Lie Group Methods in Geometric Integration

by

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Dedicated

To My Parents

Abstract

Geometric integrators are numerical methods for the approximate solution of differential equations with invariants. The main aim of geometric integrators is to produce numerical solutions with the correct qualitative behavior as possed by differential equations.
If the domain of the differential equation is Euclidean space, standard numerical methods work, however if the domain is manifold or in particular a Lie group which is a differential manifold then method of choice will be special geometric integrators known as Lie group methods.
In this thesis, we shall look at some of the basic concepts behind the two main classes of Lie group methods, Magnus series expansion and Runge–Kutta–Munthe–Kaas (RKMK) methods. These Lie group methods are applied to solve differential equations on manifold. The results of the Lie group integrators are then compared with the standard numerical methods such as the classical Runge–Kutta methods. Results indicate that Lie group methods are able to produce numerical solution which mimic the qualitative features of exact solution of differential equation which we initially solve.

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May Allah bless them all.

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Contents

Chapter 1

Introduction

Geometric integrators are those numerical methods which are used for computing the solution of differential equations with invariants. The aim of a geometric integrator is to produce numerical solutions with correct qualitative behavior as possessed by the flow of differential equation. If the differential equation models a dynamical system then it is important to preserve its phase space. A first aspect of a dynamical system that is important to preserve is its phase space. If the phase space is $\Re^n$, numerical solution can easily be achieved by using any one-step numerical method, and the solution remains in $\Re^n$. If, on the other hand, phase space is a more complicated manifold, then more sophisticated methods are called for. If, for example, the phase space is a Lie group, traditional one step numerical methods for example Runge–Kutta methods generally do not work, and one must use a Lie group integrator.
In this thesis we have employed Lie group methods to solve differential equations on manifold. In this regard the main tool is to find associated Lie algebra of particular Lie group G, then finding the solution in Lie algebra setting and map the solution back from Lie algebra to its Lie group by appropriate map. This is because Lie group is a nonlinear space, while Lie algebra is linear space.
The plan of thesis is as follows: Chapter 1 contains a review of the relevant background of the work presented in this thesis. In Chapter 2, our main emphasis is on the study of some of the Lie group methods such as Magnus series expansion and Runge–Kutta–Munthe–Kaas methods. In Chapter 3, Lie group methods are used to solve differential equations evolving on a manifold and numerical results are displayed. The last chapter of this thesis is about the conclusion of our work.

1.1 Differential Manifold

- A ***manifold*** is a topological space which resembles Euclidean space locally. Thus for an n-dimensional manifold M, every point $p \in M$ has a neighborhood $Q \subseteq M$ that is homeomorphic to an open subset $\overline{Q} \subseteq \Re^n$, such that

$$\varphi : Q \to \overline{Q},$$

is a homeomorphism.

- A ***chart*** on a manifold M, is a pair (Q_i, φ_i).
- An ***Atlas*** on a manifold M, is a collection of all charts on a manifold M.
- A ***differential manifold*** is a manifold such that, for any two charts (Q_i, φ_i) and (Q_j, φ_j) such that the $Q_i \cap Q_j$ is nonempty, the map,

$$\varphi_{ij} = \varphi_j \circ \varphi_i^{-1} : \varphi_i(U_i \cap U_j) \to \varphi_i(U_i \cap U_j),$$

is infinitely differentiable for all pairs of i, j.

1.1.1 Examples

- Any open subset O of $\Re^n$ is a manifold of dimension n.
- The unit circle $S^1 = \{(x, y) \in \Re^2 \mid x^2 + y^2 = 1\}$ is a manifold of dimension two.
- The set $O(N)$ of all $N \times N$ orthogonal matrices is a manifold.

1.2 Lie Group

- A ***Lie group*** is a group G which is a differentiable manifold, and for which the product is a differentiable mapping $G \times G \to G$. Since a Lie group G is a group, then there is a group operation, $\cdot : G \times G \to G$, satisfying the following properties

  1. $g.(h.k) = (g.h).k \ \forall\, g, k \in G$, (Associativity)
  2. $e.g = g = g.e, \ \forall g \in G$, (Identity element)
  3. $g^{-1}.g = g.g^{-1} \ \forall\, g \in G$. (Inverse)

- Lie groups which are subgroups of general linear group $GL(n)$, the group of invertible $n \times n$ matrices with the usual matrix product as the group operation are called ***matrix Lie Groups***.

1.2.1 Examples of Matrix Lie Group

- The general linear group of all $n \times n$ matrices, given as

$$GL(n) = \{Y | detY \neq 0\}.$$

- The special linear group of all $n \times n$ matrices, given as

$$SL(n) = \{Y | detY = 1\}.$$

- The orthogonal group of all $n \times n$ matrices, given as

$$O(n) = \{Y | Y^T Y = I\}.$$

1.3 Lie Group Action

Let M be a differential manifold and G be the Lie group. A left Lie group action on M is a smooth mapping $\wedge : G \times M \to M$ such that [1],

1. $\wedge(e, p) = e.p = p, \quad \forall p \in M$ and the identity element $e \in G$,

2. $\wedge(g_1.g_2, p) = \wedge(g_1, \wedge(g_2, p)), \ \forall p \in M$, and $g_1, g_2 \in G$.

$\wedge : G \times M \to M$ is a local Lie group action. Moreover $\wedge$ is a transitive action on M [2]. That is for every pair $m_1, m_2 \in M$, there exists at least one element $g \in G$ such that $\wedge(g, m_1) = m_2$.

1.4 Tangent Bundle

- Let M be a d-dimensional manifold and suppose that $p(t) \in M$ is a smooth curve such that $p(0) = p$. A ***tangent vector*** at p is defined as

$$a = \left.\frac{dp(t)}{dt}\right|_{t=0}.$$

- The set of all tangents at p is called the ***tangent space*** at p and is denoted by $TM\big|_p$. It has the d-dimensional linear space structure, as if $a, b \in TM\big|_p$ then $a + b \in TM\big|_p$ and $\alpha a \in TM\big|_p$ for any real number α.

- The collection of all tangent spaces at all points $p \in M$ is called the ***tangent bundle*** of M and is denoted by $TM = \bigcup_{p \in M} TM\big|_p$.

1.5 Vector Field

- A ***vector field*** F is simply a map $F : M \to TM$, such that for a point $p \in M$, $F(p) \in T_pM$. The set of all vector field on M is denoted by $\chi(M)$.

1.6 Differential Equations on Manifold

- Matrix differential equations of the form

$$\dot{y}(t) = A(t, y)y, \ \ t \geq O, \ \ y(0) = y_0 \in O(n),$$

where $A : R^+ \times O(n) \to so(n)$, are called ***orthogonal matrix flows***.

- Matrix differential equations of the form

$$\dot{y}(t) = B(t, y)y - yB(t, y), \ \ t \geq O, \ \ y(0) = y_0 \in s(n),$$

where $B : \Re^+ \times s(n) \to so(n)$, are called ***isospectral matrix flows***.

1.7 Left and Right Trivialization

Most of the definitions given in this thesis are based on the right trivialization, for example differential equations on Lie group given by $\dot{y}(t) = A(t)y_0$, where $A(t) \in g$ and $y \in G$. One important difference between the left and right trivialization is that the left trivialization denotes calculations done in the space coordinates of a moving object, while the right trivialization denotes that of the body coordinates of the object. The space coordinate is a frame fixed in space, while the body coordinates is a frame fixed within the body, so that this frame is moving with the body, observed with respect to the space coordinates. Right trivialization can be calculated by

$$R_a(b) = b.a \quad R : G \times G \to G.$$

$$R_a^{'}(b) = b.a \quad R : G \times G \to G, \;\; R^{'} : g \to T_pG.$$

1.8 Lie Algebra

- Given a particular Lie group G, it has an associated ***Lie algebra*** $g = T_eG$, which is the tangent space at the identity e of the Lie group G. In particular, if G is finite-dimensional, then its Lie algebra g is a linear space of the same dimension.

- Lie algebra g is closed under the bilinear and skew-symmetric operation given by the ***Lie Bracket***, $[.,.] : g \times g \to g$, defined as,

  $$[u, v] = uv - vu \;\; \forall u, v \;\in\; g.$$

  This Lie bracket must satisfy the following axioms for all $u, v, w \in g$, and α,$\beta \in \Re$ as constants

  1. $[\alpha u + \beta v, w] = \alpha[u, w] + \beta[v, w]$,
  2. $[u, v] = -[v, u]$,
  3. $[u, [v, w]] + [v, [w, u]] + [w, [u, v]] = 0$.

  For $a \in G$, $v \in g = T_eG$, using right trivialization we get the following

  $$R'_a(v) = v.a, \tag{1.1}$$

  where $'$ denotes derivative. Hence, the tangent space at any point $a \in G$ can be found with $g \in T_eG$ using R'_a, as follow for all $a \in G$ [6]

  $$T_aG = R'_a(v) \;\; where \;\; v \in g.$$

1.8.1 Example

Consider the following rotation matrix,

$$Y = \begin{bmatrix} \cos t & -\sin t \\ \sin t & \cos t \end{bmatrix},$$

differentiate Y with respect to t

$$Y' = \begin{bmatrix} -\sin t & -\cos t \\ \cos t & -\sin t \end{bmatrix},$$

at $t = 0$

$$Y'|_{t=0} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix},$$

which is a skew symmetric matrix and is the associated Lie algebra $so(2)$ of Lie group $SO(2)$.

1.9 Lie algebra action

The Lie algebra action on manifold M is denoted by a smooth function $\lambda : g \times M \to M$. Each fixed element $v \in g$ generates a vector field on M, denoted by $\lambda_*(v) : M \to TM$,

$$(\lambda_* v)(p) = \frac{d}{dt}\lambda(tv, p)\big|_{t=0}, \quad \forall p \in M. \tag{1.2}$$

Where $v \in g$ corresponds to the vector field $\lambda_*(v)$, and vector field is known as the infinitesimal generator, then the infinitesimal generator of the action corresponding to $v \in g$ is denoted by [3],

$$v_m = (\lambda_* v).$$

Definition 1. *If $\wedge : G \times M \to M$ is a left Lie group action, then the Lie algebra action $\lambda : g \times M \to M$ is given by*

$$\lambda(v, p) = \wedge(\exp(v), p), \tag{1.3}$$

for $v \in g$ close to identity, and $p \in M$.
This is a connection between Lie algebra action and Lie group action.

Corollary 1. *Let $\wedge : G \times M \to M$ be the Lie group action, with Lie algebra g on the manifold M. Then the infinitesimal generator of the action corresponding to $v \in G$ is given by*

$$v_M(p) = \frac{d}{dt} \wedge (\exp(tv), p)\big|_{t=0}, \quad \forall p \in M. \tag{1.4}$$

This infinitesimal generator is the vector field $F(p)$ on M.

1.10 Equivariant Map

Let M and N be two manifolds, and let G be a Lie group acting on a point $x \in M$, by the Lie group action $\wedge_1 : G \times M \to M$, and also acting on a point $y \in N$ by $\wedge_2 : G \times N \to N$. A smooth map $f : M \to N$ is an equivariant map with respect to the actions $\wedge_1$ and $\wedge_2$ if, for all $g \in G$

$$f(\wedge_1(g, x)) = \wedge_2(g, f(x)), \quad where \;\; x \in M \; and \; y = f(x) \in N.$$

1.11 Exponential Map

One of the link between Lie group G and its associated Lie algebra g is the exponential map exp. it is defined as the map exp : $g \to G$, such that for all matrices $v \in g$

$$exp(v) = \sum_{k=0}^{\infty} \frac{v^k}{k!}.$$

The exponential map is a local diffeomorphism (smooth map with inverse) in the neighborhood of $0 \in g$, by the inverse function theorem [4]. Also, given the nature of the exponential map, it maps $0 \in g$ to the identity element $e \in G$.

1.12 Linear Adjoint operator

The Adjoint representation of the Lie group, $Ad_a : g \to G$ for all $a \in G$ is defined as

$$Ad_a(v) = ava^{-1}, \quad for \;\; a \in G, \;\; and \;\; v \in g,$$

while the adjoint operator $ad_u : g \to g$ is the derivative of the adjoint representation Ad_a, with respect to the element $a \in G$ at the identity $e \in G$, in the direction of $u \in g$ [5]. The adjoint operator $ad_u : g \to g$ is the Lie bracket

$$ad_u(v) = [u, v] = uv - vu, \quad \forall u, v \in g.$$

1.13 The Differential of the Exponential Map and its Inverse

For $u \in G$, the derivative of the exponential map is given by $exp(u + t)' : g \to T_{exp(u)}G$, such that when applied to $v \in g$

$$\frac{d}{dt} \exp(u + tv)\big|_{t=0} = \exp(u + tv)'\big|_{t=0} = R'_{\exp(u)} \circ d\exp_u(v). \tag{1.5}$$

Where $R'_{exp(u)} : g \to T_{exp(u)}G$. The differential of the exponential map $d\exp_u : g \to g$ is the linear map, such that when applied to $v \in g$

$$d\exp_u(v) = \frac{exp(ad_u) - Id}{ad_u}(v) = \sum_{k=0}^{\infty} \frac{1}{(k+1)!} ad_u^k(v), \tag{1.6}$$

and the inverse of $d\exp_u$ is

$$d\exp_u^{-1}(v) = \frac{ad_u}{\exp(ad_u) - Id}(v) = \sum_{k=0}^{\infty} \frac{B_k}{k!} ad_u^k(v), \tag{1.7}$$

where B_k are the Bernoulli numbers.

Chapter 2

Lie Group Methods

2.1 Runge-Kutta-Munthe-Kaas Methods

Runge-Kutta-Munthe-Kaas Methods are important class of methods that allow to use the classical Runge-Kutta (RK) methods to indirectly solve the differential equations evolving on Lie groups. Runge-Kutta-Munthe-Kaas methods, were first developed by Munthe-Kaas and Zanna [2]. On linear spaces, standard classical integrators will produce solutions that reside thereon. In general, a Lie group is not such a space. Its Lie algebra, however, is linear. We can exploit this fact by translating the differential equation on the Lie group, which we want to solve, to a corresponding equation on its Lie algebra. On the Lie algebra, we use classical integrators and translate the solution back to the original space, the Lie group. By these means, we assure that the solution will reside in the Lie group. A good candidate for the translation from a Lie algebra to a Lie group is the exponential map.

2.2 The RKMK Class

The main idea behind the RKMK class of integrators is to rewrite a differential equation evolving on M, into one that evolves on g. This is because g has structure of a vector space, and classical RK method can be applied to numerically solve this equivalent differential equation on g. To do this, an equivariant map will be constructed

$$\wedge(\Psi(\cdot), p) \to M \quad for \quad p \in M,$$

where g is a Lie algebra associated with the Lie group G acting on M, and the $\Psi : g \to G$, is coordinate map, then elements of $v \in g$, can be found such that infinitesimal generater can be constructed (Section 1.8), which describes the original differential equation in terms of the Lie group action

$$\wedge : G \times M \to M.$$

We want to solve the differential equation on M

$$\dot{y} = F(y), \quad t \geq 0, \; y(0) = y_0 \in M,$$

where at each point $y(t) \in M$ for $t \in R$, the vector field $F(y(t))$ can be written in terms of the infinitesimal generator v_M

$$F(y) = v_m(y) = \frac{d}{dt} \wedge (\exp(tv), y),$$

for some $v \in g$ which relates to the differential equation on M. Once v is found, the transformation to an equivalent system on g is done by solving the differential equation given by

$$\dot{u} = d\Psi_u^{-1}(v), \quad u(0) = u_0.$$

Where $\Psi : g \to G$ is a coordinate map and $u \in g$ with respect to the infinitesimal generator v_M.

Hence $u(t)$, for $t \in \Re$, is the solution of the equivalent differential equation evolving on g. Once $u(t)$ is approximated using the classical integrators like the RK methods, then the corresponding solution $y(t) \in M$ can be found by Lie group action with respect to the known point say $y_0 \in M$

$$y(t) = \wedge(\Psi(u(t)), y_0).$$

To relate the element $v \in g$ to the original differential equation on M, v is defined as the map $f : R \times M \to g$, with respect to point $y(t)$ on M, given by the Lie group action $\wedge : G \times M \to M$ [1]. That is

$$v(t) = f(t, \wedge(\Psi(u(t)), y(t))) \quad for\; t \in R.$$

This differential equation evolves on the homogeneous space M and can be described in terms of as an infinitesimal generator v_m.

2.3 Canonical Coordinates of First kind

Consider the equation

$$\dot{Y} = A(t, Y)Y, \quad Y(0) = Y_0. \tag{2.1}$$

The map

$$A \;\in g \to \;\exp m(A)Y_0 \;\in\; G, \tag{2.2}$$

is called canonical coordinates of the first kind. This defines a smooth invertible map between a neighborhood $0 \;\in\; g$ and $Y_0 \;\in\; G$ by the inverse function theorem generalized for manifolds. If we identify the Lie algebra g with a subset of $\Re^n$, the inverse of this map gives us a chart that is centered about $Y_0 \;\in\; G$.

In [6], it is given that for small $t \geq 0$ the solution of eq (2.1) is given by

$$Y(t) \;= \exp m(\Theta(t))Y_0, \tag{2.3}$$

where $\Theta(t) \;\in\; g$ satisfies the differential equation

$$\dot{Theta}(t) = dexp^{-1}_{\Theta(t)}(A(t, Y)), \;\; \Theta(0) = 0. \tag{2.4}$$

This can be seen as follows.

$$Y(t) = \exp m(\Theta(t))Y_0,$$

as a solution of eq (2.1). Now differentiate eq (2.3) to get

$$\dot{Y}(t) = d\exp_{\Theta(t)}(T\dot{h}eta(t))\exp(\Theta(t))Y_0 = d\exp_{\Theta(t)}(T\dot{h}eta(t))Y(t). \tag{2.5}$$

Compare eq (2.5) and eq (2.1) we get

$$A(t, y) = d\exp_{\Theta(t)}(T\dot{h}eta(t)),$$

$$\Rightarrow \quad T\dot{h}eta(t) = dexp^{-1}_{\Theta(t)}(A(t, Y)).$$

The map $dexp^{-1}_u : \mathbf{g} \to \mathbf{g}$ is expressed in terms of commutators through the infinite series as follows

$$dexp^{-1}_u(v) = \sum_{k=0}^{\infty} \frac{B_k}{k!} ad^k_u(v) = v - \frac{1}{2}[u, v] + \frac{1}{12}[u, [u, v]] + ...,$$

where $ad^0_u(v) = v$ and $ad^k_u(v) = [u, ad^{k-1}_u v]$ and B_k are Bernoulli numbers. The idea of Munthe-Kass is to approximate the solution of eq (2.4) by means of classical RK methods, and then transform the results back to $\mathbf{M}$ by setting

$$y_(n+1) = \exp(\Theta'(t))y_n,$$

where y_n and $y_{n+1} \in G$.

2.4 Magnus Series Expansions

Consider the matrix Lie group equation

$$\dot{y}(t) = A(t)y(t), \quad y(0) = y_0, \tag{2.6}$$

where $y(t) \in G$, the Lie group and $A(t) \in g$, corresponding Lie algebra. In the general non-commutative case, we want to search for a matrix function $\Omega(t)$ such that the solution $y(t)$ for eq (2.6) is described as

$$y(t) = exp(\Omega(t))y_0. \tag{2.7}$$

To find the explicit expression for $\Omega(t)$, another differential equation will be solved

$$\dot{\Omega}(t) = d\exp^{-1}_{\Omega(t)}(A(t)), \quad \Omega(0) = 0, \tag{2.8}$$

where $d\exp^{-1}$ is differential of inverse of exp function as given in Section 1.13.
To derive eq (2.8), let us assume eq (2.7) holds and we differentiate it with respect to t.

$$\frac{d}{dt}y(t) = \frac{d}{dt}(exp(\Omega(t))y_0),$$

$$\dot{y}(t) = R'_{exp(\Omega(t)} \circ d\exp_{\Omega(t)}(\frac{d}{dt}\Omega(t)).y_0,$$

$$= d\exp_{\Omega(t)}(\dot{\Omega}(t)).\exp(\Omega(t)).y_0. \tag{2.9}$$

Where R' is right trivialization. Comparing eq (2.6) with eq (2.7) and eq (2.9), it is found that

$$A(t) = d\exp_{\Omega}(t)(\dot{\Omega}(t)).$$

Inverting the above yields the desired relationship in eq (2.7).
eq (2.8) can further be expanded by the definition given in (Section1.13)

$$\dot{\Omega}(t) = A(t) - \frac{1}{2}[\Omega(t), A(t)] + \frac{1}{12}[\Omega(t), [\Omega(t), A(t)]] + ..., \tag{2.10}$$

an explicit approximation to $\Omega(t)$ can be found by applying Picard iterations [11]. This approximation is called the ***Magnus series expansion*** [7], and is derived according to the steps below.
Let Ω_0 be the initial estimate to the solution $\Omega(t)$, we can let our initial estimate be $\Omega_0 = 0$. After substituting this into eq (2.10), we are left with

$$\dot{\Omega}(t) = A(t), \quad \Omega(0) = \Omega_0 = 0,$$

and integrate with respect to t

$$\int_0^t \dot{\Omega}(\xi)d\xi = \int_0^t A(\xi)d\xi.$$

So, the first iteration, denoted by $\Omega_1(t)$ yields the following approximation to $\Omega(t)$

$$\Omega_1(t) - \Omega(0) = \int_0^t A(\xi)d\xi,$$

$$\Omega_1(t) = \int_0^t A(\xi)d\xi + \Omega(0) = \int_0^t A(\xi)d\xi. \tag{2.11}$$

Now, after substitution eq (2.11) into eq (2.10)

$$\dot{\Omega}(t) = A(t) - \frac{1}{2}[\Omega_1(t), A(t)] + \frac{1}{12}[\Omega_1(t), [\Omega_1(t), A(t)]] - ..., \tag{2.12}$$

where [ ] denotes Lie brackets as given in Section1.8.
Integrate eq (2.12) to find the second iterate $\Omega_2(t)$

$$\Omega_2(t) = \int_0^t A(\xi)d\xi - \frac{1}{2}\int_0^t [\Omega_1(\xi), A(\xi)]d\xi + \frac{1}{12}\int_0^t [\Omega_1(\xi), [\Omega_1(\xi), A(\xi)]]d\xi + ... \tag{2.13}$$

Similarly, substitution of eq (2.13) in eq (2.10) will be required to find third iterate $\Omega_3(t)$. Hence, the Magnus series expansion can be rewritten as a summation of terms $H_k(t)$, where each H_k is a linear combination of terms that include exactly $k+1$ integrals and k commutators

$$\Omega(t) = \sum_{k=0}^{\infty} H_k(t), \tag{2.14}$$

where the first few terms in eq (2.14) are given by

$$
\begin{aligned}
H_0(t) &= \int_0^t A(\xi_1)d\xi_1, \\
H_1(t) &= -\frac{1}{2}\int_0^t \left[\int_0^{\xi_1} A(\xi_2)d\xi_2, A(\xi_1)\right]d\xi_1, \\
H_2(t) &= \frac{1}{4}\int_0^t \left[\int_0^{\xi_1}\left[\int_0^{\xi_2} A(\xi_3)d\xi_3, A(\xi_2)\right]d\xi_2, A(\xi_1)\right]d(\xi_1) \\
&\quad + \frac{1}{12}\int_0^t \left[\int_0^{\xi_1} A(\xi_2)\right]d\xi_2, \left[\int_0^{\xi_1} A(\xi_3)d\xi_3, A(\xi_1)\right]\Bigg]d\xi_1.
\end{aligned}
$$

The terms in the Magnus series expansion are becoming increasingly complex for terms involving high values of k and each term is made out of integrals and commutators on the matrix function $A(t)$. A shorthand notation using rooted binary trees has been extensively developed by A. Iserles [6] to represent each term in the Magnus expansion. The idea is similar to the idea of John Butcher for representing order conditions of an RK methods by rooted trees as given in [6].

2.5 Rooted Trees

Some important terminologies of graph theory are,

- Graph: The pair $G = \langle V, E \rangle$, where $V = v_1, ..., v_r$ are vertices and $E \subseteq V \times V$ are the edges, represents a graph.
- A graph is connected if all vertices are connected by a path and it is a tree if such path is unique.
- Rooted tree: The pair $T = (G, w)$, where G is a tree and w (the root) is one of its vertices.
- A rooted tree admits a natural partial ordering of ancestor/successor and parent/child. Root has no parent. Vertices with no children are called leaves.
- A binary tree is a tree in which each vertex has at most two children. A strictly binary tree is a binary tree, where each vertex has exactly two children or is a leaf.

Each term in Magnus series expansion can be grouped together by k commutators and $(k+1)$ integrals. if we, for a moment, ignore the outer most integral from 0 to t in eq (2.13) then each term in the expansion has equal number of commutators and integrals. Such terms will be denoted as $C_\tau(\xi)$, their scalar constants as $\alpha(t)$, and the binary tree as $\tau \in T_k$, where set T_k includes all trees with the same number of k commutators and k integrals. After splitting the expansion once more, functions will have exactly k integrals and k commutators. Hence, approximation in eq (2.14) can be rewritten as

$$\Omega(t) = \sum_{k=0}^{\infty} H_k(t) = \sum_{k=0}^{\infty} \sum_{\tau \epsilon T_k} \alpha(\tau) \int_0^t \boldsymbol{C}_\tau(\xi) d\xi. \tag{2.15}$$

From the Picard iteration, it follows that every $\boldsymbol{C}_\tau$ can be constructed by the following composition rules.

1. $T_0 = \tau_0$ and $C_{\tau_0}(t) = A(t)$.
2. If $\tau_1 \in T_{m_1}$ and $\tau_2 \in T_{m_2}$ then there exists a $\tau \in T_{m_1+m_2+1}$ such that

$$\boldsymbol{C}_\xi = \left[\int_0^\xi \boldsymbol{C}_{\tau 1}(\xi_1) d\xi_1, \boldsymbol{C}_{\tau 2}(\xi) \right]. \tag{2.16}$$

The index sets become sets of rooted binary trees. In general, T_k represent different terms. Pictorially, vertical branch represents an integral and two branches joined by a common root represents commutator.

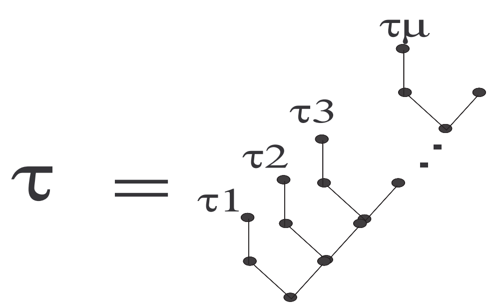
1. We identify T_0 with a rooted tree consisting of one vertex only, $\bullet$, and

$$\bullet \longrightarrow A(t)$$

2. If $T_{m_1} \ni \tau_1$ and $T_{m_2} \ni \tau_2 \to C_{\tau_2}$, then,

$$\boldsymbol{T}_{m_1+m_2+1} \ni \rightarrow \left[\int_0^t \boldsymbol{C}_{\tau_1}(\xi) d\xi, \boldsymbol{C}_{\tau_2}(t) \right],$$

this construction will give all terms of the Magnus expansion. Also, the constant $\alpha(\tau)$ can be defined by the rooted tree theory. Generally, a binary rooted tree τ representing the terms in the Magnus series expansion has the form, for $\mu \geq 1$,



with eq (2.16), the constant $\alpha(\tau)$ is calculated by [6]

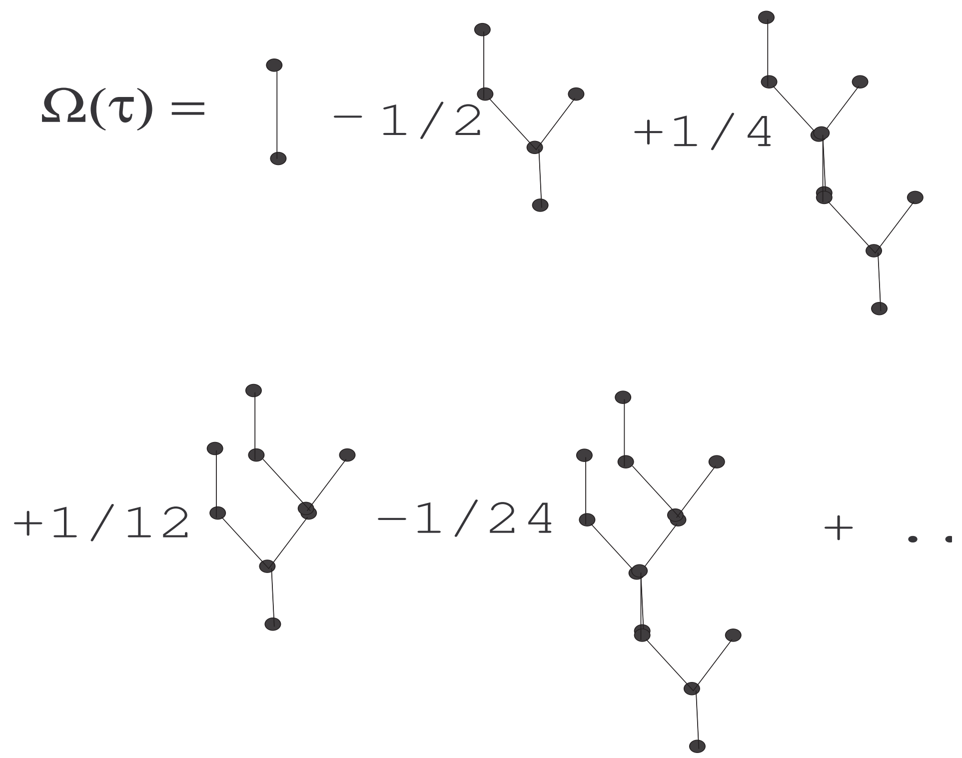
$$\alpha(\tau_0) = \alpha(.) = 1,$$

$$\alpha(\tau) = \frac{B_s}{s!} \prod_{i=1}^{s} \alpha(\tau_i), s \in Z_+,$$

where B_s are the Bernoulli numbers. Hence, higher order terms in the Magnus series expansion eq (2.15) can be derived with the help of rooted trees. Furthermore, for smooth matrix function $A(t)$, for $t \in Z_+$

$$\int_0^t C_\tau(\xi)d\xi = O(t^{k+1}) \Rightarrow \tau \in T_k. \tag{2.17}$$

In eq (2.15), $C_\tau(\xi)$ is integrated once more from 0 to t. Hence, to accurately represent the terms in the Magnus series expansion, we need to add a vertical branch to the bottom root of each tree. Now Magnus series expansion can be written in terms of the rooted trees, so eq (2.15) is given by,



2.5.1 Power m of a Rooted Tree

We have the rooted tree theory for the construction of terms in the Magnus series expansion up to any k number of commutators. Now we need to construct an approximation $\Omega_p(t)$ of a specific order p, such that

$$\Omega(t) \approx \Omega_p(t) + O(t^{p+1}).$$

From eq (2.16),

$$C_\tau(\xi) = \left[\int_0^\xi C_{\tau_1}(\xi_1)d\xi_1, C_{\tau_2}(\xi)\right].$$

If a tree $\tau \in T_k$ is of power m, where $m \geq 0$ is the smallest integer such that for a smooth matrix function $A(t)$ then,

$$C_\tau(t) = O(t^m).$$

If we denote F_m as the set of all rooted trees of power m, then the truncated Magnus series expansion of order p is given by,

$$\Omega_p(t) = \sum_{m=0}^{p-1} \sum_{\tau \in F_m} \alpha(\tau) \int_0^t C_\tau(\xi) d(\xi). \tag{2.18}$$

In the eq (2.18), the largest value of the power m is not equal to order p. This is because power m represents the order of the rooted tree associated with $C_\tau(\xi)$, and not the integral of $C_\tau(\xi)$. Another integration from 0 to t must be done in eq (2.18), so that the actual order p of $\Omega(t) \approx \Omega_p(t)$ is given by,

$$p = m + 1.$$

From eq (2.18), we know that $\tau \in T_k$, then the same tree τ is in the set F_m for the power $m \geq k$. To find m for the tree τ, we need to find the relationship between the power m for $C_\tau(t)$ and the powers m_1 and m_2 with respect to $C_{\tau_1}(t)$ and $C_{\tau_2}(t)$ in eq (2.16). This can be done by writing $C_{\tau_i}(t)$ as a series in power $O(t^{m_i})$, such that

$$C_{\tau_i}(t) = a_i t^{m_i} + b_i t^{m_{i+1}} + c_i t^{m_{i+2}} + ... \quad for \;\; i = 1, 2, ...,$$

and then substitute this series into eq (2.16). If $C_{\tau_1}(t)$ is of power m_1, such that $C_{\tau_1}(t) = O(t^{m_1})$, then the integral inside the commutator in eq (2.16) becomes

$$\begin{aligned} \int_0^t C_{\tau_1}(\xi) d\xi &= \int_0^t (a_i \xi^{m_i} + b_i \xi^{m_{i+1}} + c_i \xi^{m_{i+2}} + ...) d\xi \\ &= \frac{a_1}{m_1+1} t^{m_1+1} + \frac{b_1}{m_1+1} t^{m_1+2} + \frac{c_1}{m_1+1} t^{m_1+3} .... \end{aligned} \tag{2.19}$$

In this way, we can find the expansion for eq (2.16), given that $C_{\tau_1}(t)$ is of power m_1 and $C_{\tau_2}(t)$ is of power m_2

$$\begin{aligned} C_\tau(t) &= \left[\int_0^t C_{\tau_1}(\xi) d\xi, C_{\tau_2}(t) \right] \\ &= \left[\frac{a_1}{m_1+1} t^{m_1+1} + \frac{b_1}{m_1+1} t^{m_1+2} + \frac{c_1}{m_1+1} t^{m_1+3} ..., \right. \\ &\left. a_2 t^{m_2} + b_2 t^{m_2+1} + c_2 t^{m_2+2} + ... \right] \\ &= (\frac{[a_1, a_2]}{m_1+1}) t^{m_1+m^2+1} + (\frac{[a_1, b_2]}{m_1+1} + \frac{[b_1, a_2]}{m_1+2}) t^{m_1+m_2+2} \\ &+ (\frac{[a_1, c_2]}{m_1+1} + \frac{[b_1, b_2]}{m_1+2} + \frac{[c_1, a_2]}{m_1+3}) t^{m_1+m_2+3} + ... = O(t^{m_1+m_2+1}). \end{aligned}$$

That is, for $\tau_1 \neq \tau_2$, power m of $C_\tau(t)$ is given by

$$m = m_1 + m_2 + 1, \tag{2.20}$$

when $\tau_1 = \tau_2$, the power m of $C_\tau(t)$ can be improved by performing a similar substitution into eq (2.16)

$$\begin{aligned} C_\tau(t) &= \left[\int_0^t C_{\tau_1}(\xi)d\xi, C_{\tau_2}(t)\right] \\ &= \Big[\frac{a_1}{m_1+1}t^{m_1+1} + \frac{b_1}{m_1+1}t^{m_1+2} + \frac{c_1}{m_1+1}t^{m_1+3}..., \\ &a_2t^{m_2} + b_2t^{m_2+1} + c_2t^{m_2+2} + ...\Big] \\ &= \frac{a_1^2 - a_1^2}{m_1+1}t^{2m_1+1} + \frac{a_1b_1 - b_1a_1}{(m_1+1)(m_1+2)}t^{2m_1+2} + \frac{2(a_1c_1 - c_1a_1)}{(m_1+1)(m_1+3)}t^{2m_1+3} + ... \\ &= \frac{[a_1, b_1]}{(m_1+1)(m_1+2)}t^{2m_1+2} + \frac{2[a_1, c_1]}{(m_1+1)(m_1+3)}t^{2m_1+3} + ... = O(t^{2m_1+2}). \end{aligned}$$

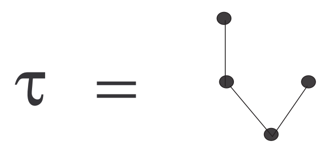
That is, for $\tau_1 = \tau_2$ the power m of $C_\tau(t)$ is given by,

$$m = 2m_1 + 2. \tag{2.21}$$

The tree of a single vertex representing $A(\xi)$ has power $m = 0$,

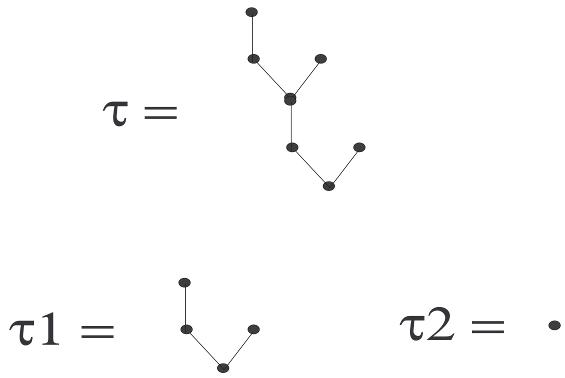
$$\tau = \bullet \in F_0, \quad where \;\; m = 0.$$

Starting with $k = 1$, we have the tree τ with subtree τ_1 and τ_2.

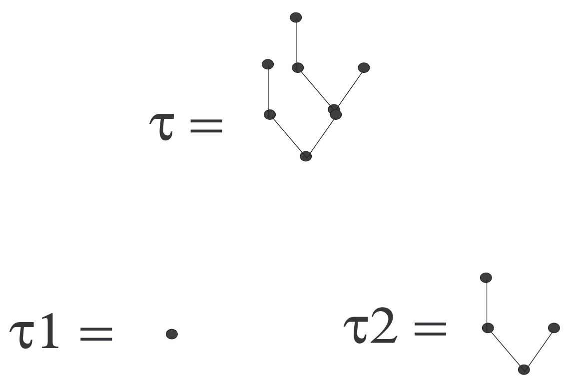


In this case, $\tau_1 = \tau_2$ and the powers $m_1 = m_2 = 0$. So by eq (2.21), the power m of $C_\tau(t)$ when $\tau \in T_1$ is $m = 2m_1 + 2 = 2$.

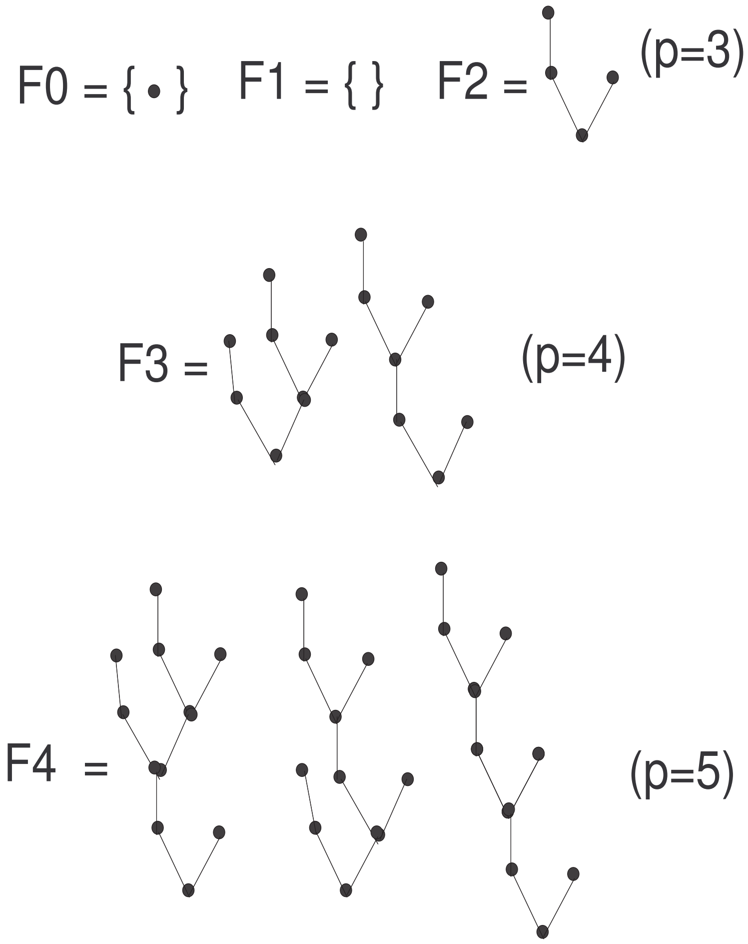
When $k = 2$, there are two trees in T_2. The first one is given by,



so that the power m of τ is τ is $m = m_1 + m_2 + 1 = 2 + 0 + 1 = 3$. Similarly, the second tree in T_2 is,



hence, for power m up to $m = 4$, the set F_m contains the following trees, which are of order $p = m + 1$ in the Magnus series expansion,



2.6 Time Symmetry and Order of the Magnus Series Expansion

Rooted trees belonging to the set F_{m+1} of power $m+1$ are also of order $p = m+1$. Hence, all the terms associated with trees from all sets of power up to F_{m+1} will be included to construct a Magnus series expansion of order p. Number of terms can further be reduced by considering time symmetry of the method [6].

Let $y(t) = \Psi_t(y_0)$ is a flow of differential equation of eq (2.6). The flow is time symmetric if $\Psi_{-t} \circ \Psi_t = I$, means that integrating from 0 to t and back to 0 yields the original initial value.

If

$$\Psi_t(y_0) = \exp(\Omega_p(t))y_0, \quad for \;\; t \geq 0,$$

then

$$\Psi_{-t} \circ \Psi_t = I.$$

Magnus series expansion that is truncated by order p also respects time symmetry [9]. Analytical time symmetric map S_t can be represented in the form $S_t = \exp(C(t))$, where

$C(t)$ is an expansion in the odd powers of t only [6]. This fact will also reduce the number of terms in the Magnus series expansion.

Theorem 1. *The function $\Omega_p(t)$ can be expanded in odd powers of t and*

$$\Omega(t) = \Omega_{2q-1}(t) + O(t^{2q+1}), \quad q \in Z_+.$$

Theorem 1 implies that for a Magnus expansion of order 4, only the terms in the sets up to F_2 are needed. This is because the linear combination of trees from F_3 is actually $O(t^5)$, and hence does not affect an order 4 approximation of $\Omega(t)$. For $q = 2$ in the Theorem 1

$$\Omega(t) = \Omega_3(t) + O(t^5).$$

So $\Omega_3(t)$ is in fact an order 4 approximation.

2.7 Multivariate Quadrature

To solve the multiple integrals in Magnus series expansion $\Omega_p(t)$, some sort of quadrature technique will be used.

2.7.1 Gauss-Legendre Quadrature

The Legendre polynomial of degree n, denoted by $P_n(x)$, is usually defined on the symmetric interval $[-1, 1]$. However, if we shift the interval to $[0, 1]$, then the Legendre polynomial, now denoted by $P_n^*(x)$ is shifted by $2x - 1$, so that $P_n^*(x) = P_n(2x - 1)$. The first few $P_n^*(x)$ are defined as

$$\begin{aligned}
P_0^*(x) &= 1, \\
P_1^*(x) &= 2x - 1, \\
P_2^*(x) &= 6x^2 - 6x + 1, \\
P_3^*(x) &= 20x^3 - 30x^2 + 12x - 1, \\
&. \\
&. \\
&. \\
&.
\end{aligned}$$

Lemma 1. *There exist polynomials $P_n^*(x) : [0, 1] \to \Re$, of degree n, for $n = 0, 1, 2, ...$ with the properties that,*

$$\int_0^1 P_m^*(x) P_n^*(x) dx = 0, \quad m \neq n.$$

$P_n^*(x)$ has n distinct real zeros in the open interval $(0, 1)$ for $n = 0, 1, 2, ...$

Theorem 1. *Suppose that c_i, for $i = 1, 2, ..., s$ are the roots of an s-degree Legendre polynomial $P_s^*(x)$, and that for each $i = 1, 2, ..., s$ the weight b_i are defined by,*

$$b_i = \int_0^1 \prod_{j=1 j\neq i}^{s} \frac{x - c_j}{c_i - c_j} dx.$$

If $\phi(x)$ is any polynomial of degree less than $2s$, then the Gauss-Legendre quadrature is given by,

$$\int_0^1 \phi(x)dx = \sum_{i=1}^{s} b_i \phi(c_i).$$

Methods having s stages and $2s$ order are called Gauss methods, an example of such Gauss method where $s = 2$ (2 stages) and order is 4 is presented as

$$\begin{array}{c|cc} \frac{1}{2} - \frac{\sqrt{3}}{6} & \frac{1}{4} & \frac{1}{4} - \frac{\sqrt{3}}{6} \\ \frac{1}{2} + \frac{\sqrt{3}}{6} & \frac{1}{4} + \frac{\sqrt{3}}{6} & \frac{1}{4} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array},$$

where c_i are zeroes of shifted Legendre polynomial $P_2^*(x)$ which are equals to $\frac{1}{2} \pm \frac{\sqrt{3}}{6}$. And b_i are the weight functions calculated by Langrange interpolating polynomials as follows,

$$b_i = \int_0^1 \prod_{j=1 j\neq i}^{s} \frac{x - c_j}{c_i - c_j} dx.$$

It can be seen that

$$b_1 = \int_0^1 \frac{x - c_1}{c_2 - c_1},$$

$$b_2 = \int_0^1 \frac{x - c_2}{c_1 - c_2}.$$

After substituting the values of c_i, from above, we have

$$b_1 = \frac{1}{2}, \qquad b_2 = \frac{1}{2}.$$

2.7.2 Multivariate Gauss-Legendre Quadrature

In most realistic cases, practical implementation of Magnus series requires the replacement of integrals by quadrature. So the numerical values of the terms in the truncated Magnus series expansion of order p can be found by applying multivariate quadrature. Similarly to the one dimensional integration, the quadrature for the multiple dimensional integration is given by the weighted sum of the multiple variable function evaluations. As a result, the weight b_i is also given by the multiple integration of the product of the Langrange interpolation polynomials. Let that each integral in the Magnus series expansion is of the form,

$$I(h) = \int_S L(A(\xi_1), A(\xi_2), ..., A(\xi_s))d\xi_s...d\xi_1, \tag{2.22}$$

where L is a multiple variable function, s is the number of integrals in the expression, and h is the stepsize. S is the integration region which is of the form polytope,

$$S = \{(\xi_1, \xi_2, ...\xi_s) \in \Re : \xi_1 \in [0\ h], \xi_l \in [0\ \xi_{m_l}], l = 2, 3, ..., s, \}$$

where $m_l \in 1, 2, ..., l-1$, for $l = 1, 2, ..s$. For example,

$$I_1 = \int_0^h A(\xi_1) d\xi_1 : \quad S_1 = \{0 \leq \xi_1 \leq 1\}, \text{(Over a line)}$$

$$I_2 = \int_0^h \int_0^{\xi_1} [A(\xi_1), A\xi(\xi_2)] d\xi_2 d\xi_1 : \quad S_2 = \{0 \leq \xi_1 \leq 1, 0 \leq \xi_2 \leq \xi_1\}, \text{(Over a triangle)}$$

$$I_3 = \int_0^h \int_0^{\xi_1} \int_0^{\xi_2} [[A(\xi_1), A(\xi_2)], A(\xi_3)] d\xi_3 d\xi_2 d\xi_1 : \quad S_3 = \{0 \leq \xi_1 \leq 1, 0 \leq \xi_2, \xi_3 \leq \xi_1\}.\text{(Over a sphere)}$$

Moreover, the integrand is, in each case, a function of the form

$$Ł(A(\xi_1), A(\xi_2), ...A(\xi_m)),$$

where L is multilinear. It has been proposed in [6] to use the quadrature formula

$$\int_{hS} Ł(A(\xi_1), A(\xi_2), ...A(\xi_s)) d\xi_s ... d\xi_1 \approx h^m \sum_{l \in C_m^v} b_l Ł(A(hc_{l_1}), A(hc_{l_2}), ...A(hc_{l_s})), \quad (2.23)$$

where $c_1, c_2, ...c_\nu$, are distinct points in $[0, 1]$ and C_s^ν is the set of all the combinations of s-tuples from the set $\{1, 2, ...\nu\}$. The weights b_l can be evaluated explicitly by the formula,

$$b_l = \int_S \prod_{i=1}^{s} \lambda_i(t_{l_i}) dt_m ... dt_1, \quad l \in C_s^\nu,$$

where $\lambda_k \in P_{\nu-1}[t]$ is the kth cardinal polynomial of Lagrange interpolation at the nodes $c_1, c_2, ...c_\nu$. Suppose that

$$\int_0^1 t^{k-1} c(t) dt = 0, \quad k = 1, 2, ...s,$$

where

$$c(t) = \prod_{i=1}^{\nu} (t - c_i).$$

Then the quadrature formula eq (2.23) is of order $\nu + s$. In other words, the order of the above multivariate quadrature is exactly the same as of the classical univariate quadrature with the same nodes. In other words, choosing $c_1, c_2, ...c_\nu$ as Gauss Legendre quadrature points in $[0, 1]$ results in order 2ν in eq (2.23) for all integrals necessary for the evaluation of truncated Magnus series. As an example, let

$$A(1) = A((\frac{1}{2} - \frac{\sqrt{3}}{6})h), \quad A(2) = A((\frac{1}{2} + \frac{\sqrt{3}}{6})h).$$

be the value of matrix A evaluated at the nodes of the fourth-order Gauss Legendre quadrature in $[0, 1]$, hence we obtain

$$\begin{aligned}
I_1 &\approx \frac{1}{2}h(A_1 + A_2),\\
I_2 &\approx \frac{\sqrt{3}}{6}h^2[A_2, A_1],\\
I_3 &\approx h^3[[A_2, A_1], (\frac{3}{80} + \frac{\sqrt{3}}{16})A_1 - (\frac{3}{80} - \frac{\sqrt{3}}{16})A_2],\\
I_4 &\approx -h^3[(\frac{3}{80} - \frac{\sqrt{3}}{16})A_1 - (\frac{3}{80} + \frac{\sqrt{3}}{16})A_2, [A_2, A_1]].
\end{aligned}$$

Although the quadrature formula (2.23) leads to remarkable savings in the number of function evaluations, it might result in considerable cost of linear algebra, since the number of terms in the sum behaves like ν^m and the computation of each such term requires $m-1$ commutators. However, very considerable reduction in the expense of linear algebra takes place when the special structure of the Lie algebra g is taken into account. To conclude this section, we combine the Magnus expansion (2.14) with the multivariate quadrature to present a fourth-order method for the solution of the differential equation,

$$\begin{aligned}
A_1 &= A(t_n + (\frac{1}{2} - \frac{\sqrt{3}}{6})h),\\
A_2 &= A(t_n + (\frac{1}{2} + \frac{\sqrt{3}}{6})h),\\
\Omega_4 &= \frac{1}{2}(A_1 + A_2) + \frac{\sqrt{3}}{6}[A_2, A_1],\\
y_{n+1} &= \exp(\Omega_4)y_n.
\end{aligned}$$

.

Chapter 3

Numerical Experiments

This chapter deals with the applications of the Lie group integrators namely Magnus series expansion and the Runge-Kutta-Munthe-Kaas (RKMK) methods, to solve matrix differential equations on the manifold also known as Lie group equation. The result from the Lie group integration are then compared with the results from explicit Runge-Kutta (RK) methods, the Gauss methods, and the built in integrator ODE45 from MATLAB. All experiments in this chapter are performed using a fixed stepsize h. All numerical methods considered in this chapter are of order 4.

3.1 Differential Equation on the Sphere

Consider differential Equation on the sphere is given by,

$$\frac{dy}{dt} = \begin{bmatrix} 0 & t & -0.4\cos t \\ -t & 0 & 0.1t \\ 0.4\cos t & -0.1t & 0 \end{bmatrix} y(t) = A(t)y(t), \quad y(0) = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}.$$

We solve this differential equation by the Magnus series expansions, Gauss, and explicit RK method. The solution $y(t) \in \Re^3$ in eq (3.1) is a vector of unit length, evolving on the unit sphere. That is the solution vector $y(t)$ that rotates around the spherical surface with respect to its origin, and naturally, the homogeneous manifold in this case is the unit sphere. In this differential equation Lie algebra is defined by the matrix $A(t)$, which in this case is $\mathbf{so}(3)$.

We want to integrate eq (3.1) for numerical experiments with the given initial condition $y(0)$, over the time interval $t = [0, 64]$ with a constant stepsize of $h = 1/20$ for the 3 integrators explicit RK, Gauss and Magnus. Then we will integrate the same problem with MATLAB's ODE45 for comparison.

The results are shown in Figures 3.1, 3.2, and 3.3,

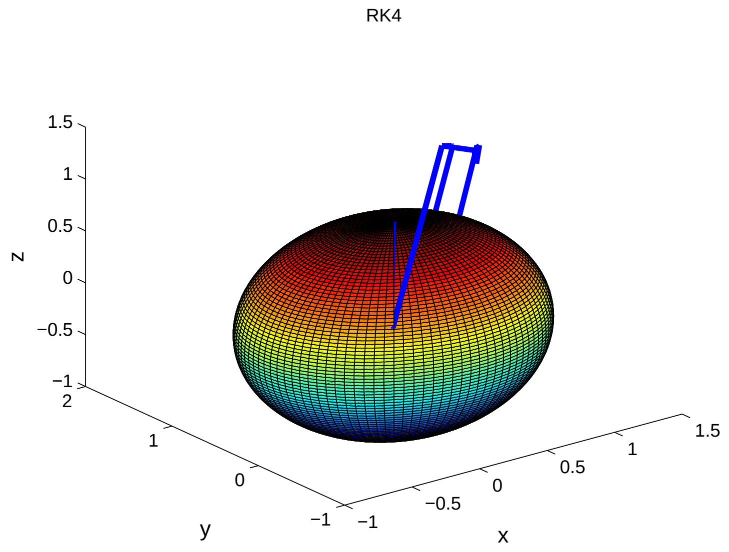


Figure 3.1: Solution of eq (3.1) from RK4 plotted on the surface of a unit sphere.

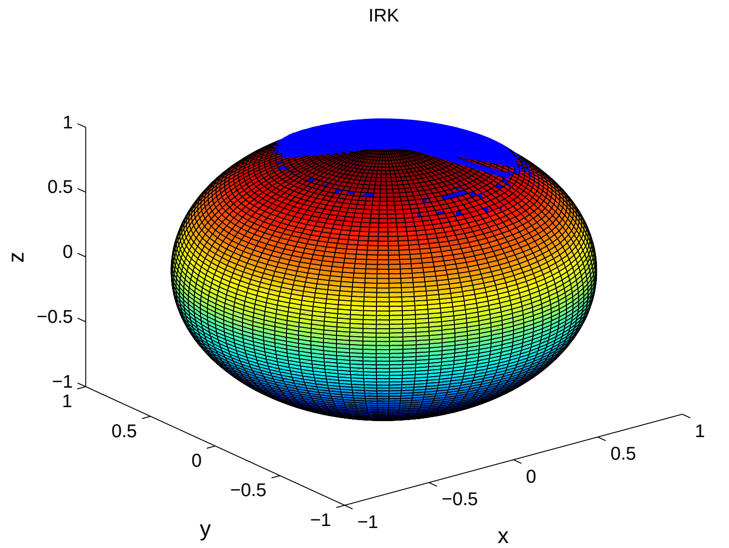


Figure 3.2: Solution of eq (3.1) from Gauss plotted on the surface of a unit sphere.

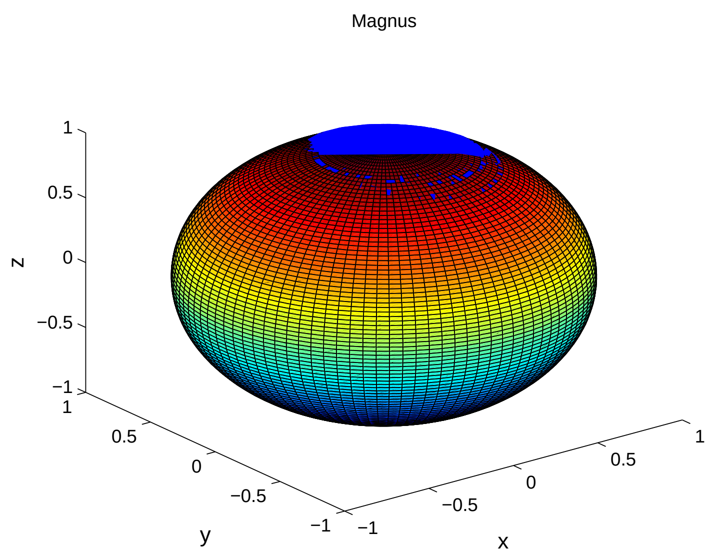


Figure 3.3: Solution of eq (3.1) from Magnus plotted on the surface of a unit sphere.

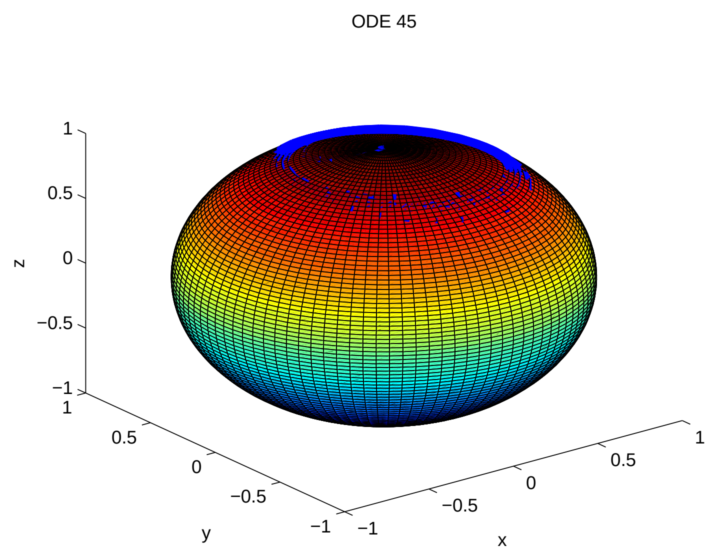


Figure 3.4: Solution of eq (3.1) from ODE45 plotted on the surface of a unit sphere.

From the Figures 3.1, 3.2, and 3.3, it is clear that solutions from explicit RK integrator drift away from the surface of the sphere, while solutions from the Gauss and Magnus stay on the sphere.

One of the advantage of using the Lie group methods such as the Magnus series expansion, for solving this type of differential equations on the sphere is that the Lie group action $\wedge$ produces special orthogonal matrices, which, when multiplied to the vector $y(t) \in \Re^3$, preserves its length in the rotation, so that solution $y(t)$ will always remain on the sphere.

3.2 Lorenz Equation

The Lorenz equation describes a complex, 3 dimensional dynamical system with 3 parameters σ, ρ and β. This system has the form

$$\dot{x} = \sigma(y - x), \tag{3.1}$$

$$\dot{y} = \rho x - y - xz, \tag{3.2}$$

$$\dot{z} = xy - \beta z. \tag{3.3}$$

These equations are nonlinear with two quadratic terms xy and xz. Solutions in the Lorenz equation are sensitive to initial conditions, and slight changes to the values of the solution in any one of the 3 components can cause drastic difference in the solution at a later time. For solving the Lorenz equations, when using the RKMK method, the manifold M is defined as the domain of groups acting on themselves, the Lie Group G is simply $\Re^n$, and the Lie algebra is also $\Re^n$ and abelian. The Lie algebra action λ is given by the standard vector addition, $\lambda(v, y) = v + y$ for v and $y \in \Re^n$, and so the mapping $f : \Re^n \times \boldsymbol{M} \to \mathbf{g}$ is simply $f : \Re^n \to \Re^n$ for this setting,

$$\dot{y}(t) = F(y),$$

where $F : \Re^n \to \Re^n$.

So the Lorenz equations can be solved by the RKMK method in its present form in eq (3.1) to eq (3.3). Also, because the Lie algebra is abelian, the adjoint operator $ad_u^0(v) = v$ and $ad_u^n(v) = 0$ for $n \geq 1$. Then, the inverse of the differential of the exponential map $d\exp_u^{-1}(v) = v$ Hence, the entire RKMK reduces to the classical Runge-Kutta method.

Now, we will follow the approach of Lorenz [8] and will use particular case when $\sigma = 10$, $\beta = \frac{8}{3}$, and $\rho = 28$. With initial condition $Y(t)$ as $Y(0) = (17, -21, 54)$, and integrate over the interval $t = [0, 10]$ with a constant stepsize of $h = 1/20$. The integrators used for solving this example are explicit RK method, Gauss method, the RKMK method, and $ODE45$.

Famous Lorenz butterfly appears with all the four methods after plotting the results.

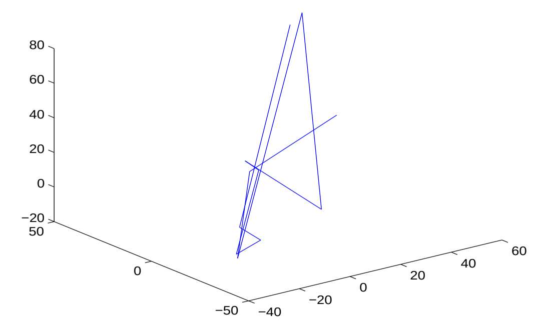


Figure 3.5: 3 dimensional graph showing the Lorenz attractor from explicit RK4, when solving eq (3.1) to (3.3).

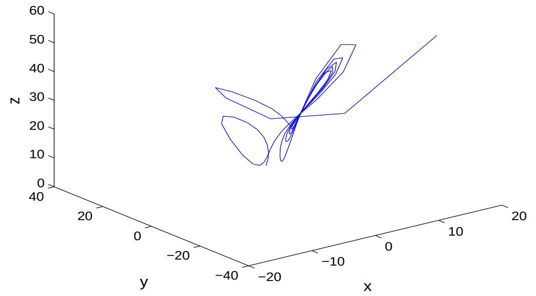


Figure 3.6: 3 dimensional graph showing the Lorenz attractor from Gauss, when solving eq (3.1) to (3.3).

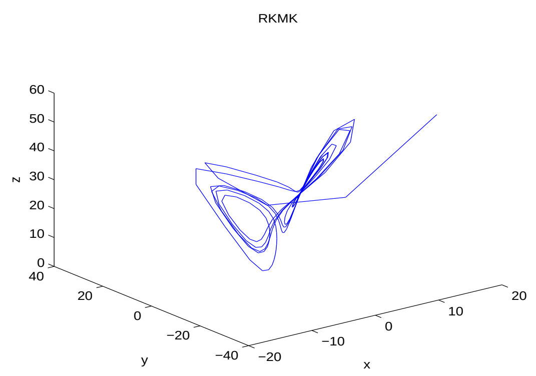


Figure 3.7: 3 dimensional graph showing the Lorenz attractor from RKMK, when solving eq (3.1) to (3.3).

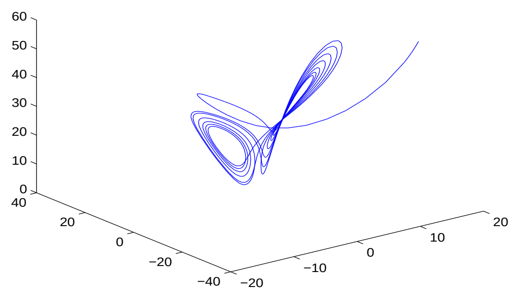


Figure 3.8: 3 dimensional graph showing the Lorenz attractor from ODE45, when solving eq (3.1) to (3.3).

Although all four attractors have the same form in three dimensions, the behavior of trajectories from different methods is not the same.

3.3 Harmonic Oscillators

Unforced harmonic oscillators can be modeled by the second order homogeneous differential equation,

$$m\frac{d^2y}{dt^2} + b\frac{dy}{dt} + ky = 0, \tag{3.4}$$

where $m, k \geq 0$, and $b \geq 0$. If $b = 0$ then the system is undamped. However, if $b > 0$, then different types of behavior are possible. For the harmonic oscillator equation, the characteristic equation is

$$\frac{-b \pm \sqrt{b^2 - 4mk}}{2m}.$$

There are three different cases for the roots of the characteristic equation [8],

- if $b^2 - 4mk < 0$, then there will be complex roots and the harmonic oscillator is said to be under damped. In this case, the system oscillates about its equilibrium position.
- if $b^2 - 4mk = 0$, then there will be repeated roots and the oscillator is critically damped.
- if $b^2 - 4mk > 0$, then the roots are real and distinct, and the oscillator is said to be over-damped and system will move to its equilibrium position without any oscillations.

Consider the second order homogeneous differential equation as an initial value problem given by,

$$\frac{d^2y}{dt^2} + 0.01t\frac{dy}{dt} + y = 0 \quad y(0) = -1, \;\; \dot{y}(0) = 2, \tag{3.5}$$

with $m = 1$, $k = 1$, $b = 0.01t$. To solve eq (3.5) with numerical integrators, this second order differential equation as a system of first order differential equations can be solved by using the substitution $dy/dt = v$, and a vector $Y(t) = [y(t), v(t)]$

$$\dot{Y}(t) = A(t)Y(t),$$

where the matrix $A(t)$ and the initial condition $Y(0)$ are given by,

$$A(t) = \begin{bmatrix} 0 & 1 \\ -1 & -0.01t \end{bmatrix}, \quad Y(0) = \begin{bmatrix} -1 \\ 2 \end{bmatrix}.$$

This system will be solved with the explicit RK4, Gauss method and Lie group methods like Magnus series expansion method, with fixed step size $h = 1/20$.

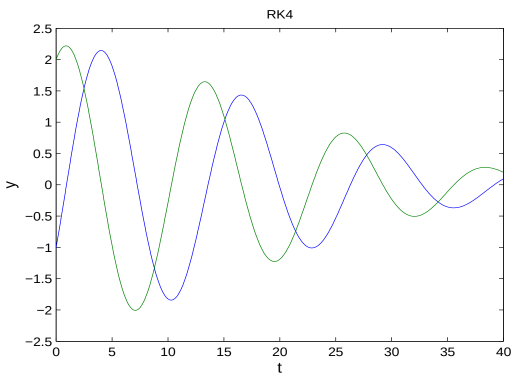


Figure 3.9: Solution of underdamped system in eq (3.5) for the interval $t \in [0, 40]$ using RK4.

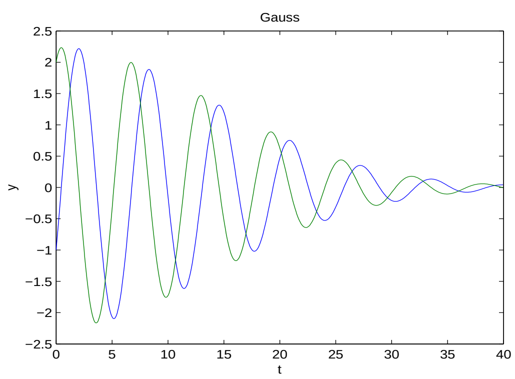


Figure 3.10: Solution of underdamped system in eq (3.5) for the interval $t \in [0, 40]$ using Gauss.

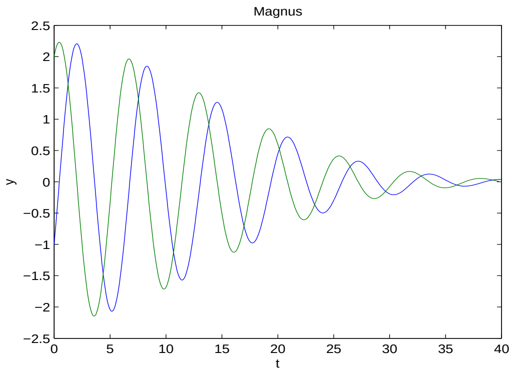


Figure 3.11: Solution of underdamped system in eq (3.5) for the interval $t \in [0, 40]$ using Magnus.

If we compare results from the 3 integrators and that of ODE45, the accuracy archived from the Magnus method is higher than that of the Runge-Kutta or the Gauss methods of same order.

Chapter 4

Conclusions

Chapter 1 introduces the basic concepts of manifolds, Lie groups and Lie algebra. It also includes Lie group actions and exponential map. Chapter 2 presents a discussion of the Magnus series expansion and Runge-Kutta-Munthe-Kaas (RKMK) method for solving linear matrix differential equations. RKMK is an important class of methods, because it allows to use the classical Runge-Kutta methods to solve differential equations on manifolds, while preserving the group structure of the manifold associated with the underlying dynamical system.

Chapter 3 contains three numerical experiments using the Magnus series expansion and RKMK method for solving Lie group equations. Observations were made regarding their performance in comparison to the classical integrators such as explicit Runge-Kutta method, and the implicit Gauss method.

In Chapter 2, the Magnus series expansion was introduced to solve the linear matrix differential equation of the form $\dot{y}(t) = A(t)y$, where the matrix A is dependent on time t only. However, when $A = A(t, y)$, then the problem becomes nonlinear and collocation methods must be used to solve such differential equations. It is something on which future work can be done.

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