Trees, Bialgebras and Intrinsic Numerical Algorithms

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Abstract

This report describes preliminary work about intrinsic numerical integrators evolving on groups. Fix a finite dimensional Lie group $G$, let $\mathfrak{g}$ denote its Lie algebra, and let $Y_1, \ldots, Y_N$ denote a basis of $\mathfrak{g}$. We give a class of numerical algorithms to approximate solutions to differential equations evolving on $G$ of the form:

$$\dot{z}(t) = F(z(t)), \quad z(0) = p \in G,$$

where

$$F = \sum_{\mu=1}^{N} a^\mu Y_\mu, \quad a^\mu \in C^\infty(G).$$

The algorithm depends upon constants $c_i$ and $c_{ij}$, for $i = 1, \ldots, k$ and $j < i$. The algorithm has the property that if the algorithm starts on the group, then it remains on the group. It also has the property that if $G$ is the abelian group $\mathbb{R}^N$, then the algorithm becomes the classical Runge-Kutta algorithm. We use the Cayley algebra generated by labeled, ordered trees to generate the equations that the coefficients $c_i$ and $c_{ij}$ must satisfy in order for the algorithm to yield an $r$th order numerical integrator and to analyze the resulting algorithms.

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1 Introduction

Fix a finite dimensional Lie group $G$, let $g$ denote its Lie algebra, and let $Y_1, \ldots, Y_N$ denote a basis of $g$. We give a class of numerical algorithms to approximate solutions to differential equations evolving on $G$ of the form:

$$\dot{x}(t) = F(x(t)), \quad x(0) = p \in G,$$

where

$$F = \sum_{\mu=1}^{N} a^\mu Y_\mu, \quad a^\mu \in C^\infty(G).$$

The algorithm depends upon constants $c_i$ and $c_{ij}$, for $i = 1, \ldots, k$ and $j < i$. The algorithm has the property that if the algorithm starts on the group, then it remains on the group. It also has the property that if $G$ is the abelian group $\mathbb{R}^N$, then the algorithm becomes the classical Runge-Kutta algorithm. Our analysis requires the Cayley algebra generated by labeled, ordered trees, introduced in [10], [11] and [6]. We use the Cayley algebra of trees to generate the equations that the coefficients $c_i$ and $c_{ij}$ must satisfy in order for the algorithm to yield an $r$th order numerical integrator and to analyze the resulting algorithms.

This is a preliminary report. A final report containing complete proofs, examples, and a further analysis of the algorithms is in preparation.

2 Families of trees

The relation between trees and Taylor's theorem goes back as least as far as Cayley [3] and [4]. Important use of this relation has been made by Butcher in his work on high order Runge-Kutta algorithms [1] and [2]. In this section and the next, we follow the treatment in [10] and [11].

By a tree we mean a rooted finite tree. If $\{F_1, \ldots, F_M\}$ is a set of symbols, we will say a tree is labeled with $\{F_1, \ldots, F_M\}$ if every node of the tree other than the root has an element of $\{F_1, \ldots, F_M\}$ assigned to it. We denote the set of all trees labeled with $\{F_1, \ldots, F_M\}$ by $\mathcal{LT}(F_1, \ldots, F_M)$. Let $k\{\mathcal{LT}(F_1, \ldots, F_M)\}$ denote the vector space over $k$ with basis $\mathcal{LT}(F_1, \ldots, F_M)$. We show that this vector space is a graded connected algebra.

We define the multiplication in $k\{\mathcal{LT}(F_1, \ldots, F_M)\}$ as follows. Since the set of labeled trees form a basis for $k\{\mathcal{LT}(F_1, \ldots, F_M)\}$, it is sufficient to describe the product of two labeled trees. Suppose $t_1$ and $t_2$ are two labeled trees. Let $s_1, \ldots, s_r$ be the children of the root of $t_1$. If $t_2$ has $n+1$
nodes (counting the root), there are \((n + 1)^r\) ways to attach the \(r\) subtrees of \(t_1\) which have \(s_1, \ldots, s_r\) as roots to the labeled tree \(t_2\) by making each \(s_i\) the child of some node of \(t_2\), keeping the original labels. The product \(t_1t_2\) is defined to be the sum of these \((n + 1)^r\) labeled trees. It can be shown that this product is associative, and that the tree consisting only of the root is a multiplicative identity; see \([5]\).

We can define a grading on \(k\{\mathcal{L}T(F_1, \ldots, F_M)\}\) by letting \(k\{\mathcal{L}T_n(F_1, \ldots, F_M)\}\) be the subspace of \(k\{\mathcal{L}T(F_1, \ldots, F_M)\}\) spanned by the trees with \(n + 1\) nodes. The following theorem is proved in \([9]\).

**Theorem 2.1** \(k\{\mathcal{L}T(F_1, \ldots, F_M)\}\) is a graded connected algebra.

If \(\{F_1, \ldots, F_M\}\) is a set of symbols, then the free associative algebra \(k\langle F_1, \ldots, F_M \rangle\) is a graded connected algebra, and there is an algebra homomorphism

\[
\phi : k\langle F_1, \ldots, F_M \rangle \rightarrow k\{\mathcal{L}T(F_1, \ldots, F_M)\}.
\]

The map \(\phi\) sends \(F_i\) to the labeled tree with two nodes: the root, and a child of the root labeled with \(F_i\); it is then extended to all of \(k\langle F_1, \ldots, F_M \rangle\) by using the fact that it is an algebra homomorphism.

We say that a rooted finite tree is ordered in case there is a partial ordering on the nodes such that the children of each node are non-decreasing with respect to the ordering. We say such a tree is labeled with \(\{F_1, \ldots, F_M\}\) in case every element, except the root, has an element of \(\{F_1, \ldots, F_M\}\) assigned to it. Let \(k\{\mathcal{L}OT(F_1, \ldots, F_M)\}\) denote the vector space over \(k\) whose basis consists of labeled ordered trees. It turns out that \(k\{\mathcal{L}OT(F_1, \ldots, F_M)\}\) is also a graded connected algebra using the same multiplication defined above. See \([9]\) for a proof of the following theorem.

We say that a rooted finite tree is heap-ordered in case there is a total ordering on all nodes in the tree such that each node precedes all of its children in the ordering. We define \(k\{\mathcal{L}HOT(F_1, \ldots, F_M)\}\) as above to be the vector space over \(k\) whose basis consists of heap-ordered trees labeled with \(\{F_1, \ldots, F_M\}\). In \([9]\) we show that \(k\{\mathcal{L}HOT(F_1, \ldots, F_M)\}\) is also a graded connected algebra \([9]\) and satisfies:

**Theorem 2.2** The map

\[
\phi : k\langle F_1, \ldots, F_M \rangle \rightarrow k\{\mathcal{L}HOT(F_1, \ldots, F_M)\}
\]

is injective.
Fix $N$ derivations $Y_1, \ldots, Y_N$ of $R$ and consider $M$ other derivations of $R$ of the form

$$F_i = \sum_{\mu=1}^{N} a_{i}^{\mu} Y_{\mu}, \quad a_{i}^{\mu} \in R, \quad i = 1, \ldots, M.$$  \hspace{1cm} (1)

Let $\text{End}(R)$ denote the endomorphisms of the ring $R$. Using the data (1), we now define a map

$$\psi : k\{\mathcal{L}T(F_1, \ldots, F_M)\} \rightarrow \text{End}(R)$$

in the following steps.

**Step 1.** Given a labeled tree $t \in \mathcal{L}T_m(F_1, \ldots, F_M)$, assign the root the number 0 and assign the remaining nodes the numbers 1, \ldots, $m$. From now on we identify the node with the number assigned to it. Let $j \in \text{nodes } t$, and suppose that $l, \ldots, l'$ are the children of $j$ and that $j$ is labeled with $F_{\eta_j}$. Fix $\mu_1, \ldots, \mu_{\nu}$ with

$$1 \leq \mu_1, \ldots, \mu_{\nu} \leq N$$

and define

$$R(j; \mu_1, \ldots, \mu_{\nu}) = Y_{\mu_1} \cdots Y_{\mu_{\nu}} a_{\eta_j}^{\mu_{\nu}}$$

if $j$ is not the root

$$= Y_{\mu_1} \cdots Y_{\mu_{\nu}}$$

if $j$ is the root .

We abbreviate this to $R(j)$. Observe that $R(j) \in R$ for $j > 0$.

**Step 2.** Define

$$\psi(t) = \sum_{\mu_1, \ldots, \mu_{m}=1}^{N} R(m) \cdots R(1) R(0).$$

**Step 3.** Extend $\psi$ to all $k\{\mathcal{L}T(F_1, \ldots, F_M)\}$ by $k$-linearity.

**Remark 2.1** In exactly the same way, we define a map

$$\psi : k\{\mathcal{L}T(F_1, \ldots, F_M)\} \rightarrow \text{End}(R),$$

by ignoring the ordering of the nodes.
Remark 2.2 Let $H$ denote one of the algebras of labeled trees above, possibly with additional structure such as an ordering or heap ordering. It is easy to check that the $\psi$ map makes $R$ into a left $H$-module.

Let $\chi$ denote the map

$$k\langle F_1, \ldots, F_M \rangle \rightarrow \text{End}(R)$$

defined by using the substitution (1) and simplifying to obtain an endomorphism of $R$.

Lemma 2.1

(i) The map $\psi$ is an algebra homomorphism

(ii) and $\chi = \psi \circ \phi$.

Proof: The proof of (i) is a straightforward verification and is contained in [8]. Since $\chi$ and $\psi \circ \phi$ agree on the generating set $E_1, \ldots, E_M$, part (ii) follows from part (i).

In the later sections, we will also require two other products defined on families of trees. Given $t_1, t_2 \in \mathcal{L}(F_1, \ldots, F_M)$, define the meld product $t_2 \circ t_1$ to be the labeled tree obtained by identifying the roots of the two trees. The meld product is then extended to all of $k\{\mathcal{L}(F_1, \ldots, F_M)\}$ by linearity. Given a derivation $F \in \text{Der}(R)$, let $t_2$ be the tree $\phi(F)$ and let $t_1 \in \mathcal{L}(F_1, \ldots, F_M)$. Recall $t_2$ is a tree consisting of a root and a node labeled $F$. We define the composition product $t_2 \circ t_1$ to be the tree formed by attaching the subtrees whose roots are the children of the root of $t_1$ to the node labeled $F$ of the tree $t_2$.

3 Trees and Taylor Series

Fix a Lie group $G$ of dimension $N$, with Lie algebra $g$, and let $R$ denote a ring of infinitely differentiable functions on $G$. We let $\exp : g \rightarrow G$ denote the exponential map. Fix a basis of the Lie algebra $g$ consisting of left invariant vector fields $Y_1, \ldots, Y_N$. We will need a map

$$\mathcal{J} : R^N \rightarrow R \otimes g, \quad (a_1, \ldots, a_N) \mapsto \sum_{\mu=1}^{N} a_\mu Y_\mu$$

and its inverse, which we denote $b$. We usually write these maps as superscripts, as in $(a_1, \ldots, a_N)^\mathcal{J}$. 

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We are interested in derivations $F$ of the form 

$$F = \sum_{\mu=1}^{N} a^{\mu} Y_{\mu}, \quad a^{\mu} \in R, \quad \mu = 1, \ldots, N$$

and the corresponding differential equation 

$$\dot{x}(t) = F(x(t)), \quad x(0) = p \in G. \quad (2)$$

Let $\exp(tF)(x)$ denote the resulting of flowing for time $t$ along the trajectory of (2) through the initial point $p \in G$. We require two lemmas concerned with Taylor series expansion of a solution of (2). These lemmas will use the maps $\phi$ and $\psi$ defined in the previous section.

If $\alpha$ is a tree, define the exponential and Meld-exponential of a tree by the formal power series 

$$\exp(t\alpha) = 1 + t\alpha + \frac{t^2}{2!}\alpha^2 + \frac{t^3}{3!}\alpha^3 + \cdots$$

$$\text{Mexp}(t\alpha) = 1 + t\alpha + \frac{t^2}{2!}\alpha \odot \alpha + \frac{t^3}{3!}\alpha \odot \alpha \odot \alpha + \cdots.$$

**Lemma 3.1** Assume $f \in R$ and $F \in \text{Der}(R)$. Then

1. 

$$(F^k f)(x) = \frac{d^k}{dt^k} f(\exp(tF)x) \big|_{t=0}.$$  

2. If $f$ is analytic near $x$, then for sufficiently small $t$,

$$f(\exp(tF)x) = \sum_{k=0}^{\infty} f(x; F^k) \frac{t^k}{k!};$$

where $f(x; F^k)$ is defined to be $(F^k f)(x)$.

3. If $f$ is analytic near $x$, then for sufficiently small $t$,

$$f(\exp(tF)x) = \psi(\exp(t\phi(F)))f|_x,$$

where $\alpha = \phi(F)$.

**Proof.** Assertions (1) and (2) can be found in [12]. Since $\phi$ is an algebra homomorphism, $\phi(F^k) = \alpha^k$. Assertion (3) then follows immediately from Assertion (2).

\[ \Box \]
Lemma 3.2 Assume $f \in R$ and $F \in \text{Der}(R)$ is left-invariant. Let $\alpha = \phi(F)$. Then

1. 
\[ f(\exp(tF)x) = f(x) + t Df(x) \cdot F(x) + \frac{t^2}{2!} D^2 f(x)(F(x), F(x)) + \cdots. \]

2. 
\[ f(\exp(tF)x) = \psi(M\exp(t\alpha)) \cdot f|_x. \]

3. If $G \in \text{Der}(R)$,
\[ \beta(G)(\exp(tF)x) = \psi(\beta \circ \text{Mexp}(t\alpha)), \]
where $\beta = \phi(G)$.

PROOF. Assertion (1) is simply Taylor’s theorem. Assertion (2) follows from Assertion (1) and the definition of the $\psi$ map, since left-invariant vector fields have “constant coefficients” with respect to the basis $Y_\mu$. Assertion (3) follows from Assertion (2) and the definition of the $\psi$, flat and sharp maps.

4 The algorithm

We are interested in numerical algorithms of the Runge-Kutta type to approximate solutions of
\[ \dot{x}(t) = F(x(t)), \quad x(0) = p \in G, \]
where $F \in \text{Der}(R)$. The algorithm depends upon constants $c_i$ and $c_{ij}$, for $i = 1, \ldots, k$ and $j < i$. For fixed constants, define the following elements of the Lie algebra $g$

\[
\begin{align*}
\bar{F}_1 &= \sum_{\mu=1}^{N} a^\mu(\nu_0) Y_\mu \in g \\
\bar{F}_2 &= \sum_{\mu=1}^{N} a^\mu(\exp(hc_{21} \bar{F}_1) \cdot \nu_0) Y_\mu \in g \\
\bar{F}_3 &= \sum_{\mu=1}^{N} a^\mu(\exp(hc_{32} \bar{F}_2) \cdot \exp(hc_{31} \bar{F}_1) \cdot \nu_0) Y_\mu \in g \\
&\vdots
\end{align*}
\]
These arise by "freezing the coefficients" of $F$ at various points along the flow of $F$.

**Algorithm 1.** Version 1. Let $x_0 = p$ and put
\[ x_{n+1} = \exp h_{c_k} \bar{F}_k \cdots \exp h_{c_1} \bar{F}_1 z_n, \]
for $n \geq 0$.

**Version 2.** Let $x_0 = p$ and put
\[ x_{n+1} = \exp (h_{c_k} \bar{F}_k + \cdots + \exp h_{c_1} \bar{F}_1) x_n, \]
for $n \geq 0$.

### 5 Necessary conditions

We prepare with two lemmas.

**Lemma 5.1** Let $f \in \mathbb{R}$ and $x_i = \phi(\bar{f}_i) \in k\{\mathcal{L}(F_1, \ldots, F_M)\}[h]$.

Then
\[
\begin{align*}
\bar{F}_1(f) &= \tilde{\psi}(\phi(\bar{F}))(f) \\
\bar{F}_2(f) &= \tilde{\psi}(\phi(\bar{F}) \circ \text{Mexp}(h_{c_1} X_1))(f) \\
\bar{F}_3(f) &= \tilde{\psi}(\phi(\bar{F}) \circ \text{Mexp}(h_{c_1} X_1 \circ \text{Mexp}(h_{c_2} X_2))(f) \\
&\vdots
\end{align*}
\]

Here $\tilde{\psi}$ is essentially the $\psi$ map followed by "freezing the coefficients" at $v_0$. More precisely,
\[
\tilde{\psi} : k\{\mathcal{L}(\bar{F}_1, \ldots, \bar{F}_M)\} \rightarrow \text{End}(\mathbb{R}).
\]

We do this in several steps.

**Step 1.** Given a labeled tree $t \in \mathcal{L}_m(\bar{F}_1, \ldots, \bar{F}_M)$, assign the root the number 0 and assign the remaining nodes the numbers 1, \ldots, $m$. From now on we identify the node with the number assigned to it. Let $j \in \text{nodes } t$, and suppose that $l, \ldots, l'$ are the children of $j$ and that $j$ is labeled with $F_{\gamma_j}$. Fix $\mu_1, \ldots, \mu_\ell$ with
\[
1 \leq \mu_1, \ldots, \mu_\ell \leq N
\]
and define

\[ R(j; \mu_1, \ldots, \mu_v) = Y_{\mu_1} \cdots Y_{\mu_v} \mu_j^\mu(\nu_0) \]

if \( j \) is not the root

\[ = Y_{\mu_1} \cdots Y_{\mu_v} \]

if \( j \) is the root.

We abbreviate this to \( R(j) \).

**Step 2.** Define

\[ \tilde{\psi}(t) = \sum_{m_1, \ldots, m_m = 1}^N R(m) \cdots R(1) R(0). \]

**Step 3.** Extend \( \psi \) to all \( k\{\mathcal{L}(F_1, \ldots, F_M)\} \) by \( k \)-linearity.

It is useful to have an intrinsic characterization of the elements \( X_i \in k\{\mathcal{L}(F_1, \ldots, F_M)\}[[h]] \). Order the labels \( F_1, \ldots, F_M \) according to their subscripts: \( F_1 < \cdots < F_M \). Let \( k\{\mathcal{LHOT}(F_1, \ldots, F_M)\} \) denote those elements of \( k\{\mathcal{L}(F_1, \ldots, F_M)\} \) satisfying

1. The nodes are heap ordered with respect to the labels \( F_1, \ldots, F_M \); in other words, the label of a child of a node is (strictly) smaller than the label of the node itself.

2. The children of a node are ordered with respect to the labels \( F_1, \ldots, F_M \); in other words, the labels of the children of a node are nondecreasing.

Using ordered, heap ordered trees it is easy to keep track of the constants \( c_i \) and \( c_{ij} \) that arise in Taylor series computations. To do this we define a map analogous to the \( \psi \) map.

Define

\[ \rho : k\{\mathcal{LHOT}(F_1, \ldots, F_M)\} \to \text{End}(R) \]

as follows

**Step 1.** Given a labeled tree \( t \in \mathcal{LHOT}(F_1, \ldots, F_M) \), with \( m + 1 \) nodes, assign the root the number 0 and assign the remaining nodes the numbers 1, \ldots, \( m \). From now on we identify the node with the number assigned to it. Fix a node \( j \) of \( t \) and let \( l, \ldots, l' \) denote its children. Let \( F_{\eta_j} \) denote the
label of node $j$. Let $p_i$ denote the number of children of $j$ labeled with the label $F_i$, for $i = 1, \ldots, M$. Let $|p|$ denote $p_1 + \cdots + p_M$. Fix $\mu_1, \ldots, \mu_\nu$ with

$$1 \leq \mu_1, \ldots, \mu_\nu \leq N$$

and define

$$R(j; \mu_1, \ldots, \mu_\nu) = \begin{cases} \frac{h^{|p|} c_{j1} \cdots c_{j\nu}}{p_1! \cdots p_M!} Y_{\mu_1} \cdots Y_{\mu_\nu} a_{ij}^\mu (v_0) & \text{if } j \text{ is not the root} \\ Y_{\mu_1} \cdots Y_{\mu_\nu} & \text{if } j \text{ is the root} \end{cases}$$

We abbreviate this to $R(j)$.

**Step 2.** Define

$$\rho(t) = \sum_{\mu_1, \ldots, \mu_m = 1}^N R(m) \cdots R(1) R(0).$$

**Step 3.** Extend $\rho$ to all $k\text{LCHOT}(F_1, \ldots, F_M)$ by $k$-linearity.

**Lemma 5.2** Let $X_i = \phi(F_i)$ and $f \in R$. Then

$$X_i(f) = \sum \rho(t)(f),$$

where the sum is over all trees $t \in \text{LCHOT}(F_1, \ldots, F_M)$ satisfying (i) $t$ consists of $i + 1$ or fewer nodes; (ii) the root of the tree has a single child labeled $F_i$.

It is now straightforward to derive the following necessary condition for a $k$th order Runge-Kutta algorithm on a group.

**Theorem 5.1** A necessary condition for a Runge-Kutta method of order $k$ on a group is that for each rooted, ordered tree $t$ consisting of $k + 1$ or fewer nodes

$$\sum \rho(t) = \frac{1}{(\#(\text{nodes}(t)) - 1)!},$$

where the sum is over all $t \in \text{LCHOT}(F_1, \ldots, F_M)$ having the same topology as $t$. 

11
References


