A survey of numerical integration techniques on manifolds

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Abstract

The following set of notes provide a very rough overview and introduction to the ideas and concepts needed to approximate differential equations evolving on homogeneous manifolds. This document mostly serves as a means to provide some basic ideas and then allow everyone else to inform me of which concepts need additional details in order to improve understanding.

Contents

1 Introduction

2 Some basic background material

The following are some basic definitions needed to discuss numerical integration on homogeneous manifolds (manifolds acted upon transitively by a Lie group). Note that the following should not be viewed as a complete list of all needed (or even relevant) topics and concepts. Any set of notes created in this way are usually incomplete, so we should either view them as a starting point from which we commence our journey to total understanding or we should discuss what further details are needed.

Definition 2.1. Let $m, d \in \mathbb{N} = \{1, 2, 3, \ldots\}$ with $m \leq d$ and let $\mathcal{M} \subseteq \mathbb{R}^d$ with $\mathcal{M} \neq \emptyset$. Then $\mathcal{M}$ is an m-dimensional smooth manifold if and only if for every $p \in \mathcal{M}$ there exist $\Omega \subseteq \mathbb{R}^d$, $U \subseteq \mathcal{M}$ with $p \in U$, and a smooth function $\varphi\colon \Omega \to \mathbb{R}^d$ such that φ is a homeomorphism and $\varphi' \circ \varphi^{-1}$ is injective. See, e.g., https://en.wikipedia.org/wiki/Manifold for more details.

Definition 2.2. Let $\mathcal{M}$ be a manifold, let $p \in \mathcal{M}$, and let $\rho\colon [0,1] \to \mathcal{M}$ be a differentiable function with $\rho(0) = p$ (cf. Definition 2.1). Then the vector

$$\left(\tfrac{\mathrm{d}}{\mathrm{d}t}\rho\right)(t)\Big|_{t=0} \tag{2.1}$$

is a tangent vector at the point p. The set of all tangent vectors at p is the tangent space at p and is denoted by $T\mathcal{M}|_p$. The collection of all tangent spaces at all points $q \in \mathcal{M}$ is called the tangent bundle of $\mathcal{M}$ and is denoted by $T\mathcal{M} = \cup_{q\in\mathcal{M}} T\mathcal{M}|_q$. See, e.g., https://en.wikipedia.org/wiki/Tangent_space for more details.

Definition 2.3. Let $\mathcal{M}$ be a manifold and let $F\colon \mathcal{M} \to T\mathcal{M}$ be a differentiable function which satisfies for all $p \in \mathcal{M}$ that $F(p) \in T\mathcal{M}|_p$ (cf. Definitions 2.1 and 2.2). Then F is a vector field on $\mathcal{M}$. The collection of all vector fields on $\mathcal{M}$ is denoted by $\mathfrak{X}(\mathcal{M})$. See, e.g., https://en.wikipedia.org/wiki/Vector_field for more details.

Definition 2.4. Let $\mathfrak{g}$ be a vector space and let $[\cdot,\cdot]\colon \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$ be a bilinear function which satisfies for all $a, b, c \in \mathfrak{g}$ that $[a,b] = -[b,a]$ and

$$[a,[b,c]] + [b,[c,a]] + [c,[a,b]] = 0. \tag{2.2}$$

Then we say that $\mathfrak{g}$ is a Lie algebra and we call the function $[\cdot,\cdot]\colon \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$ the Lie bracket on $\mathfrak{g}$. See, e.g., https://en.wikipedia.org/wiki/Lie_algebra for more details.

Problem 2.5. Let $\mathfrak{g} = \mathfrak{so}(3) = \{a \in \mathbb{R}^{3\times 3}\colon a^* = -a\}$ and let $[\cdot,\cdot]\colon \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$ satisfy for all $a, b \in \mathfrak{g}$ that $[a,b] = ab - ba$. Show that $\mathfrak{g}$ is a Lie algebra (cf. Definition 2.4).

Solution to Problem 2.5.

The solution to Problem 2.5 is thus complete. □

Problem 2.6. Let $\mathcal{M}$ be a manifold, let $C^\infty(\mathcal{M})$ be the set of smooth function on $\mathcal{M}$, let $\mathfrak{g} = \mathfrak{X}(\mathcal{M})$, and let $[\cdot,\cdot]\colon \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$ satisfy for all $X, Y \in \mathfrak{X}(\mathcal{M})$, $f \in C^\infty(\mathcal{M})$ that $[X,Y](f) = (X \circ Y)(f) - (Y \circ X)(f)$ (cf. Definitions 2.1 and 2.3). Show that $\mathfrak{g}$ is a Lie algebra (cf. Definition 2.4).

Solution to Problem 2.6.

The solution to Problem 2.6 is thus complete. □

Definition 2.7. Let $\mathfrak{g}$ be a Lie algebra (cf. Definition 2.4). Then we define $\operatorname{ad}^n\colon \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$, $n \in \mathbb{N}_0 = \{0\} \cup \mathbb{N}$, to be the functions which satisfy for all $n \in \mathbb{N}$, $u, v \in \mathfrak{g}$ that $\operatorname{ad}^0(u, v) = v$ and

$$\operatorname{ad}^n(u, v) = [u, \operatorname{ad}^{n-1}(u, v)]. \tag{2.3}$$

See, e.g., https://en.wikipedia.org/wiki/Adjoint_representation for more details.

Definition 2.8. Let $\mathcal{G}$ be a manifold (cf. Definition 2.1). We say that $\mathcal{G}$ is a Lie group if and only if there exists a function $\cdot\colon \mathcal{G} \times \mathcal{G} \to \mathcal{G}$ and $e \in \mathcal{G}$ such that

(i) it holds for all $p, q, r \in \mathcal{G}$ that $p \cdot (q \cdot r) = (p \cdot r) \cdot q$,

(ii) it holds for all $p \in \mathcal{G}$ that $p \cdot e = e \cdot p = p$,

(iii) it holds for all $p \in \mathcal{G}$ that there exists $p^{-1} \in \mathcal{G}$ such that $p^{-1} \cdot p = e$, and

(iv) it holds that $\cdot\colon \mathcal{G} \times \mathcal{G} \to \mathcal{G}$ and $\mathcal{G} \ni p \mapsto p^{-1} \in \mathcal{G}$ are smooth.

See, e.g., https://en.wikipedia.org/wiki/Lie_group for more details.

Problem 2.9. Let $\mathcal{G} = \{a \in \mathbb{R}^{3\times 3}\colon a^{-1} = a^*\}$ and let $\cdot\colon \mathcal{G} \times \mathcal{G} \to \mathcal{G}$ satisfy for all $a, b \in \mathcal{G}$ that $a \cdot b = ab$. Show that $\mathcal{G}$ is a Lie group (cf. Definition 2.8). *Note:* We have not defined matrix manifolds, but we can easily update this definition to allow for such things (e.g., via representations).

Solution to Problem 2.9.

The solution to Problem 2.9 is thus complete. □

Definition 2.10. Let $\mathcal{G}$ be a Lie group and let $e \in \mathcal{G}$ satisfy for all $p \in \mathcal{G}$ that $p \cdot e = e \cdot p = p$ (cf. Definition 2.8). Then we define the Lie algebra of a Lie group to be $\mathfrak{g} = T\mathcal{G}|_e$ (cf. Definitions 2.2 and 2.4). The Lie bracket on $\mathfrak{g}$ is the function $[\cdot,\cdot]\colon \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$ which satisfies for all $u, v \in \mathfrak{g}$, $g, h\colon [0,1] \to \mathcal{G}$ with g and h being differentiable, $g(0) = h(0) = e$, $g'(0) = u$, and $h'(0) = v$ that

$$[u, v] = \frac{\partial^2}{\partial t \partial s} g(t) \cdot h(s) \cdot g^{-1}(t)\bigg|_{t=s=0}. \tag{2.4}$$

See, e.g., https://en.wikipedia.org/wiki/Lie_group%E2%80%93Lie_algebra_correspondence for more details.

Problem 2.11. Let $\mathcal{G} = \mathrm{SO}(3) = \{a \in \mathbb{R}^{3\times 3}\colon a^{-1} = a^*,\ \det(a) = 1\}$ and let $\cdot\colon \mathcal{G} \times \mathcal{G} \to \mathcal{G}$ satisfy for all $a, b \in \mathcal{G}$ that $a \cdot b = ab$. Show that $\mathfrak{g} = \mathfrak{so}(3)$ is the Lie algebra of $\mathcal{G}$ (cf. Definition 2.10).

Solution to Problem 2.11.

The solution to Problem 2.11 is thus complete. □

Definition 2.12. Let $\mathcal{M}$ be a manifold, let $\mathcal{G}$ be a Lie group, let $e \in \mathcal{G}$ satisfy for all $p \in \mathcal{G}$ that $p \cdot e = e \cdot p = p$, and let $\Lambda\colon \mathcal{G} \times \mathcal{M} \to \mathcal{M}$ be a smooth function which satisfies for all $p, q \in \mathcal{G}$, $y \in \mathcal{M}$ that

$$\Lambda(e, y) = y \qquad \text{and} \qquad \Lambda\big(p, \Lambda(q, y)\big) = \Lambda(p \cdot q, y) \tag{2.5}$$

(cf. Definitions 2.1 and 2.8). Then we say that Λ is an (left) action of $\mathcal{G}$ on $\mathcal{M}$. See, e.g., https://en.wikipedia.org/wiki/Lie_group_action for more details.

Definition 2.13. Let $\mathcal{G}$ be a Lie group, let $e \in \mathcal{G}$ satisfy for all $p \in \mathcal{G}$ that $p \cdot e = e \cdot p = p$, and let $\mathfrak{g}$ be the Lie algebra of $\mathcal{G}$ (cf. Definitions 2.8 and 2.10). Then we define the function $R_v\colon \mathcal{G} \to \mathcal{G}$, $v \in \mathcal{G}$, to be the function which satisfies for all $u, v \in \mathcal{G}$ that $R_v(u) = u \cdot v$. Moreover, we have that for all $v \in \mathcal{G}$ it holds that $R'_v = T|_e R_v\colon \mathfrak{g} \to T\mathcal{G}|_v$ (cf. Definition 2.2). See, e.g., https://math.stackexchange.com/questions/1740179/differential-of-the-multiplication-and-inverse-maps-on-a-lie-group for more details.

Definition 2.14. Let $\mathcal{G}$ be a Lie group, let $e \in \mathcal{G}$ satisfy for all $p \in \mathcal{G}$ that $p \cdot e = e \cdot p = p$, let $\mathfrak{g}$ be the Lie algebra of $\mathcal{G}$, and let $\sigma_a\colon [0,1] \to \mathcal{G}$, $a \in \mathfrak{g}$, be a differentiable function satisfying for all $a \in \mathfrak{g}$, $t \in [0,1]$ that $\sigma_a(0) = e$ and

$$\sigma'_a(t) = R'_{\sigma_a(t)}(a) \tag{2.6}$$

(cf. Definitions 2.4, 2.8, 2.10, and 2.13). Then we define the exponential map $\exp\colon \mathfrak{g} \to \mathcal{G}$ to be the function which satisfies for all $a \in \mathfrak{g}$ that $\exp(a) = \sigma_a(1)$. See, e.g., https:

//en.wikipedia.org/wiki/Exponential_map_(Lie_theory)#:~:text=In%20the%20theory%20of%20Lie,tool%20for%20studying%20Lie%20groups. for more details.

Problem 2.15. Let $d \in \mathbb{N}$, let $\mathcal{G} = \mathrm{GL}(d;\mathbb{R}) = \{a \in \mathbb{R}^{d\times d} \colon \det(a) \neq 0\}$, and let $\cdot \colon \mathcal{G}\times\mathcal{G} \to \mathcal{G}$ satisfy for all $a, b \in \mathcal{G}$ that $a \cdot b = ab$.

a. Show that $\mathfrak{gl}_d = \mathbb{R}^{d\times d}$ is the Lie algebra of $\mathcal{G}$ (cf. Definition 2.10).

b. Show that for all $a \in \mathcal{G}$ it holds that $\exp(a) = \sum_{k=0}^{\infty} \frac{1}{k!} a^n$ (cf. Definition 2.14).

c. Determine an action of $\mathcal{G}$ on the manifold $\mathbb{R}^d$ (cf. Definition 2.12). Is this action unique?

Solution to Problem 2.15.

The solution to Problem 2.15 is thus complete. □

Lemma 2.16. Let $\mathcal{M}$ be a manifold, let $\mathcal{G}$ be a Lie group, let $e \in \mathcal{G}$ satisfy for all $p \in \mathcal{G}$ that $p \cdot e = e \cdot p = p$, let $\mathfrak{g}$ be the Lie algebra of $\mathcal{G}$, let $\Lambda\colon \mathcal{G} \times \mathcal{M} \to \mathfrak{g}$ be an action, let $T \in (0, \infty)$, $y_0 \in \mathcal{M}$, $a \in \mathfrak{g}$, let $\rho\colon [0,1] \to \mathcal{G}$ be a differentiable function satisfying that $\rho(0) = e$ and $\rho'(0) = a$, and let $y\colon [0,T] \to \mathcal{M}$ be a differentiable function satisfying for all $t \in [0,T]$ that $y(0) = y_0$ and

$$\big(\tfrac{\mathrm{d}}{\mathrm{d}t} y\big)(t) = \tfrac{\mathrm{d}}{\mathrm{d}s} \Lambda\big(\rho(s), y(t)\big)\Big|_{s=0} \tag{2.7}$$

(cf. Definitions 2.1, 2.4, 2.8, 2.10, and 2.12). Then it holds for all $t \in [0,T]$ that

$$\big(\tfrac{\mathrm{d}}{\mathrm{d}t} y\big)(t) = \Lambda\big(\exp(ta), y_0\big) \tag{2.8}$$

(cf. Definition 2.14).

Proof of Lemma 2.16. The proof of Lemma 2.16 is thus complete. □

3 Approximating differential equations on manifolds

We now begin our exploration of how we may approximate solutions to differential equations evolving on (homogeneous) manifolds. To that end, let $\mathcal{M}$ be a manifold, let $T \in (0, \infty)$, $y_0 \in \mathcal{M}$, let $F\colon [0,T] \times \mathcal{M} \to T\mathcal{M}$, and let $y\colon [0,T] \to \mathcal{M}$ be a differentiable function which satisfies for all $t \in [0,T]$ that $y(0) = y_0$ and

$$\big(\tfrac{\mathrm{d}}{\mathrm{d}t} y\big)(t) = F(t, y(t)) \tag{3.1}$$

(cf. Definitions 2.1 and 2.2). Our goal is to approximate the solution to Eq. (3.1) in a manner which preserves the fact that for all $t \in [0,T]$ it holds that $y(t) \in \mathcal{M}$ (you should convince yourself that this is indeed true). While this may seem trivial, it is easy to see that many *classical* numerical methods fail to preserve this property. For an example of such a failure, please see Problem 3.1 below.

Problem 3.1. Let $T \in (0, \infty)$, $a \in \mathbb{R}^3$, let $y_0 = (y_0^1, y_0^2, y_0^3) \in \mathbb{R}^3$ satisfy that $(y_0^1)^2 + (y_0^2)^2 + (y_0^3)^2 = 1$, let $(\cdot,\cdot)\colon \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}^3$ satisfy for all $u = (u^1, u^2, u^3) \in \mathbb{R}^3$, $v = (v^1, v^2, v^3) \in \mathbb{R}^3$ that $(u, v) = (u^2v^3 - u^3v^2, u^3v^1 - u^1v^3, u^1v^2 - u^2v^1)$, and let $y\colon [0,T] \to \mathbb{R}^3$ be a differentiable function which satisfies for all $t \in [0,T]$ that $y(0) = y_0$ and

$$\big(\tfrac{\mathrm{d}}{\mathrm{d}t} y\big)(t) = \big(a, y(t)\big). \tag{3.2}$$

a. Show that for all $t \in [0,T]$ it holds that $y(t) \in \mathrm{SO}(3)$ (cf. Problem 2.11).

b. Let $w\colon [0,T] \to \mathbb{R}^3$ satisfy for all $t \in [0,T]$ that $w(0) = y_0$ and

$$w(t) = w_0 + t\big(a, w_0\big). \tag{3.3}$$

Show that for all $t \in (0,T]$ it holds that $w(t) \notin \mathrm{SO}(3)$. *Note:* The function in Eq. (3.3) is actually known as Euler's method and is the basic tangent line approximation to a vector field.

Solution to Problem 3.1.

The solution to Problem 3.1 is thus complete. □

In order to circumvent the issues observed in Problem 3.1 above, we assume that there exist a Lie group $\mathcal{G}$ with Lie algebra $\mathfrak{g}$ and $e \in \mathcal{G}$ satisfying for all $p \in \mathcal{G}$ that $p \cdot e = e \cdot p = p$, an action $\Lambda\colon \mathcal{G} \times \mathcal{M} \to \mathfrak{g}$, a function $a\colon [0,T] \times \mathcal{M} \to \mathfrak{g}$, and a differentiable function $\rho_{t,x}\colon [0,1] \to \mathcal{G}$, $t \in [0,T]$, $x \in \mathfrak{g}$, which satisfies for all $s \in [0,1]$, $t \in [0,T]$, $x \in \mathfrak{g}$ that $\rho_{t,x}(0) = e$, $\rho'_{t,x}(0) = a(t,x)$, and

$$\left(\tfrac{\mathrm{d}}{\mathrm{d}t} y\right)(t) = \tfrac{\mathrm{d}}{\mathrm{d}s} \Lambda\big(\rho_{t,a(t,y(t))}(s), y(t)\big)\Big|_{s=0} \tag{3.4}$$

(cf. Definitions 2.1, 2.4, 2.8, 2.10, and 2.12 and Eq. (3.1)).

Remark 3.2. While the above assumptions may seem restrictive, it is important to note that Sophus Lie's third fundamental theorem guarantees that Eq. (3.4) will always hold *locally* (cf., e.g., https://en.wikipedia.org/wiki/Lie%27s_third_theorem). Thus, we may construct such actions locally throughout the interval of interest and then use the semigroup property of the exponential map to "piece these solutions together." However, in practice, one rarely runs into such pathological issues (at least, when trying to utilize structure-preserving methods).

Definition 3.3. Let $\mathcal{G}$ be a Lie group and let $\mathfrak{g}$ be the Lie algebra of $\mathcal{G}$ (cf. Definitions 2.4 and 2.8). Then we define $\operatorname{dexp}\colon \mathfrak{g}\times\mathfrak{g}\to\mathfrak{g}$ to be the function which satisfies for all $u, v \in \mathfrak{g}$ that

$$\big(\tfrac{\mathrm{d}}{\mathrm{d}t}\exp\big)(u)(v) = R'_{\exp(u)} \circ \operatorname{dexp}_u(v) \tag{3.5}$$

(cf. Definitions 2.13 and 2.14). See, e.g., https://en.wikipedia.org/wiki/Derivative_of_the_exponential_map for more details.

Lemma 3.4. Let $\mathcal{G}$ be a Lie group and let $\mathfrak{g}$ be the Lie algebra of $\mathcal{G}$ (cf. Definitions 2.4 and 2.8). Then it holds for all $u, v \in \mathfrak{g}$ that

$$\operatorname{dexp}_u(v) = \big(\operatorname{ad}^1(u,v)\big)^{-1}\Big[\exp\big(\operatorname{ad}^1(u,v)\big) - v\Big] = \sum_{k=0}^{\infty} \frac{1}{(k+1)!}\operatorname{ad}^k(u,v) \tag{3.6}$$

(cf. Definitions 2.7, 2.14, and 3.3).

Proof of Lemma 3.4. The proof of Lemma 3.4 is thus complete. □

Lemma 3.5. Let $\mathcal{G}$ be a Lie group, let $\mathfrak{g}$ be the Lie algebra of $\mathcal{G}$, and let $B_0, B_1, B_2, \ldots \in \mathbb{R}$ satisfy for all $n \in \mathbb{N}_0$ that $B_n = \sum_{i=0}^{n}\sum_{j=0}^{i}(-1)^j\binom{i}{j}{}^{j^n}/_{(i+1)}$ (cf. Definitions 2.4 and 2.8). Then it holds for all $u, v \in \mathfrak{g}$ that

$$\begin{aligned}\operatorname{dexp}_u^{-1}(v) &= \sum_{k=0}^{\infty}\frac{B_k}{k!}\operatorname{ad}^k(u,v)\\ &= v - \tfrac{1}{2}\operatorname{ad}^1(u,v) + \tfrac{1}{12}\operatorname{ad}^2(u,v) - \tfrac{1}{720}\operatorname{ad}^4(u,v) + \tfrac{1}{30240}\operatorname{ad}^6(u,v) - \ldots\end{aligned} \tag{3.7}$$

(cf. Definitions 2.7 and 3.3).

Proof of Lemma 3.5. The proof of Lemma 3.5 is thus complete. □

Remark 3.6. The sequence of rational numbers $B_0, B_1, B_2, \ldots \in \mathbb{R}$ which satisfy for all $n \in \mathbb{N}_0$ that

$$B_n = \sum_{i=0}^{n}\sum_{j=0}^{i}(-1)^j\binom{i}{j}\frac{j^n}{(i+1)} \tag{3.8}$$

are known as *Bernoulli's numbers* (cf., e.g., https://en.wikipedia.org/wiki/Bernoulli_number). Eq. (3.8) is just one of many representations of these numbers.

Lemma 3.7. Let $\mathcal{M}$ be a manifold, let $T \in (0, \infty)$, $y_0 \in \mathcal{M}$, let $\mathcal{G}$ be a Lie group, let $e \in \mathcal{G}$ satisfy for all $p \in \mathcal{G}$ that $p \cdot e = e \cdot p = p$, let $\mathfrak{g}$ be the Lie algebra of $\mathcal{G}$, let $\Lambda \colon \mathcal{G} \times \mathcal{M} \to \mathfrak{g}$ be an action, let $a \colon [0, T] \times \mathcal{M} \to \mathfrak{g}$, let $\rho_{t,x} \colon [0, 1] \to \mathcal{G}$, $t \in [0, T]$, $x \in \mathfrak{g}$, be a differentiable function which satisfies for all $s \in [0, 1]$, $t \in [0, T]$, $x \in \mathfrak{g}$ that $\rho_t(0) = e$ and $\rho_t'(0) = a(t, x)$, let $y \colon [0, T] \to \mathcal{M}$ be a differentiable function which satisfies for all $t \in [0, T]$ that $y(0) = y_0$ and

$$\left(\tfrac{\mathrm{d}}{\mathrm{d}t} y\right)(t) = \tfrac{\mathrm{d}}{\mathrm{d}s} \Lambda\left(\rho_{t,a(t,x)}(s), y(t)\right)\Big|_{s=0}, \tag{3.9}$$

and let $\Theta \colon [0, T] \to \mathfrak{g}$ satisfy for all $t \in [0, T]$ that $\Theta(0) = O$ and

$$\left(\tfrac{\mathrm{d}}{\mathrm{d}t} \Theta\right)(t) = \operatorname{dexp}^{-1}_{\Theta(t)}\Big(a\big(t, y(t)\big)\Big) = \operatorname{dexp}^{-1}_{\Theta(t)}\bigg(a\Big(t, \Lambda\big(\exp\big(\Theta(t)\big), y_0\big)\Big)\bigg) \tag{3.10}$$

(cf. Definitions 2.1, 2.2, 2.4, 2.8, 2.10, 2.12, 2.14, and 3.3). Then there exists $T_* \in (0, T]$ such that for all $t \in [0, T_*]$ it holds that

$$y(t) = \Lambda\Big(\exp\big(\Theta(t)\big), y_0\Big). \tag{3.11}$$

Proof of Lemma 3.7. The proof of Lemma 3.7 is thus complete. □

Note how the assumptions employed in Lemma 3.8 below differ from, e.g., Lemma 3.7 above. Due to the particular structure we have encountered in our actual project, Lemma 3.8 below utilizes a slightly simplified setting in order to reduce the cumbersome of the ensuing notation.

Lemma 3.8. Let $\mathcal{M}$ be a manifold, let $T \in (0, \infty)$, $y_0 \in \mathcal{M}$, let $\mathcal{G}$ be a Lie group, let $e \in \mathcal{G}$ satisfy for all $p \in \mathcal{G}$ that $p \cdot e = e \cdot p = p$, let $\mathfrak{g}$ be the Lie algebra of $\mathcal{G}$, let $\Lambda \colon \mathcal{G} \times \mathcal{M} \to \mathfrak{g}$ be an action, let $a \colon [0, T] \to \mathfrak{g}$, let $\rho_t \colon [0, 1] \to \mathcal{G}$, $t \in [0, T]$, be a differentiable function which satisfies for all $s \in [0, 1]$, $t \in [0, T]$ that $\rho_t(0) = e$ and $\rho_t'(0) = a(t)$, let $y \colon [0, T] \to \mathcal{M}$ be a differentiable function which satisfies for all $t \in [0, T]$ that $y(0) = y_0$ and

$$\left(\tfrac{\mathrm{d}}{\mathrm{d}t} y\right)(t) = \tfrac{\mathrm{d}}{\mathrm{d}s} \Lambda\left(\rho_{t,a(t)}(s), y(t)\right)\Big|_{s=0}, \tag{3.12}$$

let $B_0, B_1, B_2, \ldots \in \mathbb{R}$ satisfy for all $n \in \mathbb{N}_0$ that $B_n = \sum_{i=0}^{n} \sum_{j=0}^{i} (-1)^j \binom{i}{j} {j^n}/{(i+1)}$, let $\Theta \colon [0, T] \to \mathfrak{g}$ satisfy for all $t \in [0, T]$ that $\Theta(0) = O$ and

$$\left(\tfrac{\mathrm{d}}{\mathrm{d}t} \Theta\right)(t) = \operatorname{dexp}^{-1}_{\Theta(t)}\big(a(t)\big) = \operatorname{dexp}^{-1}_{\Theta(t)}\big(a(t)\big), \tag{3.13}$$

and let $\Theta^{[k]} \colon [0, T] \to \mathfrak{g}$, $k \in \mathbb{N}_0$, satisfy for all $k \in \mathbb{N}$, $t \in [0, T]$ that $\Theta^{[0]}(t) = O$ and

$$\Theta^{[k]}(t) = \int_0^t \operatorname{dexp}^{-1}_{\Theta^{[k-1]}(\xi)}\big(a(\xi)\big)\, \mathrm{d}\xi \tag{3.14}$$

(cf. Definitions 2.1, 2.2, 2.4, 2.8, 2.10, 2.12, 2.14, and 3.3). Then

(i) it holds for all $k \in \mathbb{N}$, $t \in [0, T]$ that

$$\Theta^{[k]}(t) = \sum_{i=0}^{\infty} \frac{B_i}{i!} \int_0^t \operatorname{ad}^i\big(\Theta^{[k-1]}(\xi), a(\xi)\big)\, \mathrm{d}\xi \tag{3.15}$$

and

(ii) there exists $T_* \in (0, T]$ such that for all $t \in [0, T_*]$ it holds that

$$\Theta(t) = \lim_{k \to \infty} \Theta^{[k]}(t) \tag{3.16}$$

(cf. Definition 2.7).

Proof of Lemma 3.8. The proof of Lemma 3.8 is thus complete. □

Remark 3.9. Armed with Lemma 3.8, we are now in a position to construct structure-preserving numerical approximations to Eq. (3.1). These approximations will proceed via two steps. First, we will choose some $m \in \mathbb{N}_0$ and utilize $\Theta^{[m]}$ in our approximation method: this requires proving a so-called *convergence result* for the Picard iterates. Next, we will construct an appropriate approximation to the exponential map: this will be accomplished via certain *rational function* approximation techniques. These two issues will be discussed further as these notes continue.

We now (informally) continue the line of thinking developed in Lemma 3.8 above. First, note that direct calculations yield that for all $t \in [0, T]$ it holds that

$$\Theta^{[1]}(t) = \int_0^t a(\xi_1)\,\mathrm{d}\xi_1, \tag{3.17}$$

$$\begin{aligned}\Theta^{[2]}(t) = {} & \int_0^t a(\xi_1)\,\mathrm{d}\xi_1 - \tfrac{1}{2}\int_0^t \left[\int_0^{\xi_1} a(\xi_2)\,\mathrm{d}\xi_2, a(\xi_1)\right]\mathrm{d}\xi_1 \\ & + \tfrac{1}{12}\int_0^t \left[\int_0^{\xi_1} a(\xi_2)\,\mathrm{d}\xi_2, \left[\int_0^{\xi_1} a(\xi_2)\,\mathrm{d}\xi_2, a(\xi_1)\right]\right]\mathrm{d}\xi_1 + \ldots,\end{aligned} \tag{3.18}$$

and

$$\begin{aligned}\Theta^{[3]}(t) = {} & \int_0^t a(\xi_1)\,\mathrm{d}\xi_1 - \tfrac{1}{2}\int_0^t \left[\int_0^{\xi_1} a(\xi_2)\,\mathrm{d}\xi_2, a(\xi_1)\right]\mathrm{d}\xi_1 \\ & + \tfrac{1}{12}\int_0^t \left[\int_0^{\xi_1} a(\xi_2)\,\mathrm{d}\xi_2, \left[\int_0^{\xi_1} a(\xi_2)\,\mathrm{d}\xi_2, a(\xi_1)\right]\right]\mathrm{d}\xi_1 \\ & + \tfrac{1}{4}\int_0^t \left[\int_0^{\xi_1}\left[\int_0^{\xi_2} a(\xi_3)\,\mathrm{d}\xi_3, a(\xi_2)\right]\mathrm{d}\xi_2, a(\xi_1)\right]\mathrm{d}\xi_1 \\ & - \tfrac{1}{24}\int_0^t \left[\int_0^{\xi_1}\left[\int_0^{\xi_2} a(\xi_3)\,\mathrm{d}\xi_3, \left[\int_0^{\xi_2} a(\xi_3)\,\mathrm{d}\xi_3, a(\xi_2)\right]\right]\mathrm{d}\xi_2, a(\xi_1)\right]\mathrm{d}\xi_1 \\ & - \tfrac{1}{24}\int_0^t \left[\int_0^{\xi_1}\left[\int_0^{\xi_2} a(\xi_3)\,\mathrm{d}\xi_3, a(\xi_2)\right]\mathrm{d}\xi_2, \left[\int_0^{\xi_1} a(\xi_2)\,\mathrm{d}\xi_2, a(\xi_1)\right]\right]\mathrm{d}\xi_1 \\ & - \tfrac{1}{24}\int_0^t \left[\int_0^{\xi_1} a(\xi_2)\,\mathrm{d}\xi_2, \left[\int_0^{\xi_1}\left[\int_0^{\xi_2} a(\xi_3)\,\mathrm{d}\xi_3, a(\xi_2)\right]\mathrm{d}\xi_2, a(\xi_1)\right]\right]\mathrm{d}\xi_1 + \ldots.\end{aligned} \tag{3.19}$$

Observe that we could have continued these calculations, but things become increasingly tedious (however, things can be simplified considerably via the use of graph theory). Next, note that even when we keep all (infinitely many) terms in Eq. (3.18) or Eq. (3.19), we are only able to approximate the function Θ with limited accuracy (this is a direct consequence of the Picard-Lindelöf theorem (cf., e.g., https://en.wikipedia.org/wiki/Picard%E2%80%93Lindel%C3%B6f_theorem). That is, let $\|\cdot\|\colon \mathfrak{g} \to [0,\infty)$ be an appropriate norm. Then, there exists $C_k \in \mathbb{R}$, $k \in \mathbb{N}_0$, and $f\colon \mathbb{N}_0 \to [0,\infty)$ such that for all $k \in \mathbb{N}_0$, $t \in [0,T_*]$ it holds that

$$\big\|\Theta(t) - \Theta^{[k]}(t)\big\| \leq C_k t^{f(k)}. \tag{3.20}$$

This indicates that keeping *all* terms in the low-level expansions is not ideal. This motivates the result in Lemma 3.10 below.

Lemma 3.10. Let $\mathcal{M}$ be a manifold, let $T \in (0,\infty)$, $y_0 \in \mathcal{M}$, let $\mathcal{G}$ be a Lie group, let $e \in \mathcal{G}$ satisfy for all $p \in \mathcal{G}$ that $p \cdot e = e \cdot p = p$, let $\mathfrak{g}$ be the Lie algebra of $\mathcal{G}$, let $\Lambda\colon \mathcal{G} \times \mathcal{M} \to \mathfrak{g}$ be an action, let $a\colon [0,T] \to \mathfrak{g}$, let $\rho_t\colon [0,1] \to \mathcal{G}$, $t \in [0,T]$, be a differentiable function which satisfies for all $s \in [0,1]$, $t \in [0,T]$ that $\rho_t(0) = e$ and $\rho_t'(0) = a(t)$, let $y\colon [0,T] \to \mathcal{M}$ be a differentiable function which satisfies for all $t \in [0,T]$ that $y(0) = y_0$ and

$$\big(\tfrac{\mathrm{d}}{\mathrm{d}t} y\big)(t) = \tfrac{\mathrm{d}}{\mathrm{d}s} \Lambda\big(\rho_{t,a(t)}(s), y(t)\big)\Big|_{s=0}, \tag{3.21}$$

let $B_0, B_1, B_2, \ldots \in \mathbb{R}$ satisfy for all $n \in \mathbb{N}_0$ that $B_n = \sum_{i=0}^n \sum_{j=0}^i (-1)^j \binom{i}{j} j^n/(i+1)$, let $\Theta\colon [0,T] \to \mathfrak{g}$ satisfy for all $t \in [0,T]$ that $\Theta(0) = O$ and

$$\big(\tfrac{\mathrm{d}}{\mathrm{d}t}\Theta\big)(t) = \operatorname{dexp}^{-1}_{\Theta(t)}\big(a(t)\big) = \operatorname{dexp}^{-1}_{\Theta(t)}\big(a(t)\big), \tag{3.22}$$

and let $\Omega^{[k]}\colon [0,T] \to \mathfrak{g}$, $k \in \mathbb{N}_0$, satisfy for all $k \in \mathbb{N}$, $t \in [0,T]$ that $\Omega^{[0]}(t) = O$ and

$$\Omega^{[k]}(t) = \sum_{i=0}^{k-1} \frac{B_i}{i!} \int_0^t \operatorname{ad}^i\big(\Omega^{[k-1]}(\xi), a(\xi)\big)\,\mathrm{d}\xi \tag{3.23}$$

(cf. Definitions 2.1, 2.2, 2.4, 2.7, 2.8, 2.10, 2.12, 2.14, and 3.3). Then

(i) there exists $T_* \in (0,T]$ such that for all $t \in [0,T_*]$ it holds that

$$\Theta(t) = \lim_{k\to\infty} \Omega^{[k]}(t) \tag{3.24}$$

and

(ii) it holds for all $k \in \mathbb{N}_0$, $t \in [0,T_*]$, and $\|\cdot\|\colon \mathfrak{g} \to [0,\infty)$ which satisfy for all $u,v \in \mathfrak{g}$, $c \in \mathbb{R}$ that $\|u+v\| \leq \|u\| + \|v\|$, $\|cu\| = |c|\|u\|$, and $\|u\| = 0$ if and only if $u = O$ that there exists $C \in \mathbb{R}$ such that

$$\big\|\Theta(t) - \Omega^{[k]}(t)\big\| \leq C t^{k+1}. \tag{3.25}$$

Proof of Lemma 3.10. The proof of Lemma 3.10 is thus complete. □

It is now important to emphasize what is implied by Lemma 3.10 above.

1. Item (i) in Lemma 3.10 above demonstrates that we can truncate the Picard iterates and still obtain the desired convergence to the true solution. *Note:* We have purposely avoided the issue of discussing/defining what a limit means in a Lie algebra, but hopefully this is clear.

2. Item (ii) in Lemma 3.10 above shows that we may choose our Picard iterate based on the amount of accuracy we desire. This can be seen in the right-hand side of Eq. (3.25).

3. It should be clear that item (ii) in Lemma 3.10 holds true if we can prove the result for one such $\|\cdot\|\colon \mathfrak{g} \to [0,\infty)$ as we are in a finite-dimensional setting.

4. Something which is hidden in the details (and often misunderstood) is the constant "C" in item (ii) in Lemma 3.10. This constant is a function of the underlying smoothness of the function a, as it will be the result of trying to bound the nested commutators within the Picard iterates. For our project we will not need to concern ourselves with this constant too much; we only need to understand its role and how it can be controlled.

Problem 3.11. Verify item (ii) in Lemma 3.10 for the case $k = 1$. Feel free to impose as much regularity (i.e., increase the assumptions on the objects introduced in Lemma 3.10) if you feel this will help.

Solution to Problem 3.11.

The solution to Problem 3.11 is thus complete. □

Problem 3.12. Verify item (ii) in Lemma 3.10 in the case where $k = 2$, $T = 1$, $\mathcal{M} = \mathcal{G} = \mathrm{SO}(3)$ and $\Lambda\colon \mathcal{G} \times \mathcal{G} \to \mathfrak{g}$ satisfies for all $a, b \in \mathcal{G}$ that $\Lambda(a, b) = ab$. If you want to simplify things further, you may let $\alpha \in \mathfrak{g}$ and choose $a\colon [0, T] \to \mathfrak{g}$ to satisfy for all $t \in [0, T]$ that $a(t) = t\alpha$.

Solution to Problem 3.12.

The solution to Problem 3.12 is thus complete. □

3.1 A first attempt at a numerical approximation

We will now (somewhat informally) motivate the construction of a numerical approximation to, e.g., Eq. (3.21). To that end, we will commence by fixing $k = 1$. This and Eq. (3.23) yield that for all $t \in [0, T_*]$ it holds that

$$\Omega^{[1]}(t) = B_0 \int_0^t \operatorname{ad}^0\big(\Omega^{[0]}(\xi), a(\xi)\big)\, \mathrm{d}\xi = \int_0^t a(\xi)\, \mathrm{d}\xi. \tag{3.26}$$

We now apply an approximation to the integral in Eq. (3.26) (since, in general, we will not be able to compute the integral exactly) to obtain that for all $t \in [0, T_*]$ it holds that

$$\Omega^{[1]}(t) \approx t a(0). \tag{3.27}$$

Problem 3.13. Let $T, L \in (0, \infty)$, let $\mathfrak{g}$ be a Lie algebra, let $\|\cdot\| \colon \mathfrak{g} \to [0, \infty)$ satisfy for all $u, v \in \mathfrak{g}$, $c \in \mathbb{R}$ that $\|u + v\| \leq \|u\| + \|v\|$, $\|cu\| = |c|\|u\|$, and $\|u\| = 0$ if and only if $u = O$, and let $a \colon [0, T] \to \mathfrak{g}$ satisfy for all $s, t \in [0, T]$ that $\|a(t) - a(s)\| \leq L|t - s|$ (cf. Definition 2.4). Show that for all $t \in [0, T]$ it holds that

$$\left\| \int_0^t a(\xi)\, \mathrm{d}\xi - t a(0) \right\| \leq \frac{Lt^2}{2}. \tag{3.28}$$

Solution to Problem 3.13.

The solution to Problem 3.13 is thus complete. □

Combining Lemmas 3.7 and 3.10 and Eq. (3.27) demonstrate that for all $t \in [0, T_*]$ it holds that

$$y(t) = \Lambda\Big(\exp\big(\Theta(t)\big), y_0\Big) \approx \Lambda\Big(\exp\big(\Omega^{[1]}(t)\big), y_0\Big) = \Lambda\Big(\exp\big(ta(0)\big), y_0\Big). \tag{3.29}$$

Provided that the group action, Λ, and $\exp(ta(0))$ can be computed with relative ease, we have arrived at a reasonable numerical approximation. Moreover, the approximations employed thus far have been linear approximations performed on objects in the Lie algebra—thus, our approximation will still lie in the original manifold for all $t \in [0, T_*]$.

Problem 3.14. Develop a similar approximation using $\Omega^{[2]}$ (cf. Lemma 3.10). Note that in this case, you will likely need to impose additional regularity assumptions (be sure to only impose precisely enough to derive your result).

Solution to Problem 3.14.

The solution to Problem 3.14 is thus complete. □

3.2 Approximating the exponential map