x_2x_0 + 0.66x_2x_2 + \cdots .
\end{aligned}
$$

The generating series of the derivatives determining the gradient of $F_{c_1}[u](t)$ and $F_{c_2}[u](t)$, respectively are computed according to Lemma 11. These are

$$
\begin{aligned}
\delta_{x_1}(c_1) = \; & 0.33\delta x_1 - 0.22x_0\delta x_1 - 0.22\delta x_1 x_0 \\
& + 0.33\delta x_1 x_1 + 0.33x_1\delta x_1 + \cdots ,
\end{aligned}
$$

$$\delta_{x_2}(c_1) = 0.22x_0\delta x_2 - 0.22x_0x_0\delta x_2 + 0.22x_0x_1\delta x_2$$
$$- 0.07x_0\delta x_2x_0 + 0.22x_0\delta x_2x_1 + \cdots,$$

$$\delta_{x_1}(c_2) = 0.22x_0\delta x_1 - 0.07x_0\delta x_1x_0 + 0.22x_0\delta x_1x_1$$
$$+ 0.22x_0x_1\delta x_1 - 0.22x_0\delta x_1x_2 + \cdots,$$

$$\delta_{x_2}(c_2) = -0.66\delta x_2 - 0.22x_0\delta x_2 - 0.22\delta x_2x_0$$
$$+ 0.66\delta x_2x_2 + 0.66x_2\delta x_2 + 0.22x_0x_0\delta x_2 + \cdots.$$

The second-order derivatives are computed using Lemma 16. These are

$$\delta_{x_1x_1}(c_1) = 0.66\delta x_1\delta x_1 - 0.44x_0\delta x_1\delta x_1 - 0.44\delta x_1\delta x_1x_0$$
$$+ 0.66\delta x_1\delta x_1x_1 + 0.66\delta x_1x_1\delta x_1 + \cdots,$$

$$\delta_{x_2x_1}(c_1) = 0.22x_0\delta x_1\delta x_2 + 0.22x_0\delta x_2\delta x_1$$
$$+ 0.22\delta x_1x_0\delta x_2 - 0.14x_0x_0\delta x_1\delta x_2 + \cdots,$$

$$\delta_{x_2x_2}(c_1) = -0.44\delta x_2\delta x_2 + 1.03x_0x_0\delta x_2\delta x_2$$
$$- 0.44x_0x_1\delta x_2\delta x_2 + 0.44x_0\delta x_2x_0\delta x_2 + \cdots,$$

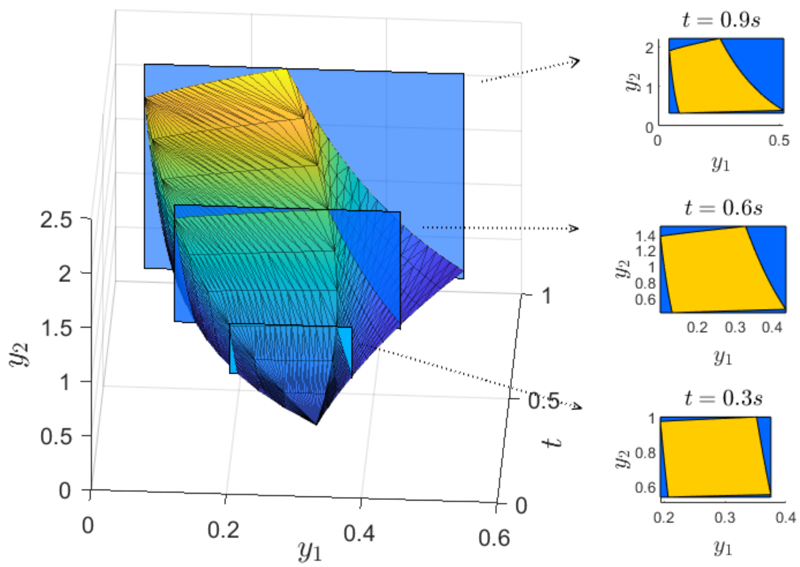


Figure 7.6: Reachable sets and minimum bounding box in Example 24 for $\mathcal{U} = \{(u_1, u_2) : 0 \leq u_1 \leq 1,\ 0 \leq u_2 \leq 1\}$ and a Chen-Flies series truncation of $N = 8$. On the right side, the graph displays the minimum bounding boxes at three different times: $t = 0.3s$, $t = 0.6s$ and $t = 0.9s$. The trust region size used was $\Delta = 1$.

$$\begin{aligned}\delta_{x_1x_1}(c_2) = &\, 0.44x_0\delta x_1\delta x_1 + 0.29x_0x_0\delta x_1\delta x_1 \\ &- 0.14x_0\delta x_1\delta x_1x_0 + 0.44x_0\delta x_1\delta x_1x_1 + \cdots ,\end{aligned}$$

$$\begin{aligned}\delta_{x_2x_1}(c_2) = &- 0.22x_0\delta x_1\delta x_2 - 0.22x_0\delta x_2\delta x_1 \\ &- 0.22\delta x_2x_0\delta x_1 + 0.14x_0x_0\delta x_1\delta_2 + \cdots ,\end{aligned}$$

$$\begin{aligned}\delta_{x_2x_2}(c_2) = &\, 1.33\delta x_2\delta x_2 + 0.44x_0\delta x_2\delta x_2 + 0.44\delta x_2x_0\delta x_2 \\ &+ 0.44\delta x_2\delta x_2x_0 - 1.33\delta x_2\delta x_2x_2 + \cdots .\end{aligned}$$

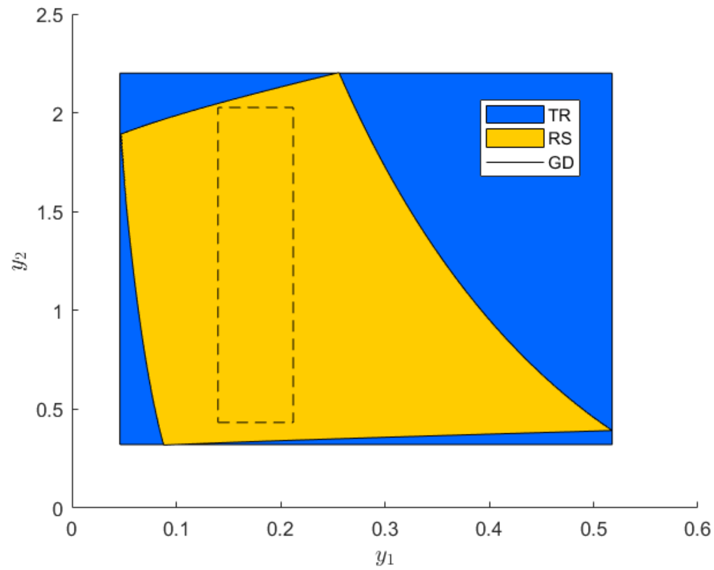


Figure 7.7: Minimum bounding box and reachable set (RS) in Example 24 at the time $t = 0.9s$ with $\mathcal{U} = \{-1 \leq u_1 \leq 1, -1 \leq u_2 \leq 1\}$ and a Chen-Fliess series truncation of $N = 8$. The trust region algorithm (TR) needed 140 iterations while the dashed box gives the minimum bounding box using the gradient descent with 140 iterations. One will need 490 iterations to a fixed step size of $\varepsilon = 0.01$ over the same number of iterations. The actual minimum bounding box is obtained through gradient descent with a step size of $\varepsilon = 0.1$ and 490 iterations.

From Lemma 17, these determine the Hessian of system. Fig. 7.6 shows the result of Algorithm 3 to compute the minimum bounding box of the reachable at different points in time (t = 0.3, 0.6 and 0.9 seconds). Fig. 7.7 compares the trust region method against the gradient descent method for the computation of the minimum bounding box of the system in Example 24. The gradient descent method produced the dashed box in Fig. 7.7 with the same number of iterations the trust regions method took to obtain the true minimum bounding box. To match the true minimum bounding box, the gradient descent method needed 490 iterations.

Chapter 8

Backward and Inner Approximation of Reachable Sets

The problem of computing the minimum bounding box of the input-output backward reachable set given the output box $[\underline{y}, \overline{y}]$ of the Chen-Fliess series $F_c[u](t)$ can be reduced to finding the minimum and maximum of u of all $u \in B_{\mathfrak{p}}^m(R)[0,T]$ subject to $F_c[u](t)$ and lying inside the box $[\underline{y}, \overline{y}]$. This is a non-convex optimization problem, and this section provides a methodology for solving it. The idea for such a method revolves around setting a *gradient descent* recursion for some initial condition u_0 that has the form

$$u_i(k) = u_i(k) - \varepsilon e_i, \tag{8.1}$$

where ε is the *learning* parameter and e_i is an appropriate gradient with respect to u_i, which is the i-th coordinate of the input u.

8.1 Pre-Image and Backward Reachable Sets

Here, finding the backward reachable set of (2.4) using a Chen-Fliess series representation is stated as an optimization problem. It is important to notice that this problem lies in the realm of infinite dimensional analysis and is in general non-tractable. Therefore, the problem is solved using a numerical method based on the *Gâteaux directional derivative* [25].

The definition of a backward reachable set for system in state-space representation can be written as

Definition 50 *The state backward reachable set at a fixed time t of (2.4) subject to a set of states taking values in $\mathcal{Z} \subset \mathbb{R}^n$ and a set of initial states $\mathcal{Z}_0 \subset \mathbb{R}^n$ is*

$$Pre(\mathcal{Z}_0, \mathcal{Z})(t) := \left\{ z \in \mathcal{Z}_0 : \exists u \in L_{\mathfrak{p}}^m[0,t],\ \phi(t,u,z_0) \in \mathcal{Z} \right\}$$

where $\phi(\tau, u, z_0)$ for $\tau \in [0,T]$ represents the trajectory of the state z satisfying (2.4a).

Before getting into the details, observe that Definition 50 does not consider an output equation. The following definition is a mild extension of the definition of the state backward reachable set.

Definition 51 *The backward reachable set at a fixed time t of (2.4) subject to a set of outputs taking values in $\mathcal{Y} \subset \mathbb{R}^\ell$ and a set of initial states $\mathcal{Z}_0 \subset \mathbb{R}^n$ is*

$$Pre(\mathcal{Z}_0, \mathcal{Y})(t) := \left\{ z \in \mathcal{Z}_0 : \exists u \in L_{\mathfrak{p}}^m[0,t], h(\phi(t,u,z_0)) \in \mathcal{Y} \right\}$$

where $\phi(\tau, u, z_0)$ for $\tau \in [0,t]$ represents the trajectory of the state z satisfying (2.4a).

This is extended to the backward reachable set of a Chen-Fliess series providing an input-output framework. For the next definition, consider for any $c \in \mathbb{R}^\ell\langle\langle X\rangle\rangle$, the power series $c' \in \mathbb{R}^\ell\langle\langle X\rangle\rangle$ such that $c' = c - (c, \emptyset)$.

Definition 52 *Given the alphabet $X = \{x_0, \cdots, x_m\}$, the formal power series $c \in \mathbb{R}^\ell\langle\langle X\rangle\rangle$ and $\mathcal{Y} \subset \mathbb{R}^m$, the input-output backward reachable set of the Chen-Fliess series $F_c[u](t)$ with outputs taking values in $\mathcal{Y}$ is the set*

$$Pre_c(\mathcal{Y}_0, \mathcal{Y})(t) = \Big\{ y_0 \in \mathcal{Y}_0 \ : \ \exists u \in L_{\mathfrak{p}}^m[0,t], y_0 + F_{c'}[u](t) \in \mathcal{Y} \Big\}.$$

In the case that the backward reachable set at $t_0 > 0$ of a given Chen-Fliess series with final output set $\mathcal{Y}$ at t_f needs to be obtained, the following set is more appropriate:

$$\mathrm{Pre}_c(y_0, \mathcal{Y})(t_0, t_f) = \Big\{ y \in \mathbb{R}^\ell \ : \ \exists u \in L_{\mathfrak{p}}^m[0,t], F_c[u](t_0, t_f) \in \mathcal{Y}, \ F_c[u](0, t_0) = y \Big\}.$$

In many branches of the analysis of systems such as control, path planning, and viability, the knowledge of the set of inputs that steer the Chen-Fliess series to a given output set is sought. For Chen-Fliess series, this set is equal to the pre-image of the given output set.

Definition 53 *Given the alphabet $X = \{x_0, \cdots, x_m\}$, the formal power series $c \in \mathbb{R}^\ell\langle\langle X\rangle\rangle$ and the output set $\mathcal{Y} \subset \mathbb{R}^m$, the pre-image of the Chen-Fliess series $F_c[u](t)$ with outputs taking values in $\mathcal{Y}$ is the set*

$$F_c^{-1}(\mathcal{Y})(t) = \{ u \in B_{\mathfrak{p}}^m(R)[0,T] \ : \ F_c[u](t) \in \mathcal{Y} \}.$$

The next result relates the state backward reachable set definition from the output perspective with the definition via Chen-Fliess series.

Theorem 18 *Consider the nonlinear affine control system in (2.4), given the output set* $\mathcal{Y} \subset \mathbb{R}^\ell$ *and the initial state set* $\mathcal{Z}_0 \subset \mathbb{R}^n$ *and the initial output set* $\mathcal{Y}_0 = h(\mathcal{Z}_0)$*, the output backward reachable set of the system in Definition 51 is equal to the backward reachable set of Chen-Fliess series in Definition 52. This is,* $h(Pre(\mathcal{Z}_0, \mathcal{Y})(t)) = Pre_c(\mathcal{Y}_0, \mathcal{Y})(t)$*.*

Proof: The proof follows straightforwardly from the fact that the Chen-Fliess series represents the output of the system in $B_{\mathfrak{p}}^m(R)[0,T]$.

$$
\begin{aligned}
y \in h(\mathrm{Pre}(\mathcal{Z}_0, \mathcal{Y})(t)) &\iff \exists z_0 \in \mathcal{Z}_0,\ \exists u \in L_{\mathfrak{p}}^m[0,t], y = h(\phi(t,u,z_0)), y_0 = h(z_0) \\
&\iff \exists u \in L_{\mathfrak{p}}^m[0,t],\ y_0 = h(z_0), y = y_0 + F_c[u](t) \\
&\iff y \in \mathrm{Pre}_c(\mathcal{Y}_0, \mathcal{Y})(t).
\end{aligned}
$$

■

For computational matters, Theorem 18 implies that the output backward reachable set can be computed using the Chen-Fliess series of the system. Naturally, the minimum bounding box of the output backward reachable set is equal to the minimum bounding box of the backward reachable using Chen-Fliess series.

The definition of an output reachable set in Definition 37 is extended to take a set of initial outputs.

Definition 54 *Given the alphabet* $X = \{x_0, \cdots, x_m\}$*, the formal power series* $c \in \mathbb{R}^\ell\langle\langle X \rangle\rangle$*, the set* $\mathcal{U} \subset B_{\mathfrak{p}}^m(R)[0,T]$ *and the set of initial outputs* $\mathcal{Y}_0$*, the reachable set*

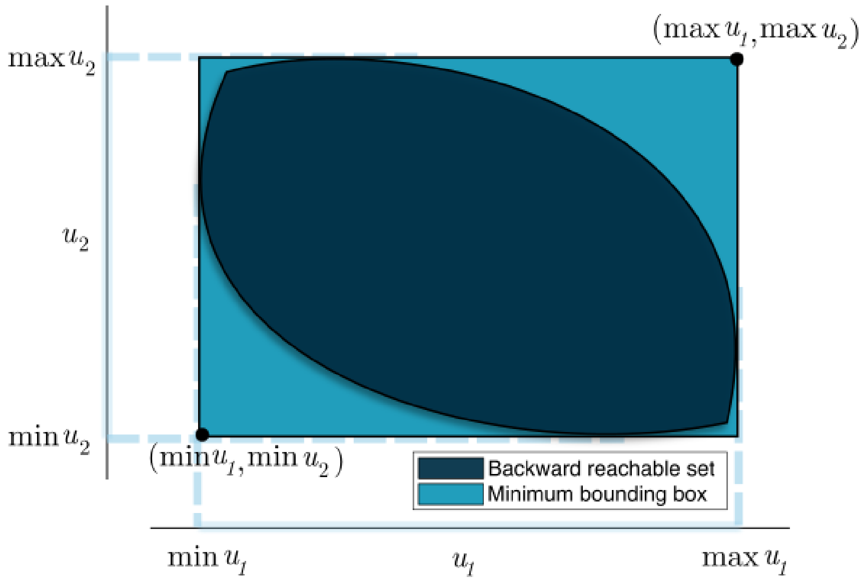


Figure 8.1: Pre-image set of a control affine system with a 2 dimensional input and its minimum bounding box in terms of its maximum and minimum inputs.

of the Chen-Fliess series $F_c[u](t)$ *with inputs taking values in* $\mathcal{U}$ *and initial outputs* $y_0 \in \mathcal{Y}_0$ *is the set*

$$Reach_c(\mathcal{U}, \mathcal{Y}_0)(t) := \left\{ y = y_0 + F_{c'}[u](t) \in \mathbb{R}^\ell : \forall u \in \mathcal{U}, \forall y_0 \in \mathcal{Y}_0 \right\}$$

The next result characterizes the reachable set of a Chen-Fliess series at any time in terms of the initial output set, the Minkowski sum and the reachable set of the power series without the drifting element.

Theorem 19 *For any* $c \in \mathbb{R}^\ell\langle\langle X \rangle\rangle$*, the reachable set satisfies*

$$Reach_c(\mathcal{U}, \mathcal{Y}_0)(t) = \mathcal{Y}_0 \oplus Reach_{c'}(\mathcal{U}, 0)(t)$$

Proof: The proof follows by definition

$$\begin{aligned} y \in \text{Reach}_c(\mathcal{U}, \mathcal{Y}_0)(t) &\iff \exists u \in \mathcal{U}, \exists y_0 \in \mathcal{Y}_0, y = y_0 + F_{c'}[u](t) \\ &\iff y \in \mathcal{Y}_0 \oplus \text{Reach}_{c'}(\mathcal{U}, 0)(t) \end{aligned}$$

■

Given the linear control system

$$\dot{x} = Ax + Bu,\ x(0) = x_0,$$

the solution is given by

$$x(t) = \exp(-At)x_0 + \int_0^t \exp(A(t-\tau))Bu(\tau)d\tau$$

then the reachable set o the linear system for $x_0 \in \mathcal{X}_0$ and $u \in \mathcal{U}$ is

$$\text{Reach}(\mathcal{U}, \mathcal{X}_0) = \text{Reach}(\mathcal{X}_0, 0) \oplus \text{Reach}(0, \mathcal{U}). \tag{8.2}$$

8.2 Backward Reachable Set Computation via Chen-Fliess Series

Theorem 19 extends the well-known result in (8.2) to the Chen-Fliess series setting. In what follows, the focus is on the computation of the minimum bounding box of the pre-image set in Definition 53. For the sake of space, denote $B = B_{\mathfrak{p}}^m(R)[0,T]$.

The idea to compute the minimum bounding box is to reduce the calculations to only two points. Figure 8.1 illustrates the idea of the computation of the minimum bounding box of the pre-image set by the optimization of the coordinates of the input. Equivalently, the following problems are solved:

$$\begin{aligned} \min_{u\in B} \quad & u_i \\ \text{s.t.} \quad & F_c[u](t) \in [\underline{y}, \overline{y}] \end{aligned} \qquad \text{and} \qquad \begin{aligned} \max_{u\in B} \quad & u_i \\ \text{s.t.} \quad & F_c[u](t) \in [\underline{y}, \overline{y}]. \end{aligned} \tag{8.3}$$

call the solution of each problem $\underline{u}_i$ and $\overline{u}_i$ respectively and form the vector $\underline{u} = (\underline{u}_1, \cdots, \underline{u}_m)$ and $\overline{u} = (\overline{u}_1, \cdots, \overline{u}_m)$ then the minimum bounding box of the backward reachable set is $[\underline{u}, \overline{u}]$. Notice that the problem of the feasibility of (8.3) is not trivial since the constraints are a set of polynomial inequalities. To tackle this problem the Positivstellensatz in Theorem (8) can be used.

Formally, the problem in (8.3) having a solution follows from the Karush-Kuhn-Tucker conditions, where the critical points of the Lagrangian function are the candidates for optimal points. Here, the Lagrangian expressions of interest are

$$L(\lambda, u) = u_i + \sum_{j=1}^{\ell} \lambda_j^1(\overline{y}_i - F_{c_i}[u](t)) + \lambda_j^2(F_{c_i}[u](t) - \underline{y}_i),$$

$$\lambda_j^1(\overline{y}_i - F_{c_i}[u](t)) = 0,$$

$$\lambda_j^2(\underline{y}_i - F_{c_i}[u](t)) = 0,$$

$$F_{c_i}[u](t) - \overline{y}_i \leq 0,$$

$$\underline{y}_i - F_{c_i}[u](t) \leq 0,$$

$$\lambda_j^k \geq 0, \forall k \in \{1, 2\}$$

for all $j \in \{1, \cdots, m\}$. The optimal points $(\lambda^*, \underline{u})$ are characterized by the set of Gâteaux partial differential equations:

$$\begin{aligned} \frac{\partial}{\partial \lambda} L(\lambda^*, u^*) = 0, \\ \frac{\partial}{\partial u} L(\lambda^*, u^*) = 0. \end{aligned} \tag{8.4}$$

Obtaining a closed-form of the solution of (8.4) is challenging even for real value functions over real coordinate domains. In recent efforts [19], the critical points characterizing the optimal values of the unconstrained optimization of a Chen-Fliess series are found analytically for simple cases. Here, the problem in (8.3) is solved numerically through a variation of the gradient descent method known as *projected gradient descent* [51]. Similar to [54–57], the constraint is enforced by projecting the solution at each iteration on the boundary of the constrained sets in the problem. This projection constitutes the difference between the method used here and the one used in [54], where in the latter the input updates were only projected over the pre-defined input constraint set. Define the set $\mathcal{P} = F_c^{-1}([\underline{y}, \overline{y}])(t) := \{u \in B_{\mathfrak{p}}^m(R)[0, T] \ : F_c[u](t) \in [\underline{y}, \overline{y}]\}$. Using Definition 53, the projected gradient descent method for the minimization of the i-th input coordinate is described in Algorithm 4 where $\text{Proj}_{\mathcal{P}}(u) := \min_{z \in \mathcal{P}} ||z - u||$.

Algorithm 4 Projected Gradient Descent

Input: N_{GD}, u_0, ε, $\mathcal{P}$

1: Initialization : u_0

2: **for** $j = 1$ to N_{GD} **do**

3: $\quad u_i^{j+1} = u_i^j - \varepsilon e_i,$

4: $\quad u_i^{j+1} \leftarrow \mathrm{Proj}_{\mathcal{P}}(u_i^{j+1})$

5: **end for**

6: **return** $u_i^{N_{GD}}$

8.3 Inner approximation of Reachable Sets via Chen-Fliess Series

In this section, a method for computing the inner approximation of a reachable set of a nonlinear affine control system in (2.4) using Chen-Fliess series is povided. Similar to [53], the approach here is based on the optimization of a Chen-Fliess series and follows along the lines of that in [43], where the method for inner approximation of the reachable set is applied to linear systems. By using the Chen-Fliess series framework, inner approximations can be obtained for a broader class of systems but with the condition that the reachable sets must be convex. Furthermore, the method in [43] computes inner approximations of the so-called viability set by using a support vector function.

Figure 8.2 shows the reachable set overapproximated by taking a sample of support vectors equal to the canonical basis of $\mathbb{R}^2$, i.e., (e_1, e_2). This results in the box

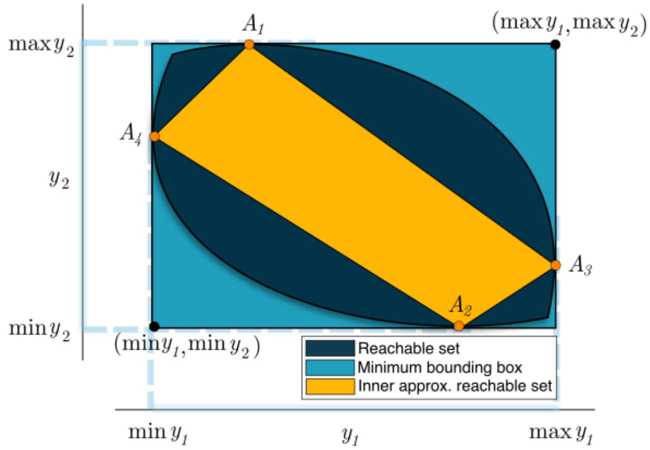


Figure 8.2: Inner-approximation of the reachable set of a control affine system with a 2 dimensional output and its minimum bounding box in terms of its maximum and minimum inputs.

$\mathcal{Y} = [\min y,\ \max y]$, which can also be expressed as

$$\mathcal{Y} = \{y \in \mathbb{R}^2 :\ y \cdot v \leq \sigma_{\mathcal{Y}}(v), v \in \{e_1, e_2, -e_1, -e_2\}\}.$$

The points defining the inner-approximation of the reachable set are the solutions to the following optimization problems:

$$\arg\min_{u\in\mathcal{U}} F_{c_i}[u](t) \quad \text{and} \quad \arg\max_{u\in\mathcal{U}} F_{c_i}[u](t) \tag{8.5}$$

Figure 8.2 shows these points explicitly and labeled as

$$
\begin{aligned}
A_1 &= (F_{c_1}[u_1^*](t), F_{c_2}[u_1^*](t)),\\
A_2 &= (F_{c_1}[u_2^*](t), F_{c_2}[u_2^*](t)),\\
A_3 &= (F_{c_1}[u_3^*](t), F_{c_2}[u_3^*](t)),\\
A_4 &= (F_{c_1}[u_4^*](t), F_{c_2}[u_4^*](t)),
\end{aligned}
$$

where

$$
\begin{aligned}
u_1^* = \arg\max_{u\in\mathcal{U}} F_{c_1}[u](t),\ \ u_2^* = \arg\min_{u\in\mathcal{U}} F_{c_2}[u](t),\\
u_3^* = \arg\max_{u\in\mathcal{U}} F_{c_2}[u](t),\ \ u_4^* = \arg\min_{u\in\mathcal{U}} F_{c_1}[u](t).
\end{aligned}
$$

Hence, the inner-approximation is given by the convex hull

$$
\mathrm{IReach}_c(\mathcal{U})(t) = \mathrm{conv}(A_1, A_2, A_3, A_4).
$$

In [43] the same set was written as

$$
\mathrm{IReach}_c(\mathcal{U})(t) = \mathrm{conv}(\{u_e : e \in \{e_1, e_2, -e_1, -e_2\}\}),
$$

where $v_{\mathcal{Y}}(e) = \arg\max_{y\in\mathcal{Y}} y \cdot e$ and $u_e \in v_{\mathcal{Y}}(e)$. Here, to obtain the reachable set inner-approximation, one computes

$$
\begin{aligned}
\underline{u}^i &= \arg\min_{u\in\mathcal{U}} F_{c_i}[u](t)\\
\overline{u}^i &= \arg\max_{u\in\mathcal{U}} F_{c_i}[u](t)\\
\underline{A}^i &= (F_{c_1}[\underline{u}^i](t), F_{c_2}[\underline{u}^i](t))\\
\overline{A}^i &= (F_{c_1}[\overline{u}^i](t), F_{c_2}[\overline{u}^i](t))
\end{aligned}
$$

for $i \in \{1, \cdots, \ell\}$, which yields the reachable set inner-approximation as

$$
\mathrm{IReach}_c(\mathcal{U})(t) = \mathrm{conv}(\underline{A}^1, \cdots, \underline{A}^\ell, \overline{A}^1, \cdots, \overline{A}^\ell).
$$

8.4 Numerical Simulations

This section presents two examples illustrating how Algorithms 4 is used to compute the MBB of the pre-image and how to compute the inner-approximation of reachable sets. The results are compared to the pre-image and reachable set computed using exhaustive evaluations. The first example considers a multiple input multiple output Lotka-Volterra system to compute the minimum bounding box of the pre-image of an output set, and in the second example, the Lorenz attractor is used to illustrate the computation of the inner-approximation of the reachable set.

Example 25 *Consider the following MISO Lotka-Volterra system given by*

$$\dot{x}_1 = -x_1x_2 + x_1u_1,$$

$$\dot{x}_2 = x_1x_2 - x_2u_2,$$

$$y = x$$

with initial condition $x_0 = (1/6, 1/6)^\top$. *The generating series of* y_1 *and* y_2 *are com-*

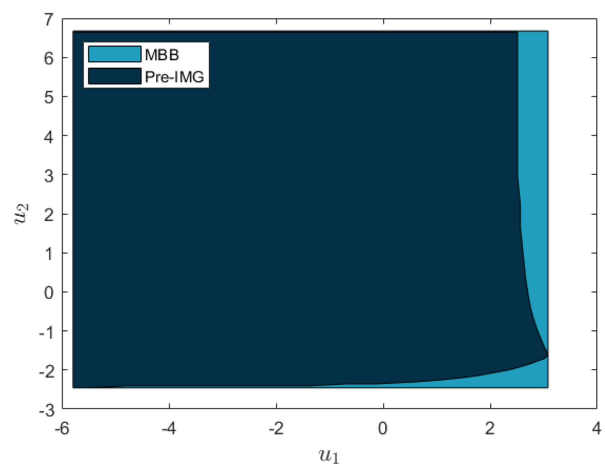


Figure 8.3: Estimation of the minimum bounding box of the pre-image (Pre-IMG) of the output set $\mathcal{Y} = [(-2, -2), (2, 2)]$ *of the system in Example 25 with initial state* $x_0 = (1/6, 1/6)$, *output set , and truncation length* $N = 8$.

puted

$$c_1 = 0.33 - 0.22x_0 + 0.33x_1 + 0.07x_0x_0 - 0.22x_0x_1 \cdots$$

$$c_2 = 0.66 + 0.22x_0 - 0.66x_2 - 0.07x_0x_0 + 0.22x_0x_1 + \cdots$$

and its derivatives

$$\delta(c_1) = 0.33\delta x_1 - 0.22x_0\delta x_1 + 0.22x_0\delta x_2 + \cdots$$
$$\delta(c_2) = 0.66\delta x_2 + 0.22x_0\delta x_1 - 0.22x_0\delta x_2 + \cdots$$

Algorithm 4 is used to compute the minimum bounding box of the pre-image as in Definition 53 of the output set $\mathcal{Y} = \{y \in \mathbb{R}^2 : \ -2 \le y_1 \le 2, -2 \le y_2 \le 2\}$.

From Figure 8.3, it is clear that the pre-image is contained in the computed minimum bounding box.

Example 26 *Consider the Lorenz attractor*

$$\begin{aligned} \dot{x}_1 &= u_1(x_2 - x_1), \\ \dot{x}_2 &= x_1(u_2 - x_3) - x_2, \\ \dot{x}_3 &= x_1x_2 - x_3, \\ y &= (x_1, x_2)^T. \end{aligned} \tag{8.6}$$

Assume the input u *is constrained* $u_1 \in [0,1]$, $u_2 \in [0,1]$ *and the initial state is* $x_0 = (0.1, 0.2, 0.3)$. *From (2.5), the generating series of* y_1 *and* y_2 *are*

$$c_1 = 0.1 + 0.1x_0 - 0.23x_1x_0 - 0.1x_1x_1 + 0.1x_1x_2 + \cdots$$
$$c_2 = 0.2 - 0.23x_0 + 0.1x_2 + 0.258x_0x_0 - 0.03x_0x_1 + \cdots$$

To perform the optimization, the derivatives of the generating series as in Definition

45 are calculated to obtain the Gâteaux derivative

$$\delta(c_1) = -0.23\delta x_1 x_0 - 0.1\delta x_1 x_1 - 0.1 x_1 \delta x_1 + \cdots$$

$$\delta(c_2) = 0.1\delta x_2 - 0.03 x_0 \delta x_1 - 0.1 x_0 \delta x_2 + 0.1\delta x_2 x_1 + \cdots$$

Figure 8.4 shows the minimum bounding box and inner-approximation of the reachable set at time $t = 0.5s$. It is clear from the plot that the inner-approximation is contained inside the reachable set.

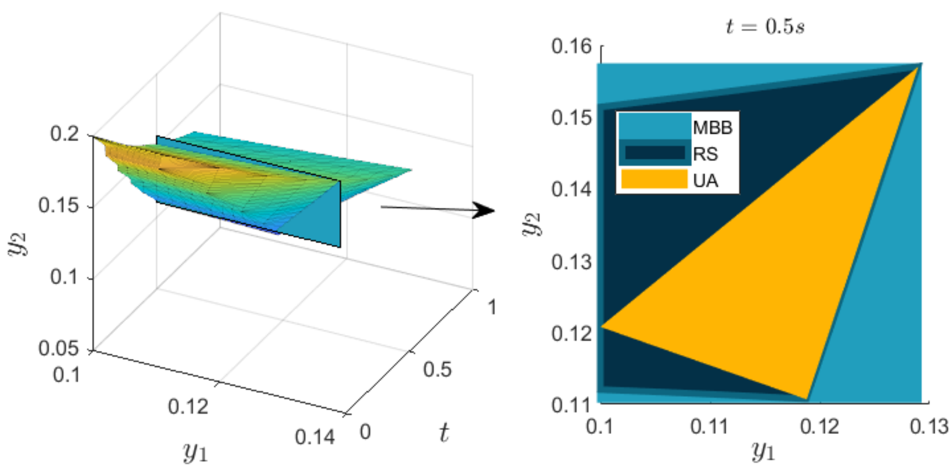


Figure 8.4: On the left, the reachable set (RS) of the system in Example 26 over a time horizon of $t \in [0, 0.8]$ is shown. On the right the estimation of the inner-approximation (UA) of the reachable set with inputs $0 \leq u_1 \leq 1$ and $0 \leq u_2 \leq 1$, and truncation length $N = 6$. The minimum bounding box is also shown.

Chapter 9

Vector Field Perturbation

In the present chapter, the problem of quantifying the effect of the perturbation of the vector field on the output which is represented by the Chen-Fliess series is addressed. To accomplish this, the definition of the iterative Lie derivative is extended to be able to take words from two languages, the original and a differential language. Then the closed-form of the Chen-Fliess series of the output associated with the nonlinear system with the perturbed vector field is obtained. With this, the Gâteaux and Fréchet derivatives are computed in a similar way as in [57].

9.1 Perturbed System

Consider the nonlinear system in (2.4) with perturbed vector fields

$$\begin{aligned} \dot{z} &= g_0(z) + e_0(z) + \sum_{i=1}^{m}(g_i(z) + e_i(z))u_i \\ y &= h(z) \end{aligned} \tag{9.1}$$

where the functions $e_i(z)$ represent the vector field perturbation. The iterative Lie derivative as defined in (2.5) does not distinguish between the original vector field and the perturbation. Consider the following example.

Example 27 *Take the iterated Lie derivative of the output of (9.1) associated with the word x_0. This is,*

$$L_{x_0}h(z) = \frac{\partial}{\partial z}h(z) \cdot (g_0(z) + e_0(z)) \tag{9.2}$$

the expressions $\frac{\partial}{\partial z}h(z)\cdot g_0(z)$ and $\frac{\partial}{\partial z}h(z)\cdot e_0(z)$ cannot be written in the notation of the iterative Lie derivative. To overcome this, consider the language $Y = \{y_0, y_1, \cdots, y_m\}$ and $Z = X \cup Y$. Now associate Z with the original vector field g_i and Y with the perturbation field e_i. Then (9.2) becomes

$$\begin{aligned} L_{x_0}h(z) &= \frac{\partial}{\partial z}h(z) \cdot (g_0(z) + e_0(z)) \\ &= L_{z_0}h(z) + L_{y_0}h(z) \end{aligned}$$

which is written in terms of Lie derivatives of the languages Z and Y.

9.2 Extended Iterative Lie Derivative

To extend the idea described in Example 27, the definition of iterative Lie derivative in (2.5) is extended to take two languages.

Definition 55 *Consider the alphabets X and δX associated to the vector fields g, e, respectively. The extended iterative Lie derivative of $\eta \in Z^*$ of the vector field (g, e)*

is given by the mapping $\mathcal{L}_\eta : L_\mathfrak{p}^m[0,T] \to \mathcal{C}[0,T]$, *where* $\mathcal{L}_\emptyset h(t) = 1$ *and*

$$\mathcal{L}_{z_i\eta} h := \begin{cases} \dfrac{\partial}{\partial z}\mathcal{L}_\eta h \cdot g_i, & z_i \in X, \\ \\ \dfrac{\partial}{\partial z}\mathcal{L}_\eta h \cdot e_i, & z_i \in \delta X. \end{cases} \tag{9.3}$$

The following lemma provides a closed-form of the Chen-Fliess series of the perturbed system in (9.1) in terms of two alphabets. This expression is later used to describe the derivatives of the Chen-Fliess series with respect to a vector field perturbation. From Definition 38, $\sigma_X(\xi) = \eta$ for any $\xi \in I_\eta$.

Lemma 20 *Let* X, Y *and* δY *be alphabets associated to* $g + e,\ g,\ e \in L_\mathfrak{p}^m[t_0, t_1]$, *respectively. Given* $c \in \mathbb{R}\langle\langle X \rangle\rangle$ *associated with the original nonlinear system (2.4), the Chen-Fliess series of the output in (9.1), with power series* $c \oplus d$, *is written as*

$$F_{c\oplus d}[u](t) = \sum_{k=0}^{\infty} \sum_{\xi \in \mathbb{S}_{Y^*, \delta Y^k}} \mathcal{L}_\xi h|_{z_0} E_{\sigma_X(\xi)}[u](t). \tag{9.4}$$

Proof: To obtain (9.4), it is first shown that

$$L_\eta h = \mathcal{L}_{\mathrm{char}(I_\eta)} h \tag{9.5}$$

for any $\eta \in X^*$. This is proved by induction over the length of the word η. Consider $|\eta| = 1$, $\eta = x_j$, then $I_\eta = \{y_j,\ \delta y_j\}$. From the linearity of the derivative and

Definition 55, it follows that

$$\begin{aligned}
L_{x_j}h &= \frac{\partial}{\partial z}h \cdot (g_j + e_j), \\
&= \frac{\partial}{\partial z}h \cdot g_j + \frac{\partial}{\partial z}h \cdot e_j, \\
&= \mathcal{L}_{y_j}h + \mathcal{L}_{\delta y_j}h, \\
&= \mathcal{L}_{\mathrm{char}(I_{x_j})}h.
\end{aligned}$$

Now assume that (9.5) holds true for any $\eta' \in X^*$ such that $|\eta'| = k$, and compute the expression for $\eta = x_i\eta'$. That is,

$$L_\eta h = \frac{\partial}{\partial z}L_{\eta'}h \cdot (g_i + e_i).$$

Since $|\eta'| = k$ and by the induction hypothesis, one has that

$$L_\eta h = \frac{\partial}{\partial z}\mathcal{L}_{\mathrm{char}(I_{\eta'})}h \cdot (g_i + e_i),$$

Hence, using linearity of the inner product $\cdot$ and (2.5) over the alphabet $Y \cup \delta Y$, it follows that

$$\begin{aligned}
L_\eta h &= \mathcal{L}_{x_i \mathrm{char}(I_{\eta'})}h + \mathcal{L}_{\delta x_i \mathrm{char}(I_{\eta'})}h \\
&= \mathcal{L}_{\mathrm{char}(I_\eta)}h.
\end{aligned}$$

Now, (2.3) can be expressed in terms of (9.3). That is,

$$\begin{aligned} F_{c\oplus d}[u](t) &= \sum_{\eta\in X^*} L_\eta h|_{z_0} E_\eta[u](t), \\ &= \sum_{\eta\in X^*} \mathcal{L}_{\mathrm{char}(I_\eta)} h|_{z_0} E_\eta[u](t), \\ &= \sum_{\eta\in X^*} \sum_{\xi\in I_\eta} \mathcal{L}_\xi h|_{z_0} E_\eta[u](t). \end{aligned}$$

Since $\eta = \sigma_X(\xi)$ for all $\xi \in I_\eta$, it then follows that

$$F_{c\oplus d}[u](t) = \sum_{\eta\in X^*} \sum_{\xi\in I_\eta} \mathcal{L}_\xi h|_{z_0} E_{\sigma_X(\xi)}[u](t). \tag{9.6}$$

Observe that if $\eta_1 \neq \eta_2$ then I_{η_1} and I_{η_2} are disjoint, then

$$Z^* = \bigcup_{\eta\in X^*} I_\eta = \bigcup_{\eta\in X^*} \{\xi :\ \xi \in I_\eta\}. \tag{9.7}$$

and

$$\sum_{\xi\in Z^*} \xi = \sum_{\eta\in X^*} \sum_{\xi\in I_\eta} \xi \tag{9.8}$$

Applying (9.8) in (9.6), one has that

$$F_{c\oplus d}[u](t) = \sum_{\xi\in Z^*} \mathcal{L}_\xi h|_{z_0} E_{\sigma_X(\xi)}[u](t). \tag{9.9}$$

Finally, $\sum_{\xi\in Z^*} \xi = \sum_{k=0}^{\infty} \sum_{\xi\in \mathbb{S}_{X^*,\delta X^k}} \xi$. Hence, (9.9) is equal to (9.4). This completes the proof. ■

9.3 The Fréchet Derivative

Next, (9.4) is used to provide the functional derivative that quantifies the vector field perturbation.

Theorem 20 *Let X, Y and δY be alphabets associated with $g+e,\ g,\ e \in L_{\mathfrak{p}}^m[t_0,t_1]$, respectively. The Chen-Fliess series is Fréchet differentiable with respect to the vector field if and only if*

$$\lim_{e\to 0}\frac{1}{\|e\|_{\mathfrak{p}}}\left(\sum_{k=2}^{\infty}\sum_{\xi\in\mathbb{S}_{Y,\delta Y^k}}\mathcal{L}_{\xi}h|_{z_0}E_{\sigma_X(\xi)}[u](t)\right)=0,$$

and its Fréchet derivative is expressed as

$$\mathbb{D}F_c[u][g,e](t)=\sum_{\eta\in X^*}\sum_{\xi\in\mathbb{S}_{\eta,\delta X}}\mathcal{L}_{\xi}h|_{z_0}E_{\sigma_X(\xi)}[u](t),$$

whenever $c\in\mathbb{R}^{\ell}_{LC}\langle\langle X\rangle\rangle$.

Proof: The proof follows by a direct application of Lemma 20 and Definition 42. Consider $\delta>0$ and h such that $\|h\|_{\mathfrak{p}}<\delta$, from (9.4), it follows that

$$F_{c\oplus d}[u](t)=\sum_{k=0}^{\infty}\sum_{\xi\in\mathbb{S}_{Y,\delta Y^k}}\mathcal{L}_{\xi}h|_{z_0}E_{\sigma_X(\xi)}[u](t).$$

For $k=0$, one has that

$$F_c[u](t)=\sum_{\xi\in\mathbb{S}_{Y^*,\delta Y^0}}\mathcal{L}_{\xi}h|_{z_0}E_{\sigma_X(\xi)}[u](t). \tag{9.10}$$

Note here that $\mathcal{L}_\xi h|_{z_0} = L_\xi h|_{z_0}$ since $\xi \in Y^*$, which is why the left-hand side of (9.10) does not depend on the perturbation e. Then, it follows that

$$F_{c\oplus d}[u](t) - F_c[u](t) - \sum_{\xi \in \mathbb{S}_{Y^*,\delta Y}} \mathcal{L}_\xi h|_{z_0} E_{\sigma_X(\xi)}[u](t) = \sum_{k=2}^{\infty} \sum_{\xi \in \mathbb{S}_{Y,\delta Y^k}} \mathcal{L}_\xi h|_{z_0} E_{\sigma_X(\xi)}[u](t).$$

Multiplying by $1/\left\|e\right\|_{\mathfrak{p}}$ and taking the limit of e to 0 gives the desired result. Finally, observe that the generating series of $\mathbb{D}F_c[u][g,e](t)$ inherits the local convergent bounds of the original series c. Therefore, for $c \in \mathbb{R}_{LC}\langle\langle X\rangle\rangle$, the Fréchet derivative $\mathbb{D}F_c[u][g,e](t)$ is convergent and well-posed, which completes the proof. ■

In this chapter, the vector field perturbation of Chen-Fliess series is measured. A closed form of this is obtained by extending the definition of Lie derivative to be able to read words from two languages where letters from one language are associated with the original vector field and the letters from the new language are associated with the perturbation of the vector field.

Chapter 10

Conclusion and Further Research

10.1 Conclusion

This work provides a closed form of an overapproximation of the reachable set of the output of a non-linear affine system represented by the Chen-Fliess operator. For this, interval arithmetic was used to compute an overestimation of the reachable set of an iterated integral, then the result was obtained by adding up all the overestimating sets of the defining reachable set. The advantage of this method is its closed form which makes computation faster than solving a non-convex optimization problem. Also, the examples show very good accuracy for short-time horizons, but as the time horizon gets larger, the accuracy decreases, which can be improved by increasing the order of the approximation.

Two methodologies of computing overestimation of the reachable set of systems represented in an input-output manner by the Chen-Fliess series formalism are provided. First, the input-output mixed-monotonicity method extended the notion of mixed-monotonicity into the Chen-Fliess series framework. Then, to obtain the minimum bounding box of output reachable sets, an optimization routine was provided for Chen-Fliess series and the gradient descent method that essentially found the input functions producing the system's maximum/minimum outputs. This second approach required finding a closed form of the Fréchet, Gâteaux derivative and the gradient in the Chen-Fliess framework along with a condition for its existence. It was shown theoretically that the reachable set obtained by optimizing the Chen-Fliess series is the minimum bounding box containing the reachable set. If the interval of time is partitioned, it was proved that the order in which the optimization is performed over each subinterval of time does not affect the result. This is important to approximate the optimal value of the Chen-Fliess series by dividing the interval of time into smaller pieces. Illustrative examples were provided in the last section, and the results were compared against reachable set overestimations computed using the mixed-monotonicity procedure.

The framework of differential languages to formalize the computation of Chen-Fliess series derivatives and provide an algebraic method to obtain such Chen-Fliess series derivatives is introduced. A closed-form of the Hessian for a Chen-Fliess series was presented, and Newton's and trust regions optimization algorithms for the computation of the minimum bounding box of reachable sets for systems represented by Chen-Fliess series were developed. To ensure the algorithm works appropriately, the second-order mean value theorem was introduced in the Chen-Fliess series context using differential-algebraic means instead of the classical chain rule approach. Illustrative examples of three control affine systems were provided in the last section showing that the over-approximations obtained from the algorithms are indeed minimum bounding boxes.

It was shown that the minimum bounding boxes are computed with fewer iterations than the gradient descent approach. The notion of input-output backward reachable set and output reachable set pre-image for systems represented by a Chen-Fliess series. Two algorithms are developed for computing such sets. The first algorithm computes the minimum bounding box of the pre-image set whereas the second algorithm computes an inner approximation of output reachable sets. Two examples were presented with the purpose of illustrating the computation of the minimum bounding box of the pre-image and the inner approximation of output reachable sets.

Finally, the measurement of the perturbation of the Chen-Fliess series with respect to the vector field is addressed. The closed form of the Fréchet derivative is obtained for this by extending the definition of the iterative Lie derivative to be able to read two languages.

10.2 Further Research

In the present section, the problem of collision avoidance using Chen-Fliess series is outlined. The idea is similar to the original ideas of the control barrier functions techniques [6,41,71]. For the sake of simplicity, the object to avoid can be represented as a circle of radius r and center c. Also, assume that the task is to avoid the obstacle with the least energy. The set-up of the problem is the following:

$$\begin{aligned} \min_{u \in B} \quad & u^T u \\ \text{s.t.} \quad & \dot{h}(t) \geq -\alpha(h(t)) \end{aligned} \tag{10.1}$$

to include the Chen-Fliess series, the function $h(t) = ||F_c[u](t) - c||^2 - r$ is considered instead where the object to avoid is the circle $||x - c||^2 \leq r$. This problem is related to control barrier functions. Since equation (10.1) is an optimization problem and in the present dissertation, the tools to optimize Chen-Fliess series were provided, this is a natural future research direction.

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PUBLICATIONS

Journal Publications:

1. **I. Perez Avellaneda** and L. A. Duffaut Espinosa and Francisco Rosales Marticorena. Feedback Dynamic Control for Exiting a Debt-Induced Spiral in a Deterministic Keen Model. PLOS ONE, 2023. under review.
2. **I. Perez Avellaneda** and L. A. Duffaut Espinosa. Second-Order Optimization of Chen-Fliess Series for Input-Output Reachability. Systems and Control Letters, 2023. under review.
3. **I. Perez Avellaneda** and L. A. Duffaut Espinosa. Input-Output Overestimation of Reachable Sets with Chen-Fliess Series. Transactions on Automatic Control, 2023. under review.

Selected Conference Publications:

1. **I. Perez Avellaneda** and L. A. Duffaut Espinosa. Backward and Inner Approximation of Output Reachable Sets via Chen-Fliess Series. 59th Annual Allerton Conference on Communication, Control, and Computing, 2023, to appear.
2. L. A. Duffaut Espinosa, W.S. Gray and **I. Perez Avellaneda**. Derivatives of Chen-Fliess Series with Applications to Optimal Control. 62nd Conference on Decision and Control, 2023, to appear.
3. **I. Perez Avellaneda** and L. A. Duffaut Espinosa. Output Reachability of Chen-Fliess series: A Newton-Raphson Approach. 57th Annual Conference on Information Science and Systems, Baltimore, Maryland, 2023, pp. 1-6.