# Linearization and Model Reduction in Zonotope-Based Reachability Analysis of Nonlinear ODEs

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**Abstract**

We report on recent work [16] on the reachability analysis of nonlinear ordinary differential equations (ODEs). Relying on Carleman linearization and Krylov projection, we describe a method that, given a nonlinear ODE system, generates a small linear approximation of the original dynamics. The construction is independent of the initial condition. Used in conjunction with zonotopes, this yields CKR, an accurate reachability analysis algorithm.

**Keywords**

Nonlinear ODEs, reachability, zonotopes, Carleman linearization, Krylov spaces.

## 1. Introduction

The analysis of systems of nonlinear ordinary differential equations (ODEs) poses formidable challenges to theoreticians and practitioners. Among the great variety of existing formal methods, many focus on computing detailed, effective descriptions of the set of reachable states over a given time horizon, see e.g. [37, 24, 22, 23, 2, 3] and references therein. These descriptions, variously called *reachsets*, *flowpipes* etc., are typically obtained in a piecewise fashion; that is, by sewing together local approximations over different regions of the state space and/or time. In particular, given a nonlinear system of ODEs in the state variables $x = (x_1, ..., x_n)^T$

$$\dot{x} = f(x_1, ..., x_n), \tag{1}$$

approximation can take place either in space, like when linearizing the system's equations around a point $x = x_0$; or in time, like when Taylor expanding the ODE's solution around a time $t = t_0$. With traditional methods, the resulting description will typically exhibit only a limited, *local* accuracy.

We describe recent work [16] studying approximations of nonlinear systems that can be accurate also non-locally, in the following sense: differently from classical linearization, our approximate model's equations do not depend on a specific expansion point $x_0$; differently from $t$-Taylor expansions, the temporal interval in which our approximation is good is not directly linked to the convergence of the solution's Taylor series around $t_0$, and is wider in concrete cases. In our method, a crucial step in achieving these goals is the computation of a 'small', hence computationally tractable, linear ODE system that approximates (1) (Section 2). Under suitable stability assumptions, this approximation admits useful and concrete error bounds. This is leveraged in a reachability analysis algorithm that works in the general, not necessarily stable case: CKR (Carleman-Krylov Reachability, Section 3). The basic idea of CKR is to perform propagation of an initial convex set, relying on the reduced, linearized system rather than on (1). Similarly to other proposals [24, 32, 38], compensation of errors resulting from nonlinearities is reduced to an optimization problem. We show that this scheme is particularly effective when the reachsets are represented as *zonotopes* [27]. Experiments conducted with a proof-of-concept implementation have shown promising results (Section 4).

**Related and Further Work** There exists a vast literature on the linearization of nonlinear systems. In particular, techniques based on Carleman embedding [6, 29] have recently received a renewed attention. Most related to our work and motivations, Jungers and Tabuada [28] have recently proposed a technique

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for global approximation of nonlinear ODEs by linear ODEs, based on *polyflows*. These are systems that are exactly linearizable via a change of variables. The technique in [28] is based on building polyflows that approximate the original system, using as a basis the Lie derivatives up to some order $N$ and as $N \to +\infty$ the approximation of [28] becomes exact. Note that this is an asymptotic result that does not easily yield concrete bounds for a fixed $N$. Systems that are exactly linearizable via polynomial changes of variables are the subject of [35, 36, 8]; see also [9, 7, 11].

In [8] we have considered Carleman embedding and Krylov-based approximations, essentially from a local point of view. Here, we provide novel analyses of both local and global errors, and leverage them in CKR, a new reachability algorithm. General error bounds for the truncated Carleman linearization have been recently considered in [4, 25]. The time interval of validity of these bounds is quite small, and they appear to be in practice more conservative, contrary to ours. In [26], efficient reachability for weakly nonlinear, dissipative systems relying on Carleman linearization is presented. In the conference version [13] an earlier, less stable version of CKR, based on polytopes, is considered.

In the field of reachability for continuous and hybrid systems, state-of-the-art tools like Flow$*$ [23] and CORA [2] employ a mix of approximations techniques [30, 22, 23, 2, 1, 3]. In particular, Flow$*$ [22, 23] is based on Taylor models, while CORA mainly relies on linearization of the ODE equations [1, 3].

The investigation reported here is part of a broader research agenda, aimed at integrating formal methods for dynamical and safety-related systems [8, 7, 9, 10, 11] with aspects concerning, in perspective, quantitative security [19, 20, 18], distributed execution with notions of failure and recovery [12], probabilistic programming, testing and verification [17, 31, 14, 15].

## 2. Carleman Linearization and Reduction via Krylov Projection

We introduce a linearization method for system (1) that is strongly related to Carleman embedding [29] and then discuss an approach to reduce the dimension of the linearized system. For $x = (x_1, ..., x_n)^T$ a vector of state variables, we consider a system of ODEs

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

where $f = (f_1, ..., f_n)^T$ is a vector field of locally Lipschitz analytic functions defined on some open subset $\Omega \subseteq \mathbb{R}^n$. For $x_0 \in \Omega$, we let $x(t; x_0)$ be the unique solution of the ODE system with the initial condition $x(0) = x_0$: the unique solution exists and is real analytic (Picard-Lindelöf theorem).

For a real analytic function $g$ defined on some open subset of $\mathbb{R}^n$ that includes the trajectories $x(t; x_0)$ for $x_0 \in \Omega$, we will be interested in studying the *observable* of the system (2) via $g$, that is the function $g \circ x(t; x_0) = g(x(t; x_0))$. Recall that $\mathcal{L}_f(g) := \langle \nabla g, f \rangle = \sum_{j=1}^{n} \frac{\partial g}{\partial x_j} \cdot f_j$ is the Lie derivative of $g$ (w.r.t. $f$), and $\mathcal{L}_f^{(k)}(g)$ is the $k$-th Lie derivative, defined inductively by $\mathcal{L}_f^{(k+1)}(g) := \mathcal{L}_f(\mathcal{L}_f^{(k)}(g))$. We shall omit the subscript $_f$ whenever it is understood from the context.

Let us fix a set $\mathcal{A} = \{\alpha_1, \alpha_2, ...\}$ of functions $\alpha_i : \mathbb{R}^n \to \mathbb{R}$. For instance $\mathcal{A}$ might be all monomial functions. We assume that there are unique $v = (\lambda_1, ..., \lambda_M)^T \in \mathbb{R}^M$ and basis vector $\alpha := (\alpha_1, ..., \alpha_M)^T$ such that

$$g = \sum_{i=1}^{M} \lambda_i \alpha_i \;=\; v^T \alpha \tag{3}$$

where $g$ is any observable function. Otherwise, all we require from the functions in $\mathcal{A}$ is that they are analytic[1], and that the Lie derivative of each $\alpha_i$ can in turn be expressed as a unique linear combination of elements from $\mathcal{A}$: $\mathcal{L}(\alpha_i) = \sum_{j \geq 1} a_{ij} \alpha_j$. We let $A$ denote the $M \times M$ matrix of the coefficients $a_{ij}$ for $1 \leq i, j \leq M$, and $B$ be the $M \times k$ matrix of possibly nonzero elements $b_{i,j} = a_{i,M+j}$; that is, $k$ is chosen large enough to ensure that, for $1 \leq i \leq M$, we have $a_{ij} = 0$ for each $j > M + k$. We let $\psi \stackrel{\triangle}{=} (\alpha_{M+1}, ..., \alpha_{M+k})^T$. The *Carleman linearization* (or embedding) of (2) is given by the following linear system in the variables $z = (z_1, ..., z_M)^T$ and initial condition

$$\dot{z} = Az + B\psi(x(t; x_0)) \tag{4}$$

[1]This can be weakened to analyticity in some open set containing all the trajectories $x(t; x_0)$ for $x_0 \in \Omega$.

$$z(0) = \alpha(x_0) \;=:\; z_0\,. \tag{5}$$

The following result is an almost immediate consequence of the existence and uniqueness of the solution of ODEs (Picard-Lindelöf). For a detailed proof, see [8, Th.3].

**Theorem 1** (Carleman linearization). *Let $x_0 \in \Omega$. Then $\alpha(x(t;x_0))$ is the unique solution of the system (4) with $z(0)$ as in (5).*

Note that we cannot *explicitly* build the system (4), as the function $\psi(x(t;x_0))$ is in general not available. This leads us to consider an approximation where we neglect the "remainder" $\psi(x(t;x_0))$, the *truncated* Carleman linearization of dimension $M$

$$\dot{z} = Az \qquad\qquad z(0) = z_0 (= \alpha(x_0))\,. \tag{6}$$

Now, we discuss a method to reduce the dimension of (6), while keeping certain, still local, accuracy guarantees. Fix $g = \langle v, \alpha\rangle$ ($v \in \mathbb{R}^M$), an observable of interest, as in (3). We consider the $m$-dimensional Krylov space[2] generated by $v$ and $A^T$, that is the subspace of $\mathbb{R}^M$

$$\mathcal{K}_m := \mathrm{span}\{v, A^T v, (A^T)^2 v, ..., (A^T)^{m-1} v\}\,.$$

Let $V = [v_1|\cdots|v_m]$ be an orthonormal basis of $\mathcal{K}_m$, represented as a $M \times m$ matrix. Consider the projection of $A^T$ onto $\mathcal{K}_m$ and represent it w.r.t. the basis $V$, that is the $m \times m$ matrix

$$H_m := V^T A^T V\,.$$

Given a vector of $m$ distinct state variables $y = (y_1, ..., y_m)^T$, we let the *reduced* linear system derived from (4) and the corresponding initial condition, derived from (5), be defined as:

$$\dot{y} = H_m^T y \tag{7}$$

$$y(0) = V^T z_0 \;=:\; y_0\,.$$

Note that the reduced equations (7) do not depend on $x_0 \in \Omega$. Informally speaking, the solution $y(t;y_0)$ of the reduced system describes the evolution of the vector $\alpha(x(t;x_0))$, projected onto the subspace $\mathcal{K}_m$, in the coordinates of the basis $V$. We note that there exists a well-known algorithm for the efficient, "on the fly" construction of the matrices $V, H_m$, the Arnoldi iteration [34]. Recalling that $g = \langle v, \alpha\rangle$ it is natural to consider the following approximation of $g(x(t;x_0))$.

**Definition 1** (reduced observable dynamics). *For each $x_0 \in \Omega$ and $y_0 = V^T x_0$, we define the function:*

$$\widehat{g}(t;x_0) := v^T V y(t;y_0)\,. \tag{8}$$

In fact, we will see that $v_1 = v/||v||_2$, while $v$ is orthogonal to $v_j$ for $j > 1$. Hence (8) can be simplified to

$$\widehat{g}(t;x_0) = ||v||_2\, y_1(t;y_0)\,. \tag{9}$$

In order to study the quality of this approximation, we introduce the error function relative to $g$

$$\epsilon_g(t;x_0) := g(x(t;x_0)) - \widehat{g}(t;x_0)\,.$$

The following result confirms that this error is small near $t = 0$. Indeed, the Taylor expansions of $\widehat{g}(t;x_0)$ and $g(x(t;x_0))$ up to order $m-1$ coincide:

**Theorem 2.** *For each $x_0 \in \Omega$, the function $\epsilon_g(t;x_0)$ is $O(t^m)$ around $t = 0$.*

Explicit local bounds of the error function can be obtained from the Taylor theorem with remainder in Lagrange form, assuming we can construct validated enclosures $S$ and $E$ of $x(\tau;\xi)$ and $\frac{\mathrm{d}^m}{\mathrm{d}t^m}\widehat{g}(\tau;\xi)$, respectively, for $(\tau,\xi)$ ranging in a small set — which is possible by standard techniques, see e.g. [33] and references therein. Under suitable, stability conditions, also a global bound of the error function $\epsilon_g$ can be given. Let $r_m$ denote the projection of $A^T v_m$ onto $\mathcal{K}_m^\perp$, the orthogonal complement of $\mathcal{K}_m$, and define the *remainder function* as $h(x) := v_m^T B\psi(x) + r_m^T \alpha(x)$. Then, for any $t > 0$ such that $x(\tau;x_0)$ is defined for $\tau \in [0,t]$ and assuming additionally $H_m$ is stable, we can prove

$$|\epsilon_g(t;x_0)| \le ||v||_2\, D \int_0^t |h(x(\tau;x_0))|\,\mathrm{d}\tau \tag{10}$$

where $D > 0$ is a constant independent of $t$. Qualitatively speaking, (10) says that, for a stable $H_m$, the behaviour of the global error is determined by $|h(x(\tau;x_0))|$: if this function decays fast enough to be integrable over $[0,+\infty)$, then $\epsilon_g(t;x_0)$ will be globally bounded.

[2] For an introduction to Krylov spaces, see e.g. [34].

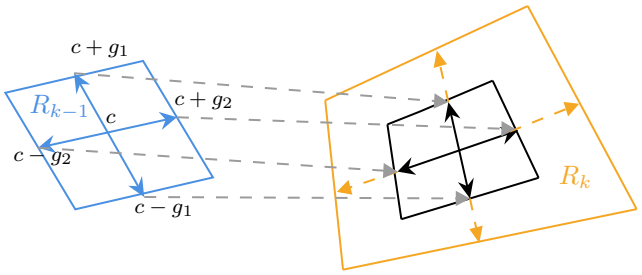


**Figure 1:** Propagation and inflation of a zonotope. The dashed arrows represent the function $\xi \mapsto \widehat{x}(\Delta_k; \xi)$.

## 3. Application to Reachability Analysis

We will apply the outlined linearization scheme to compute an approximation $\widehat{x}(t; x_0)$ of the flow $x(t; x_0)$, and then use it to compute an overapproximation of the reachable set of the nonlinear system (1) at fixed times: $t_1, t_2, ....$ This goal will be achieved by applying the scheme of Section 2 to each of the observable functions $g = x_i$, for $i = 1, ..., n$ in turn. Using the notation in that section, for each $i = 1, ..., n$, let $v^{(i)}$ the coefficient vector of $x_i$ in the chosen basis $\alpha$, that is $x_i = v^{(i)T}\alpha$, and $V^{(i)}, H_m^{(i)}$ the corresponding basis and reduced matrix. We define the approximate flow by $\widehat{x}(t; x_0) := (\widehat{x}_1(t; x_0), ..., \widehat{x}_n(t; x_0))^T$ where, as an instance of (9), we have

$$\widehat{x}_i(t; x_0) := ||v^{(i)}||_2 \, y_1^{(i)}(t; y_0) \quad (i = 1, ..., n) \tag{11}$$

with $y^{(i)}(t; y_0)$ the solution of the linear initial value problem (7) for $g = x_i$. As the solution of a linear system of ODEs, each component in (11) can be written explicitly as $\widehat{x}_i(t; x_0) = ||v^{(i)}||_2 \left(\mathrm{e}^{tH_m^{(i)T}}\right)_1 V^{(i)T}\alpha(x_0)$ for $i = 1, ..., n$, where $(\mathrm{e}^{(\cdots)})_1$ denotes the first row of the exponential matrix. Note that, as a function of $x_0$, for a fixed $t$, $\widehat{x}_i(t; x_0)$ is a linear combination of the components of the basis $\alpha(x_0)$. It is also convenient to introduce the following *error vector*: $\epsilon(t; x_0) := x(t; x_0) - \widehat{x}(t; x_0)$.

In what follows, we will consider the case where an initial set $X_0$ is given, rather than an individual initial state $x_0$. The general idea of the algorithm is to use $\widehat{x}(\Delta; \cdot)$ to propagate a reachset from one time point to the next, by a time-step of $\Delta$. The propagated set needs then to be 'inflated' to compensate for approximation errors. The concrete way in which propagation and inflation are carried out will depend on the representation that will be adopted for sets of reachable states. We will give a generic description of the method, independent of the type of representation. Then we will instantiate it to a concrete method by considering a specific set representations, zonotopes [27].

Let $X_0$ be a compact set of initial states and $t > 0$ be such that $x(\tau; x_0)$ is well-defined for each $x_0 \in X_0$ and $\tau \in [0, t]$. In the interval $[0, t]$, choose $N$ time points $0 = t_0, t_1, \cdots, t_N = t$, with $\Delta_k := t_k - t_{k-1} > 0$ for $1 \leq k \leq N$. The algorithm, which we christen CKR for *Carleman-Krylov Reachability*, builds a sequence of compact sets $R_0, R_1, ..., R_N \subseteq \mathbb{R}^n$, the *reachsets*, s.t.

(a) $R_k$ is an overapproximation of the set of reachable states at time $t_k$: $R_k \supseteq x(t_k; X_0) = \{x(t_k, \xi) : \xi \in X_0\}$, in particular $R_0 = X_0$;

(b) $R_k$ belongs to a pre-specified class of *compact* subsets of $\mathbb{R}^n$, say $\mathcal{C}$ (e.g. polytopes, zonotopes,...).

The method essentially applies three set operations on $\mathbb{R}^n$ to build $R_k$ given $R_{k-1}$:

- *propagation*: propagates linearly a reachset $R_{k-1}$ from $t_{k-1}$ to $t_k$, thus obtaining $\widetilde{R}_k$;
- *enclosure computation*: generates a compact set $E_k$ that includes the error vector $\epsilon$ at $t_k$;
- *inflation*: computes a bloated version $R_k$ of the propagated reachset $\widetilde{R}_k$ that includes $\widetilde{R}_k + E_k$, where $+$ denotes here Minkowski sum[3].

A formal description of these operations, as well as a proof of correctness of the general method, can be found in the journal version [16].

Now, let us consider a specific set representation: zonotopes. Given a column vector $c \in \mathbb{R}^n$ (*center*) and a matrix formed by $p \geq 1$ column vectors $G = [g_1| \cdots |g_p] \in \mathbb{R}^{n \times p}$ (*generators*), the corresponding

[3]For $A, B \subseteq \mathbb{R}^n$, $A + B := \{a + b : a \in A, b \in B\}$.

*zonotope* is the set $\mathrm{Z}(c, G) := \{c + G \cdot \lambda : \lambda \in [-1, 1]^p\} \subseteq \mathbb{R}^n$. We represent the initial set as well as the successive reachsets $R_0, R_1, R_2, ...$ as zonotopes $\mathrm{Z}(c, G)$, such that, for a fixed integer $p$ ($n \leq p \leq 2n$), $G \in \mathbb{R}^{n \times p}$ has row rank $n$ (i.e. $G$ is full rank). Informally speaking, the basic idea is to use the maps $\xi \mapsto \widehat{x}(\Delta_k; \xi)$ ($k = 1, 2, ...$) to propagate a zonotope $R_{k-1} = \mathrm{Z}(c, G)$ from time $t_{k-1}$ to time $t_k$. We first build an auxiliary $\widetilde{R}_k$ by propagating $R_{k-1}$ *as if* the map $\widehat{x}(\Delta_k; \cdot)$ were linear. In more detail, we determine the auxiliary zonotope $\widetilde{R}_k := \mathrm{Z}(\widetilde{c}, \widetilde{G})$ by taking as $\widetilde{c}$ the center of mass of the $2p$ vectors obtained by linear propagation, $v_1^{\pm} := \widehat{x}(\Delta_k; c \pm g_1), ..., v_p^{\pm} := \widehat{x}(\Delta_k; c \pm g_p)$, and then choosing the generators $\widetilde{g}_j$'s from the 'direction' vectors $v_j^{\pm} - \widetilde{c}$. To obtain $R_k$, we 'stretch' the resulting $\widetilde{R}_k$, by multiplying the generators $\widetilde{g}_j$'s by suitable factors $\lambda_j^*$'s, so as to compensate for approximation and linearization errors (see Figure 1). Error compensation is based on the fact that, for each vector $z \in \widehat{x}(\Delta_k; R_{k-1}) + E_k$, we can compute a solution $\lambda \in \mathbb{R}^p$ of the system $\widetilde{G}\lambda + \widetilde{c} = z$ using the *pseudoinverse* of $\widetilde{G}$, and can then maximize $\lambda$ componentwise. See [16] for a detailed description.

## 4. Reachsets: Comparison with Flow∗ and CORA

Flow∗ [23] and CORA [2] are state-of-the-art tools for reachability analysis; they are quite effective at building (over-approximations of) reachsets. In [16], we have compared the reachsets $R_k$ produced by CKR with those produced by Flow∗ and CORA on different benchmarks drawn from [5, 21]: Jet Engine, Brusselator, Van Der Pol, Lorenz, Roessler, coupled Van Der Pol and Lotka-Volterra.

We quantify the accuracy of the returned sequence of reachsets using two different measures: (1) the *volume of the final reachset*; (2) only for CORA and CKR, the *average volume of the reachsets* at times $t_0, ..., t_N = T$. CKR is extremely accurate for all the models we have considered. In particular the final reachsets produced by CKR are tighter than those produced by the other two tools in all cases, often significantly so. With one exception, CKR is the most accurate algorithm, also when considering average accuracy across different examples. In terms of execution time, Flow∗ is the most effective tool on the considered examples. CKR times are in line with, or at least comparable with, Flow∗'s. As an example, we report in Fig. 2 a graphical comparison of the reachsets produced by the three algorithms when applied to the Van der Pol system. Numerical values and full details on experiments can be found in [16].

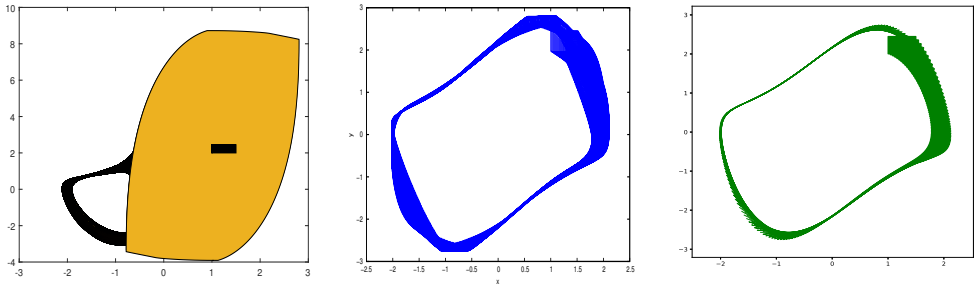

**Figure 2:** Reachsets computed with CORA (**left**), Flow∗ (**center**) and CKR (**right**) for Van der Pol model [16].

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## Declaration on Generative AI

The authors have not employed any Generative AI tools.

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