MAGNUS' EXPANSION AS AN APPROXIMATION TOOL FOR ODES

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A

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Abstract

Magnus' expansion approximates the solution of a linear, nonconstant-coefficient system of ordinary differential equations (ODEs) as the exponential of an infinite series of integrals of commutators of the matrix-valued coefficient function. It generalizes a standard technique for solving first-order, scalar, linear ODEs. However, much about the convergence of Magnus' expansion and its efficient computation is not known.

In this thesis, we describe in detail the derivation of Magnus' expansion. We review Iserles' ordering for efficient calculation. We explore the convergence of the expansion and we apply known convergence estimates. Finally, we demonstrate the expansion on several numerical examples, keeping track of convergence as it depends on parameters. These examples demonstrate the failure of current convergence estimates to correctly account for the degree of commutativity of the matrix-valued coefficient function.

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1 Introduction

In various engineering and physics applications, often a system of coupled ordinary differential equations arises when attempting to model the physical system being studied. Numerous techniques and methods have been used to find solutions, whether they are analytic or numerical. Examples include finding an integrating factor to create an exact differential; Runge-Kutta numerical methods for computing a solution; and Picard iteration for an approximate analytical solution.

Recently, an alternative method for numerical computation based on an approximate analytical solution has been proposed [1], [18]. This method's inspiration dates to the work done by Wilhelm Magnus in the 50's.

Using this method, we examine the possibility for finding and approximating a fundamental solution for a general linear differential equation

$$D_t Y(t) + A(t)Y(t) = \mathbf{0}, \qquad Y(t_0) = Y_0 \tag{1.1}$$

where $A(t)$ is a matrix-valued function, entry-wise continuous in the variable t, and $Y(t)$ is a matrix-valued function of t with each entry continuous.

We are principally concerned with the analytical aspects of what's known as Magnus' expansion. Much recent work has been concerned with the numerical aspects of Magnus' expansion. We diverge from the work of [1] who develop a time-stepping numerical algorithm for solution to certain systems of ODEs. Instead, we address the limits of 'long-time' use of Magnus' expansion. While the numerical implementation of Magnus' expansion is quite powerful, the analytical foundations for implementing the numerical algorithm are far from being well established. We will find analytical approximations e^{Ω_m} to the solution of (1.1) (Magnus' expansion), for which we want to answer four important questions. These questions are:

1. For what values of t does $\Omega_m(t)$ converge to $\Omega(t)$ as $m \to \infty$?

2. If $\Omega_m(t)$ converges, how close is $\Omega_m(t)$ to $\Omega(t)$ for a given m?

3. For what values of t is $e^{\Omega(t)} = \Phi(t)$, the fundamental solution to (1.1)?

4. Exactly how close is $e^{\Omega_m(t)}$ to $\Phi(t)$ for a given m?

This thesis provides approximate answers to these questions in several examples; furthermore, this thesis develops the minimum theoretical framework necessary to attack these questions.

Notation. *For this paper, let M_n denote $n \times n$ matrices with complex entries. We use the notation D_t for $\frac{d}{dt}$, as well as D_t^n for $\frac{d^n}{dt^n}$. We will use m, n, k, p, q for natural numbers $\mathbb{N}$, and A, B, Ω, W, X, Y for elements of M_n. We use $[A, B]$ as the Lie commutator of $A, B \in M_n$, defined by $[A, B] = AB - BA$.*

1.1 Motivation: Systems Arising from Machining Applications

Suppose one wants to find an approximation to the system of delay-differential equations (DDE's), with l fixed delays $\tau_j > 0$,

$$D_t x(t) + A(t) x(t) + \sum_{j=1}^{l} B_j(t) x(t - \tau_j) = \mathbf{0} \tag{1.2}$$

where $x(t) \in \mathbb{R}^n$ and A, B_j are continuous "$n \times n$ matrix functions" of time $t \geq 0$. Specifically, for systems of equations derived from models of machining processes, the functions A and B_j are periodic functions of time, due to the nature of machining [27].

To solve this DDE, we first consider finding the fundamental solution to the homogeneous first order linear differential equation

$$D_t x(t) + A(t) x(t) = \mathbf{0} \tag{1.3}$$

If we find a fundamental solution $\Phi(t)$ to (1.3) with $\Phi(t_0) = \mathbf{I}$, then (1.2) can be solved by a "variation-of-parameters" [8] method; yielding a solution

$$x(t) = \Phi(t) x(t_0) + \sum_{j=0}^{l} \int_{t_0}^{t} \Phi(t) \Phi^{-1}(s) B_j(s) x(s - \tau_j) ds \tag{1.4}$$

For the equations appearing in machining applications, the coefficients are periodic functions $A(t)$ and $B_j(t)$, with T such that $A(t) = A(T+t)$ and $B_j(t) = B_j(T+t)$ for all j. From Floquet theory, in the ODE case ($B_j = 0$ for all j) it can be shown that the solution $\Phi(t)$ is stable if at the end of the principal period T, $\Phi(T) = e^{AT}$, then the real parts of the eigenvalues of A are all negative. Finding $\Omega(t)$, stability is determined by the eigenvalues of $\Omega(t)$ having real part < 0, in contrast to stability determined from the eigenvalues of $e^{\Omega(t)}$ having magnitude < 1.

In order to determine stability for the general DDE case (1.2), the goal is to compute a reasonably accurate approximation of $\Phi(t)$. If we can find $\Omega(t)$, such that $\Phi(t) = e^{\Omega(t)}$, in some neighborhood of t_0, then we can determine the stability of the DDE by finding the eigenvalues of $\Omega(t)$, giving us stability for $\Phi(t)$ in (1.4). This is the main motivation for finding a fundamental solution of the form $e^{\Omega(t)}$.

1.2 Geometric Integration

Traditional numerical analysis approaches a differential equation with the idea that the derivative of a function is a *local phenomenon*. That is, for the differential equation

$$D_t f(t) = g(t, f(t)), \; f(0) = f_0 \tag{1.5}$$

we approximate

$$D_t f(t) \approx Dctz(f, h, f_0)$$

with $Dctz(f, h, f_0)$ some discretization of $D_t f$ at f_0 using f and a step size of h in t. Then, through a careful selection of step size and discretization, the solution is (hopefully) accurate at some predefined level.

While traditional numerical analysis techniques succeed in producing small error for each step, the approach of geometric integration suggests better approximations for larger time scales. The approach of geometric integration to the differential equation (1.5) is to identify some *global* property of $f(t)$, such as some constraint on the problem like a conserved quantity (energy, momentum, etc...) or some other intrinsic property. Then, using the global property as a guide, devise some numerical scheme which minimizes the error while preserving this global property.

The geometric integration technique of Lie-group methods, of which Magnus' expansion is one, takes advantage of the symmetries of (1.5) [18]. Let's consider an ODE which evolves on the unit circle (the Lie group S^1). An example would be where $D_t r = 0$ and $D_t \theta = f(t, \theta)$ with (r, θ) the polar coordinates of S^1, for instance in the concrete example of a pendulum. Notice that the differential equation is described nicely in polar coordinates (only a simple scalar equation needs to be solved), while in euclidean coordinates (x, y) we have a pair of nonlinear coupled differential equations with an additional constraint. Consider the numerical scheme applied to the differential equations in euclidean coordinates. With a standard numerical scheme, we would propagate errors in both the x and the y directions, not necessarily remaining within the constraint that $x^2 + y^2 = 1$.

But suppose instead that we had applied a numerical scheme to the differential equation in polar coordinates. With this approach, any error of the solution would only be in the θ coordinate and there would be no error in the r coordinate, since it's change for any (realistic) scheme would remain 0. In this way, the solution to the differential equation could satisfy the constraint of remaining on the unit circle. The geometry of the numerical solution remains consistent with any analytical solution for θ.

The significance of the Lie theory is that the symmetries of an ODE are usually described by a Lie group, a manifold. No matter how nonlinear the manifold, its tangent space (at the algebraic identity, the Lie algebra) is a linear vector space. For Magnus' expansion, the main idea is the analytic approximation of the solution to a linear, first order ODE can be most easily done by first finding a solution to the associated ODE in the tangent space, then analytically approximating the solution to the original ODE through the use of the exponential map (the map that takes the Lie algebra to the Lie group).

2 General Theory of ODEs

A general system of ordinary differential equations is

$$D_t Y(t) + f(Y(t), t) = \mathbf{0} \tag{2.1}$$

where $Y(t) \in \mathbb{R}^n$ is a vector-valued function of t. In this thesis we deal primarily with linear systems (1.1) and their fundamental solutions. The fundamental solution has the properties: 1)$\Phi(t)$ is an $n \times n$ matrix-valued function of time, 2)$D_t\Phi(t) = A(t)\Phi(t)$ and 3)$\Phi(t_0) = I$, the $n \times n$ matrix identity, yet we are also concerned with non-linear systems given by (2.1).

2.1 Existence and Uniqueness of Solutions

First Order Linear Scalar ODEs

Consider the simple linear scalar homogeneous ordinary differential equation

$$D_t y(t) + a(t)y(t) = 0 \quad \text{with } y(t_0) = c_0. \tag{2.2}$$

The solution of (2.2) on the interval $[t_0, t_f)$ is given by the function

$$y(t) = c_0 e^{-\int_{t_0}^{t} a(\xi)d\xi} \tag{2.3}$$

This solution can be found by 1) the method of finding an integrating factor so that (2.2) is reduced to the derivative of a constant (easily integrated), or by 2) moving $D_t y(t)$ to the other side of the equation, then integrating with respect to dt.

A single, first order linear scalar ODE is fairly simple and doesn't account for the differential equations that arise in most situations. Many other possibilities exist and are encountered quite frequently; for instance, n_{th} order ODEs, coupled systems, etc... Countless examples of second order scalar equations occur naturally in the application of Newton's laws of motion, and higher order coupled systems occur when studying the Hamiltonian of a system.

N*th* Order Linear Scalar ODEs

Consider now the n*th* order linear scalar homogeneous ordinary differential equation

$$D_t^n y(t) + p(t)D_t^{(n-1)} y(t) + ... + b(t)D_t y(t) + a(t)y(t) = 0 \qquad (2.4)$$

with initial conditions

$$y(t_0) = c_0, y(t_0) = c_1, ..., D_t^{(n-1)} y(t_0) = c_{n-1} \text{ where } c_j \in \mathbb{R} \qquad (2.5)$$

In this case, the solution isn't found as easily as the first order scalar equation (2.2). Finding an integrating factor is, for nearly all cases, impossible to find analytically.

Proposition 1 *Equation (2.4) is equivalent to a matrix formulation of equation (2.2). The equivalence is if $y(t)$ is a solution of (2.4), then the vector $Y(t) = \left(y(t), D_t y(t), ..., D_t^{(n-1)} y(t)\right)^T$ of n-1 derivatives of $y(t)$, is a solution of (1.1), where*

$$A(t) = \begin{pmatrix} 0 & 0 & \cdots & 0 & 1 \\ 0 & 0 & \cdots & 1 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 1 & \cdots & 0 & 0 \\ -a(t) & -b(t) & \cdots & -n(t) & -p(t) \end{pmatrix} \text{ and } Y(t_0) = \left(y(t_0), D_t y(t_0), ..., D_t^{(n-1)} y(t_0)\right)^T.$$

The question of existence of solutions for first and n*th* order linear ODEs is answered through an application of the following theorem,

Theorem 2 (Linear Existence and Uniqueness) *Let $A(t)$ be a matrix-valued function of t, with each entry a continuous function on (t_i, t_f). There exists a unique solution of the initial value problem (1.1) on (t_i, t_f).*

One proof of this theorem is by Picard iteration. See section 3.

We will be interested in a particular nonlinear ODE as well, namely Hausdorff's equation (4.2) for $\Omega(t)$. The right side of equation (4.2) is reasonably well-behaved, and the general existence and uniqueness theorem [5] could perhaps be applied to give short-time existence. However, the existence of $\Phi(t) = e^{\Omega(t)}$ is not in doubt as $\Phi(t)$ solves the linear equation (3.1). The issue of existence and uniqueness is unimportant relative to the construction of approximations to $\Omega(t)$, and thus to $\Phi(t)$. One construction, Magnus' expansion, is the topic of this thesis.

Systems of ODEs

So, how does one find a solution for (2.4); or, more generally, (1.1)? If $A(t)$ is a constant matrix-valued function, e.g. $A(t) = A_0 \; \forall t \in (t_i, t_f)$, then we can find an integrating factor $\mu = e^{-\int_{t_0}^{t} A_0 d\xi} = e^{-A_0(t-t_0)}$ such that

$$\mu D_t Y(t) + \mu A_0 Y(t) = D_t (\mu Y(t)) = \mathbf{0}$$

$$\Rightarrow Y(t) = e^{-A_0 t} \left(e^{A_0 t_0} Y_0 \right) \tag{2.6}$$

is a solution to equation (1.1).

Now, if $A(t)$ is not a constant matrix, we run into difficulties. At time $t = t_1$, $A(t_1) Y(t_1)$ is in the tangent space of the curve $Y(t)$ at t_1 and at time $t = t_2$, $A(t_2) Y(t_2)$ is in the tangent space of the curve $Y(t)$ at t_2. By being in the tangent space, we can see that $A(t_1)$ and $A(t_2)$ contain some information about the 'direction' the curve Y is evolving. So if we start at point Y_0 and follow along with the motion of $A(t_1) Y(t_1)$, then follow the motion of $A(t_2) Y(t_2)$, we end up at, say, point Y_{12}. Suppose also that we start at point Y_0 and follow the motion of $A(t_2) Y(t_2)$, then follow the motion of $A(t_1) Y(t_1)$ a small distance, and we end up at point Y_{21}. If $Y_{21} \neq Y_{12}$, then the motion prescribed by $A(t)$ doesn't allow us to simply integrate along $A(t)$ and then exponentiate for a solution.

It turns out that the question regarding the exponentiation of the integral of $A(t)$ as a solution of (1.1) becomes "does $A(\xi)A(\zeta) = A(\zeta)A(\xi)$?"

Definition 3 *A square matrix valued fuction of time $A(t)$ is* commutative *if and only if $A(\xi)A(\zeta) = A(\zeta)A(\xi)$ for all ζ, ξ. Likewise, we refer to $A(t)$ as* noncommutative *if $A(\xi)A(\zeta) \neq A(\zeta)A(\xi)$ for some ξ, ζ.*

Proposition 4 *If $A(\xi)A(\zeta) = A(\zeta)A(\xi)$ for all $\zeta, \xi \in \mathbb{R}$, then*

$$Y(t) = Y(t_0)e^{-\int_{t_0}^{t} A(\xi)d\xi} \tag{2.7}$$

with $Y(t_0)$ the vector of initial conditions solves (1.1).

Proof. The proof, based on Magnus' expansion, is deferred until appendix C. ■

The following is an easy-to-prove sufficient condition for commutativity.

Lemma 5 *A matrix function of time $A(t) \in \mathbb{R}^{n \times n}$ is commutative iff all eigenvectors of $A(t)$ are constant, independent of t.*

Proof. $\Leftarrow$) Suppose all eigenvectors of $A(t)$, an $n \times n$ matrix function of t, are constant, independent of t. Let $v \in \mathbb{R}^n$ and let $\lambda_j(t), e^j$ be the $m \leq n$ eigenvalues and normalized eigenvectors respectively, of $A(t)$. Then we have

$$\begin{aligned} A(x)\,A(y)\,v &= A(x)\sum_{j=1}^{m} c_j \lambda_j(y)\, e^j \\ &= \sum_{j=1}^{m} c_j \lambda_j(x)\, \lambda_j(y)\, e^j \\ &= A(y)\sum_{j=1}^{m} c_j \lambda_j(x)\, e^j \\ &= A(y)A(x)v \end{aligned}$$

$\Rightarrow$) Suppose $A(x)A(y) = A(y)A(x)$. Take $e_x \neq \mathbf{0}$ such that $A(x)e_x = \lambda_x e_x$. Now,

$$A(x)\left(A(y)e_x\right) = A(y)A(x)e_x = \lambda_x \left(A(y)e_x\right)$$

which means that $A(y)e_x$ is a scalar multiple of a nonzero eigenvector of $A(x)$. In particular, $A(y)e_x = c_1(x,y)e'_x$, for e'_x a nonzero eigenvector of $A(x)$ and $c_1(x,y)$ a scalar function of x and y. By the same process,

$$\begin{aligned} A(y)e_x &= c_1(x,y)e'_x \\ A(y)e'_x &= c_2(x,y)e''_x \\ &\vdots \\ A(y)e_x^{m-1} &= c_m(x,y)e_x^m \end{aligned}$$

So, there is a $k \leq m$ such that $A^k(y)e_x = c_1(x,y)c_2(x,y)\cdots c_k(x,y)e_x = c(x,y)e_x$. This means that e_x is an eigenvector of $A^k(y)$

$$e_x = s(x)e_y$$

where e_y is some eigenvector of $A^k(y)$. But the left side of $\frac{e_x}{s(x)} = e_y$ is dependent only on x and the right side is dependent only on y, so that $\frac{e_x}{s(x)}$ and e_y must be constant, independent of the variables $x,\ y$. Thus, the eigenvectors of A must be constant. ∎

What if $A(t)$ is noncommutative? Do we have hope for constructing a solution? One method of solution is Picard iteration as discussed in section 3.

2.2 Fundamental Solutions

By the general existence and uniqueness theorem 2, we know that there exists a unique $Y(t)$ which solves equation (1.1).

Definition 6 *A spanning set of solution vectors on $(t_i, t_f) \subset \mathbb{R}$ to the linear homogeneous differential equation (*1.1*) is called a* fundamental set *if the solution vectors are linearly independent for all $t \in (t_i, t_f)$.*

Definition 7 *A matrix-valued function $\Phi : (t_i, t_f) \to \mathbb{R}^{n\times n}$ is a fundamental solution if the columns of $\Phi(t)$ form a fundamental set.*

That is, if $\left\{\phi_j(t)\right\}_{j=1}^{n}$ forms a fundamental set, then we can create a fundamental solution $\Phi(t)$ on (t_i, t_f) associated with the differential equation (1.1) by taking column p of $\Phi(t)$ to be $\phi_p(t)$.

The importance of finding a fundamental solution is that *every* solution to (1.1) can be written as a linear combination of the columns of $\Phi(t)$. In particular, the solution to (1.1) with initial condition Y_0 is

$$Y(t) = \Phi(t)\left(\Phi(t_0)\right)^{-1} Y_0.$$

3 Classical Methods for Approximating a Fundamental Solution

Much of numerical analysis focuses on approximating the solution to a given differential equation. Methods include Euler's method, Taylor series methods, and predictor-corrector methods as well as Picard iteration. It is often necessary to approximate the fundamental solution using a numerical method, since a closed form analytic solution may not always be possible to find. We restrict our attention here to the linear case

$$D_t\Phi(t) + A(t)\Phi(t) = \mathbf{0} \qquad \Phi(t_0) = I \tag{3.1}$$

We will suppose $A(t)$ is bounded and integrable.

In the following, we discuss Picard iteration of ODEs. Note that finite Picard iteration is used later in this thesis to provide an approximation for a given differential equation.

3.1 Picard Iteration

Picard iteration is the integral analogue of Taylor expansion.

Consider equation (3.1). If we integrate $D_t\Phi(\eta)$ with respect to η from t to t_0, using the fundamental theorem of calculus we get

$$\Phi(t) - \Phi(t_0) = \int_{t_0}^{t} D_t\Phi(\eta)d\eta = \int_{t_0}^{t} A(\eta)\Phi(\eta)d\eta$$

This gives us an integral formulation for the ODE (3.1):

$$\Phi(t) = I + \int_{t_0}^{t} A(\eta)\Phi(\eta)d\eta \tag{3.2}$$

Assuming that $A(t)$ is integrable, we can start an iterative scheme with the (relatively poor) approximation that $\Phi_0(t) = I$ so that

$$\Phi_1(t) = I + \int_{t_0}^{t} A(\eta) d\eta$$

Continuing on we get

$$\begin{aligned}
\Phi_p(t) &= I + \int_{t_0}^{t} A(\eta)\Phi_{(p-1)}(\eta) d\eta \qquad (3.3)\\
&= I + \int_{t_0}^{t} A(\eta_{p-1}) d\eta_{p-1} + \int_{t_0}^{t} A(\eta_{p-1}) \int_{t_0}^{\eta_{p-1}} A(\eta_{p-2}) d\eta_{p-2} d\eta_{p-1} + \\
&\quad ... + \int_{t_0}^{t} A(\eta_{p-1}) \int_{t_0}^{\eta_{p-1}} A(\eta_{p-2}) ... \int_{t_0}^{\eta_1} A(\eta_0) d\eta_0 d\eta_1 ... d\eta_{p-1}.
\end{aligned}$$

This sequence of iterations of $\Phi_p(t)$ converges to the fundamental solution $\Phi(t)$. Let $\|A(t)\| = \widetilde{a}$ and estimate

$$\begin{aligned}
\|\Phi_p(t) - \Phi_{p+1}(t)\| &= \left\| \int_{t_0}^{t} A(\eta_p) \int_{t_0}^{\eta_{p-1}} A(\eta_{p-1}) ... \int_{t_0}^{\eta_1} A(\eta_0) d\eta_0 d\eta_1 ... d\eta_{p-1} d\eta_p \right\| \\
&\leq \int_{t_0}^{t} \|A(\eta_p)\| \int_{t_0}^{\eta_{p-1}} \|A(\eta_{p-1})\| ... \int_{t_0}^{\eta_1} \|A(\eta_0)\| d\eta_0 d\eta_1 ... d\eta_p \\
&= \widetilde{a}^p \int_{t_0}^{t} \int_{t_0}^{\eta_{p-1}} ... \int_{t_0}^{\eta_2} \int_{t_0}^{\eta_1} 1 d\eta_0 d\eta_1 ... d\eta_{p-1} d\eta_p = \widetilde{a}^p \frac{(t-t_0)^p}{p!}
\end{aligned}$$

So that

$$\|\Phi_p(t) - \Phi_k(t)\| \leq \sum_{r=k}^{p} \widetilde{a}^r \frac{(t-t_0)^r}{r!} \to 0 \qquad (3.4)$$

provided $\widetilde{a}(t-t_0) < \infty$, as $p, k \to \infty$. That is, $\{\Phi_p(t)\}$ is Cauchy in the $\|\cdot\|$ norm, so $\Phi(t) = \lim_{p\to\infty} \Phi_p(t)$ and also

$$\|\Phi(t) - \Phi_k(t)\| \leq \sum_{r=k}^{\infty} \widetilde{a}^r \frac{(t-t_0)^r}{r!} \qquad (3.5)$$

We see that $\Phi_k(t) \to \Phi(t)$ pointwise and in norm. Actually, we have uniform convergence for t in any fixed neighborhood of t_0.

The general existence and uniqueness theorems can be proven using Picard iteration as a constructive method. See [5]

In the case of $A(t)$ a constant matrix, i.e. $A(t) = A$, Picard iteration gives us

$$\begin{aligned}
\Phi_1(t) &= I + \int_{t_0}^{t} A\Phi_{(0)}(\eta)d\eta = I + A\left(t - t_0\right) \\
\Phi_2(t) &= I + \int_{t_0}^{t} A\left(I + A\left(\eta - t_0\right)\right)d\eta = I + A\left(t - t_0\right) + \frac{A^2\left(t - t_0\right)^2}{2} \\
\Phi_p(t) &= I + A\left(t - t_0\right) + \frac{A^2\left(t - t_0\right)^2}{2} + ... + \frac{A^p\left(t - t_0\right)^p}{p!} = \sum_{k=0}^{p} \frac{A^k\left(t - t_0\right)^k}{k!}
\end{aligned}$$

which in the limit as $p \rightarrow \infty$ we get $\Phi(t) = e^{A(t-t_0)}$ the correct solution.

4 Hausdorff's equation

Motivated by the scalar case (2.2) with fundamental solution $\phi(t) = e^{-\int_{t_0}^{t} a(\xi)d\xi}$, we seek to find an $\Omega(t)$, such that the fundamental solution to (3.1) is $\Phi(t) = e^{\Omega(t)}$. We follow the footsteps of Hausdorff, finding an expression for $\Omega(t)$ in terms of $A(t)$ from (3.1).

4.1 Derivation of Hausdorff's equation for $D_t\Phi = A\Phi$.

Consider equation (3.1) and assume $\Phi(t) = e^{\Omega(t)}$ for $\Omega(t) \in M_n$. Note $\Omega(t_0) = \mathbf{0}$. From now on we suppress the "t": $\Omega = \Omega(t)$, etc...

Since $\Phi(t_0) = I$ and Φ is continuous, Φ is invertible in a neighborhood of $t = t_0$, and $\Phi^{-1} = e^{-\Omega}$, (3.1) is algebraically equivalent to the equation

$$\left(D_t e^{\Omega}\right) e^{-\Omega} = A \tag{4.1a}$$

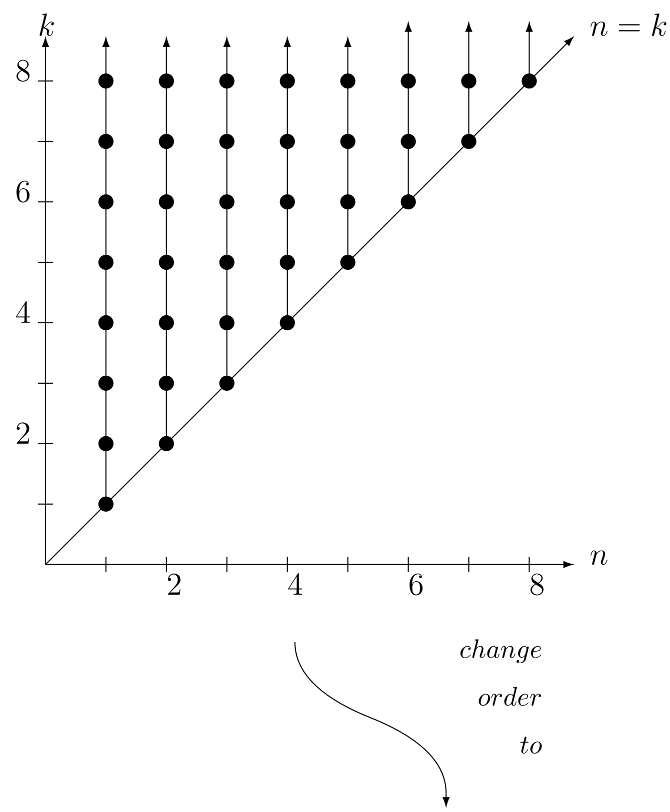
Since $e^{\Omega} = \sum\limits_{m=0}^{\infty} \frac{\Omega^m}{m!}$, and $D_t(\Omega^m) = \sum\limits_{q=1}^{m} \Omega^{q-1}(D_t\Omega)\Omega^{m-q}$, (4.1a) becomes

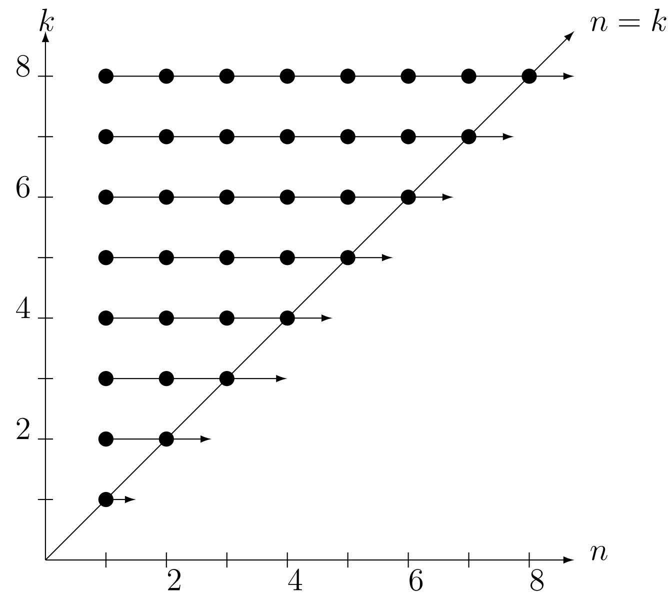
$$\begin{aligned}
A &= \left(D_t e^{\Omega}\right) e^{-\Omega} \\
&= \left(\sum_{n=1}^{\infty} \frac{D_t(\Omega^n)}{n!}\right) \cdot \left(\sum_{m=0}^{\infty} \frac{(-1)^m \Omega^m}{m!}\right) \\
&= \left(\sum_{n=1}^{\infty} \frac{1}{n!} \sum_{q=1}^{n} \Omega^{n-q}(D_t\Omega)\Omega^{q-1}\right) \cdot \left(\sum_{m=0}^{\infty} \frac{(-1)^m \Omega^m}{m!}\right) \\
&= \sum_{n=1}^{\infty} \sum_{q=1}^{n} \sum_{m=0}^{\infty} \left(\frac{(-1)^m}{m!} \frac{1}{n!} \left\{\Omega^{q-1}(D_t\Omega)\Omega^{m+n-q}\right\}\right)
\end{aligned}$$

Switching the order of the m and q sums and letting $m + n = k$, we have

$$\begin{aligned} A &= \sum_{n=1}^{\infty}\sum_{k=n}^{\infty}\sum_{q=1}^{n}\left(\frac{(-1)^{k-n}}{(k-n)!}\frac{1}{n!}\left\{\Omega^{q-1}\left(D_t\Omega\right)\Omega^{k-q}\right\}\right) \\ &= \sum_{n=1}^{\infty}\sum_{k=n}^{\infty}\sum_{q=1}^{n}\left(\frac{(-1)^{k}(-1)^{n}}{k!}\begin{pmatrix} k \\ n \end{pmatrix}\left\{\Omega^{q-1}\left(D_t\Omega\right)\Omega^{k-q}\right\}\right) \\ &= \sum_{n=1}^{\infty}\sum_{k=n}^{\infty}\sum_{q=1}^{n}\left((-1)^{n}\frac{(-1)^{k}}{k!}\begin{pmatrix} k \\ n \end{pmatrix}\left\{\Omega^{q-1}\left(D_t\Omega\right)\Omega^{k-q}\right\}\right) \end{aligned}$$

We want to switch the order of summation between k and n in order to reduce to a simpler expression for A. The easiest way to see this is to draw a picture:





Note that originally, $k \in \{n, \ldots, \infty\}$, and $n \in \{1, \ldots, \infty\}$. In the second picture, $n \in \{1, \ldots, k\}$, and $k \in \{1, \ldots, \infty\}$ and we still cover all the same lattice points. So,

$$A = \sum_{k=1}^{\infty} \sum_{n=1}^{k} \sum_{q=1}^{n} \left((-1)^n \frac{(-1)^k}{k!} \begin{pmatrix} k \\ n \end{pmatrix} \left\{ \Omega^{q-1} \left(D_t \Omega \right) \Omega^{k-q} \right\} \right)$$

Next we want to also swap summation over indices q and n. Using the same idea, but for finite sets of indices, we change the order of summation from $q \in \{1, \ldots, n\}$, $n \in \{1, \ldots, k\}$ to $q \in \{1, \ldots, k\}$, $n \in \{q, \ldots, k\}$, so that the expression for A becomes

$$A = \sum_{k=1}^{\infty} \frac{(-1)^k}{k!} \left\{ \sum_{q=1}^{k} \sum_{n=q}^{k} \left((-1)^n \binom{k}{n} \left\{ \Omega^{q-1} \left(D_t \Omega \right) \Omega^{k-q} \right\} \right) \right\} \tag{4.1b}$$

Lemma 8 *Let* $p, q \in \mathbb{N}$. *Then* $\sum_{r=p}^{q} (-1)^r \begin{pmatrix} q \\ r \end{pmatrix} = (-1)^p \begin{pmatrix} q-1 \\ p-1 \end{pmatrix}$

Proof. See [25]. ■

Note that $\left[\Omega^{q-1} \left(D_t \Omega \right) \Omega^{k-q} \right]$ does <u>not</u> depend on n, and (4.1b) becomes

$$A = \sum_{k=1}^{\infty} \frac{(-1)^k}{k!} \left(\sum_{q=1}^{k} (-1)^q \begin{pmatrix} k-1 \\ q-1 \end{pmatrix} \left\{ \Omega^{q-1} \left(D_t \Omega \right) \Omega^{k-q} \right\} \right)$$

by the lemma. Upon re-indexing both sums,

$$A=\sum_{k=0}^{\infty}\frac{(-1)^k}{(k+1)!}\left(\sum_{q=0}^{k}(-1)^q\left(\begin{array}{c}k\\ \\ q\end{array}\right)\left\{\Omega^q\left(D_t\Omega\right)\Omega^{k-q}\right\}\right) \tag{4.2}$$

Definition 9 *Fix $X\in M_n$. The map $ad_X : M_n\to M_n$ is defined by $ad_X(Y)=XY-YX=[X,Y]$ for $Y\in M_n$. This is extended recursively: $ad_X^p(Y)=X\cdot ad_X^{p-1}(Y)-ad_X^{p-1}(Y)\cdot X=\left[X,ad_X^{p-1}(Y)\right]$, for $Y\in M_n$ and $ad_X^0(Y)=Y$.*

Lemma 10 $\forall X,Y\in M_n$, $\forall p\in\mathbb{N}$,

$$ad_X^p(Y)=\sum_{q=0}^{p}(-1)^q\binom{p}{q}\left\{X^{p-q}YX^q\right\}$$

Proof. By induction. First, $ad_X^0(Y)=Y$, $ad_X^1(Y)=-[Y,X]=[X,Y]$. Second, suppose $ad_X^{p-1}(Y)=\sum\limits_{q=0}^{p-1}(-1)^q\binom{p-1}{q}\left\{X^{p-1-q}YX^q\right\}$ holds. Then,

$$\begin{aligned}
ad_X^p(Y) &= (-1)\left\{\left(\sum_{q=0}^{p-1}(-1)^q\binom{p-1}{q}\left\{X^{p-1-q}YX^q\right\}\right)\cdot X-X\cdot\left(\sum_{q=0}^{p-1}(-1)^q\binom{p-1}{q}\left\{X^{p-1-q}YX^q\right\}\right)\right\}\\
&= \left(\sum_{q=0}^{p-1}(-1)^q\binom{p-1}{q}\left\{X^{p-q}YX^q\right\}\right)-\left(\sum_{q=0}^{p-1}(-1)^q\binom{p-1}{q}\left\{X^{p-1-q}YX^{q+1}\right\}\right)\\
&= \left(\sum_{q=0}^{p-1}(-1)^q\binom{p-1}{q}\left\{X^{p-q}YX^q\right\}\right)-\left(\sum_{q=1}^{p}(-1)^{q-1}\binom{p-1}{q-1}\left\{X^{p-q}YX^q\right\}\right)\\
&= X^pY+\left(\sum_{q=1}^{p-1}(-1)^q\binom{p-1}{q}\left\{X^{p-q}YX^q\right\}\right)+\left(\sum_{q=1}^{p-1}(-1)^q\binom{p-1}{q-1}\left\{X^{p-q}YX^q\right\}\right)+(-1)^pYX^p\\
&= X^pY+\left(\sum_{q=1}^{p-1}(-1)^q\left\{\binom{p-1}{q}+\binom{p-1}{q-1}\right\}\left\{X^{p-q}YX^q\right\}\right)+(-1)^pYX^p\\
&= X^pY+\left(\sum_{q=1}^{p-1}(-1)^q\binom{p}{q}\left\{X^{p-q}YX^q\right\}\right)+(-1)^pYX^p\\
&= \sum_{q=0}^{p}(-1)^q\binom{p}{q}\left\{X^{p-q}YX^q\right\}
\end{aligned}$$

∎

Note that ad_X^p is linear: $ad_X^p(\alpha Y+\beta Z)=\sum\limits_{q=0}^{p}(-1)^{p+q}\binom{p}{q}\left\{X^{p-q}(\alpha Y+\beta Z)X^q\right\}=\alpha ad_X^p(Y)+\beta ad_X^p(X)$.

Notice that since $ad_A^1(B) = -ad_B^1(A)$,

$$\begin{aligned} ad_X^p(Y) &= \sum_{q=0}^{p} (-1)^q \binom{p}{q} \left\{X^{p-q} Y X^q\right\} \\ &= (-1)^p \sum_{q=0}^{p} (-1)^{p-q} \binom{p}{q} \left\{X^{p-q} Y X^q\right\} \\ &= (-1)^p \sum_{q=0}^{p} (-1)^q \binom{p}{q} \left\{X^{q} Y X^{p-q}\right\} \end{aligned}$$

Our expression for A from (4.2) is then

$$A = \sum_{k=0}^{\infty} \left(\frac{ad_\Omega^k (D_t\Omega)}{(k+1)!} \right) \tag{4.3}$$

Lemma 11 *Let $X \in M_n$, such that $\|X\| = M < \infty$. Then $ad_X^k : M_n \to M_n$ is a bounded linear operator. In particular, $\left\|ad_\Omega^k\right\| \le (2\|\Omega\|)^k$.*

Proof. Let $W \in M_n$, such that $\|W\| = 1$, and $\alpha, \beta \in \mathbb{C}$.
$\left\|ad_X^k W\right\| = \left\| \sum\limits_{q=0}^{k} (-1)^{k+q} \binom{k}{q} \left\{X^{k-q} W X^q\right\} \right\| \le \sum\limits_{q=0}^{k} \binom{k}{q} \left\|\left\{X^{k-q} W X^q\right\}\right\|$
$\le \sum\limits_{q=0}^{k} \binom{k}{q} \|X\|^{k-q} \|W\| \|X\|^q = \sum\limits_{q=0}^{k} \binom{k}{q} \|X\|^k = \|X\|^k 2^k$ ■

If we regard the right side of (4.3) as a linear operator on $D_t\Omega$, we get the expression

$$A = \sum_{k=0}^{\infty} \left(\frac{ad_\Omega^k}{(k+1)!} \right) (D_t\Omega) \tag{4.4}$$

What we would like to do is solve this linear equation for $D_t\Omega$. This will require the functional calculus [12].

4.2 Solving the linear operator equation for $D_t\Omega$.

The power series $\sum\limits_{n=0}^{\infty} \frac{z^n}{(n+1)!}$ is analytic and entire in the complex plane. Note

$$\sum_{n=0}^{\infty} \frac{z^n}{(n+1)!} = \frac{1}{z} \sum_{n=0}^{\infty} \frac{z^{n+1}}{(n+1)!} = \frac{1}{z} \left(-1 + \sum_{n=0}^{\infty} \frac{z^n}{n!} \right) = \frac{1}{z} \left(-1 + e^z\right).$$

Lemma 12 *Let $\Theta_\Omega : M_n \to M_n$, be the operator given by*

$$\Theta_\Omega = \sum_{k=0}^{\infty} \frac{ad_\Omega^k}{(k+1)!}$$

Then, Θ_Ω is a bounded linear operator and $\|\Theta_\Omega\| \leq \frac{e^M-1}{M}$ if $M = 2\|\Omega\|$

Proof. Linearity is obvious. From lemma (11) we have

$\left\|ad_\Omega^k\right\| \leq (2\|\Omega\|)^k = M^k$. In fact, if $W \in M_n$ and $\|W\| = 1$, then $\|\Theta_\Omega(W)\| = \left\|\sum_{k=0}^{\infty} \frac{ad_\Omega^k(W)}{(k+1)!}\right\| \leq \sum_{k=0}^{\infty} \frac{\left\|ad_\Omega^k(W)\right\|}{(k+1)!} \leq \sum_{k=0}^{\infty} \frac{M^k}{(k+1)!} = \frac{e^M-1}{M}$. ■

From the functional calculus of finite dimensional operators [12], we have

Definition 13 *The* spectrum σ *of a linear operator T in a finite dimensional space Z is the set of complex numbers μ such that $T - \mu I$ is not a bijection. Note that T, an operator on Z, is not a bijection if and only if there exists $v \in Z$ such that $Lv = 0$. Thus the spectrum $\sigma(T)$ of T is exactly the eigenvalues of T.*

Definition 14 *We denote by $\mathfrak{F}(T)$ the class of functions which are complex analytic on some neighborhood B of $\sigma(T)$. If $f \in \mathfrak{F}(T)$ then we define $f(T)$ as*

$$f(T) = \frac{1}{2\pi i} \oint_{\partial A} f(\gamma)(\gamma I - T)^{-1} d\gamma \tag{4.5}$$

where $A \subset B$ such that A is an open set of $\mathbb{C}$ with finitely many connected components that contain the spectrum of T, i.e. $\sigma(T) \subset A$, and the boundary of A, $\partial A \subset B$ is a closed Jordan curve.

For each $\mu \in \sigma(T)$, and for all $g \in \mathfrak{F}(T)$, expand g as a power series so that

$$g(T) = \sum_{n=0}^{\infty} \frac{\left(D^{(n)}g\right)(\mu)}{n!} (T - \mu I)^n \tag{4.6}$$

where $g(T)$ is defined by (4.5). In this manner, all functions of an operator T, analytic on a neighborhood of $\sigma(T)$, are given as power series of T.

Theorem 15 *Let $f, g \in \mathfrak{F}(T)$. Then $(f \cdot g)(T) = f(T) \cdot g(T)$.*

Proof. [11]. ■

From (4.4) and (4.5), and if

$$f(z) = \sum_{k=0}^{\infty} \frac{z^k}{(k+1)!} = \frac{1}{z}\left(-1 + e^z\right),$$

the expression for A becomes

$$A = \sum_{k=0}^{\infty} \left(\frac{ad_{\Omega}^{k}}{(k+1)!} \right) (D_t \Omega) = \Theta_{\Omega}(D_t\Omega) = f(ad_{\Omega})(D_t\Omega) \tag{4.7}$$

If $f, g \in \mathfrak{F}(T)$ such that $g(z) \cdot f(z) = 1 \ \forall z \in \sigma(T) \subset \mathbb{C}$, then

$$T = I(T) = (g \cdot f)(T) = g(T) \cdot f(T)$$

Recall equation (4.4). Provided we can find an analytic function g such that $g(z) \cdot f(z) = 1$, we can apply $g\left(ad_{\Omega}^{k}\right)$ to (4.4) in order to isolate $D_t\Omega$. We want the function g to satisfy

$$g(z)\left(\frac{1}{z}\left(-1+e^z\right)\right) = g(z)\left(\sum_{k=0}^{\infty} \frac{z^k}{(k+1)!}\right) = 1 \tag{4.8}$$

So $g(z) = \frac{z}{e^z - 1}$. It turns out that

$$g(z) = \sum_{k=0}^{\infty} B_k \frac{z^k}{k!}$$

where B_k are the Bernoulli numbers [2].

Neglecting convergence temporarily, let $\Theta_{\Omega}^{-1} : M_n \to M_n$ be the operator given by

$$\Theta_{\Omega}^{-1} = \sum_{k=0}^{\infty} B_k \frac{ad_{\Omega}^{k}}{k!} = g(ad_{\Omega})$$

In equation (4.7) for A, apply Θ_{Ω}^{-1} to both sides. This gives us the expression

$$\Theta_{\Omega}^{-1}(A) = \Theta_{\Omega}^{-1}\left(\Theta_{\Omega}(D_t\Omega)\right) = D_t\Omega$$

This leads us to

$$D_t\Omega = \Theta_{\Omega}^{-1}(A) = \sum_{k=0}^{\infty} B_k \frac{ad_{\Omega}^{k}(A)}{k!} \tag{4.9}$$

where we have isolated the expression for $D_t\Omega$, and (4.9) is known as *Hausdorff's equation* [1].

But, what are the conditions necessary for the given series Θ_Ω^{-1} to be convergent? According to Definition 14, we must have g analytic on some neighborhood that contains $\sigma\left(ad_\Omega\right)$. With $g\left(z\right) = \frac{z}{e^z-1}$, we can see that there are poles for $e^z - 1 = 0$, or $z = 2\pi ni$, $n \in \mathbb{Z}$. But notice that there is a removable singularity for $z = 0$, since $g\left(z\right) \equiv \frac{1}{\frac{e^z-1}{z}} = \frac{1}{1+\frac{z}{2}+\frac{z^2}{6}+\ldots}$, which is analytic at $z = 0$. So $g\left(z\right)$ is analytic in the complex plane except for the points $z = 2\pi ni$, $n \in \mathbb{Z}-\left\{0\right\}$. Provided $\left\{2\pi ni\right\}_{n\in\mathbb{Z}-\{0\}} \cap \sigma\left(ad_\Omega\right) = \phi$, then Θ_Ω^{-1} exists, is convergent, and is the inverse of Θ_Ω. See appendix D for a discussion regarding the relationship between the spectrum of Ω and the spectrum of ad_Ω.

5 Magnus' Expansion

In the late 1940's, while reviewing some algebraic problems concerning linear operators in quantum mechanics, Wilhelm Magnus considered Hausdorff's equation (4.9) and approximated a solution through the use of Picard iteration. He was able to show that the solution to Hausdorff's equation (4.9) is given by the series

$$\begin{aligned}\Omega(t) &= \int_0^t A(\zeta_1)d\zeta_1 - \frac{1}{2}\int_0^t \left[\int_0^{\zeta_1} A(\zeta_2)d\zeta_2, A(\zeta_1)\right] d\zeta_1 \\ &+\frac{1}{4}\int_0^t \left[\int_0^{\zeta_1}\left[\int_0^{\zeta_2} A(\zeta_3)d\zeta_3, A(\zeta_2)\right] d\zeta_2, A(\zeta_1)\right] d\zeta_1 \\ &+\frac{1}{12}\int_0^t \left[\int_0^{\zeta_1} A(\zeta_2)d\zeta_2, \left[\int_0^{\zeta_1} A(\zeta_2)d\zeta_2, A(\zeta_1)\right]\right] d\zeta_1 + ...\end{aligned}$$

in some neighborhood of $t = t_0$ only " if certain unspecified conditions of convergence are satisfied." [20] Later, in the same paper, Magnus gives the condition that a solution to $D_t\Phi(t) = A(t)\Phi(t), \quad \Phi(t_0) = I$of the form $\Phi(t) = e^{\Omega(t)}$ exists in a neighborhood of $e^{\Omega(t_0)}$ " if and only if none of the differences between any two of the eigenvalues of $\Omega(t_0)$ equals $2\pi ni$, where $n \in \mathbb{Z} - \{0\}$."[20]. See appendix (D).

Following much work on attempting to find analytic expressions for $\Omega(t)$, notably by [21], [28], and [13], in the late 1990's Arieh Iserles 'rediscovered' Magnus' expansion in his study of geometric integration. Specifically, Iserles [1], found the first few terms of Magnus' expansion useful for a numerical approximation method that capitalized on the symmetries preserved under the exponential map. We follow Iserles' in exploring Magnus' expansion.

5.1 Iserles' Ordering of Magnus' Expansion

Consider equation (4.9) , Hausdorff's equation, a nonlinear differential equation of the form (2.1) derived from (3.1).

$$D_t\Omega(t) = \sum_{m=0}^{\infty}\frac{B_m}{m!}ad_{\Omega}^m(A) \qquad \Omega(0) = 0 \tag{5.1}$$

Let us suppose that following infinitely many Picard iterations, we can write the solution to (5.1) in the form

$$\Omega(t) = \sum_{k=0}^{\infty}\left(\sum_{\tau\in\mathbb{T}_k}\alpha_\tau\int H_\tau\right) \tag{5.2}$$

where k is the index for the indexing set $\mathbb{T}_k$ to be defined later, and H_τ is a matrix function of time indexed by $\tau\in\mathbb{T}_k$.

Differentiating this expression with respect to time and using (5.1), we find that

$$\begin{aligned} D_t\Omega &= \sum_{k=0}^{\infty}\left(\sum_{\tau\in\mathbb{T}_k}\alpha_\tau H_\tau\right) = \sum_{m=0}^{\infty}\frac{B_m}{m!}ad_\Omega^m(A) \\ &= \sum_{m=0}^{\infty}\frac{B_m}{m!}ad^m_{\left\{\sum_{k=0}^{\infty}\left(\sum_{\tau\in\mathbb{T}_k}\alpha_\tau\int H_\tau\right)\right\}}(A) \\ &= A + \sum_{m=1}^{\infty}\frac{B_m}{m!}ad^m_{\left\{\sum_{k=0}^{\infty}\left(\sum_{\tau\in\mathbb{T}_k}\alpha_\tau\int H_\tau\right)\right\}}(A) \end{aligned} \tag{5.3}$$

Now,

$$ad^m_{\left\{\sum_{k=0}^{\infty}\left(\sum_{\tau\in\mathbb{T}_k}\alpha_\tau\int H_\tau\right)\right\}}(A) = \tag{5.4}$$

$$\begin{aligned} &= \left[\sum_{k=0}^{\infty}\left(\sum_{\tau\in\mathbb{T}_k}\alpha_\tau\int H_\tau\right), ad^{m-1}_{\left\{\sum_{k=0}^{\infty}\left(\sum_{\tau\in\mathbb{T}_k}\alpha_\tau\int H_\tau\right)\right\}}(A)\right] \\ &= \sum_{k=0}^{\infty}\left(\sum_{\tau\in\mathbb{T}_k}\alpha_\tau\left[\int H_\tau, ad^{m-1}_{\left\{\sum_{k=0}^{\infty}\left(\sum_{\tau\in\mathbb{T}_k}\alpha_\tau\int H_\tau\right)\right\}}(A)\right]\right) \\ &= \sum_{k_1=1}^{\infty}\cdots\sum_{k_m=1}^{\infty}\left(\sum_{\tau^1\in\mathbb{T}_{k_1}}\cdots\sum_{\tau^m\in\mathbb{T}_{k_m}}\alpha_{\tau^1}\ldots\alpha_{\tau^m}\left[\int H_{\tau^1},\left[\ldots,\left[\int H_{\tau^m},A\right]\ldots\right]\right]\right) \end{aligned}$$

We find, after inserting the expression from (5.4) into (5.3), that for $\tau\in T_k$,

$$H_\tau = R(H_{\tau^1}, H_{\tau^2}, \ldots, H_{\tau^m}) \text{ and } \alpha_\tau = r\left(\alpha_{\tau^1}, \alpha_{\tau^2}, \ldots, \alpha_{\tau^m}\right) \tag{5.5}$$

where $R : M_n^m \to M_n$ is multilinear, $r : \mathbb{R}^m \to \mathbb{R}$, and H_{τ^n} is indexed by elements $\tau^n \in \mathbb{T}_j$ for $j < k$ and $n \in \{1, 2, ..., m\}$.

For example, let n=2. We have

$$\sum_{\tau\in\mathbb{T}_2} \alpha_\tau H_\tau = \frac{B_2}{2!} \sum_{\tau^a\in\mathbb{T}_1} \alpha_{\tau^a} \left[\int H_{\tau^a}, A\right] \tag{5.6}$$

$$+ \frac{B_1}{1!}\frac{B_1}{1!} \sum_{\tau^b\in\mathbb{T}_0} \sum_{\tau^c\in\mathbb{T}_0} \alpha_{\tau^b}\alpha_{\tau^c} \left[\int H_{\tau^b}, \left[\int H_{\tau^c}, A\right]\right]$$

From this we can see that building the H_τ's as n-integrals of commutators depends on the ways of combining k-integrals of commutators with p-integrals of commutators, such that $k + p = n$.

Note that for $k = 0$ we end up with

$$\sum_{\tau\in\mathbb{T}_0} \alpha_\tau H_\tau = A$$

This gives us a starting point for defining the successive terms H_τ for $k \in \mathbb{N}$. Next is $k = 1$, for which there is only one possible way to combine an integral of A with A, giving

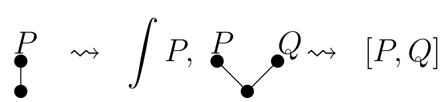
$$for\ \tau\in \mathbb{T}_1,\ H_\tau\in \{A\} \tag{5.7}$$

$$for\ \tau\in \mathbb{T}_2,\ H_\tau\in \left\{\left[\int A, A\right]\right\}$$

$$for\ \tau\in \mathbb{T}_3,\ H_\tau\in \left\{\left[\int A, \left[\int A, A\right]\right], \left[\int \left[\int A, A\right], A\right]\right\} \text{ as seen in } (5.6).$$

5.2 Tree and Forest Construction.

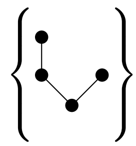
Following Iserles [1], we use the representation



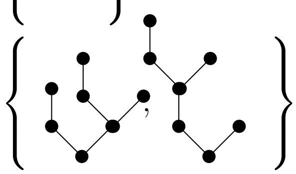
for integration and commutation respectively. Let A from (5.7) be represented by $\bullet$, that is, each vertex at the end of a branch, a leaf, represents A. We build the indexing set $\mathbb{T}_k$ by constructing the representatives $\tau \in \mathbb{T}_k$ using these elements. The first three *index sets* corresponding to (5.7) are given by

$$\mathbb{T}_0 = \left\{ \bullet \right\} \qquad \text{(Forests)}$$

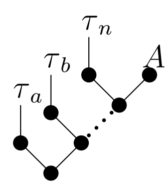
$\mathbb{T}_1 =$



$\mathbb{T}_2 =$

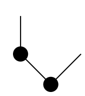


Each tree $\tau \in \mathbb{T}_k$ can be written in the form



(5.8)

where each τ on a branch is a tree from the previous index sets. All trees begin with a foundation of



(5.9)

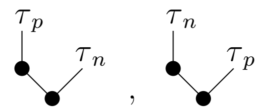
corresponding to $\left[\int H_\tau, ad_\Omega^{m-1}(A)\right]$. See (5.4). By induction, all trees (elements) in each forest (indexing set), that is, each $\tau \in \mathbb{T}_k$, $k \in \mathbb{N}$, can be written with (5.9), in the form of (5.8). The tree from (5.8) directly corresponds to the function $H_\tau = \left[\int H_{\tau^a}, \left[\int H_{\tau^b}, ..., \left[\int H_{\tau^n}, A\right] ...\right]\right]$.

5.3 Algorithm for constructing $\mathbb{T}_k$, for $k \in \mathbb{N}$.

1. Find the set $\mathbb{T}_0$ by Picard iteration on (5.1).

$$\mathbb{T}_0 = \left\{ \bullet \right\}$$

2. Take the foundation (5.9). Our possibilities for $\mathbb{T}_k$ are



(5.10)

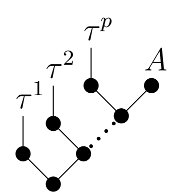
for $\tau_n \in \mathbb{T}_n, \tau_p \in \mathbb{T}_p$. So we recursively build $\mathbb{T}_k$ by collecting all trees created from $\mathbb{T}_n$ and $\mathbb{T}_p$ such that $n + p = k$ exactly like in (5.10).

5.4 Coefficient Construction Indexed by Each $\tau \in \mathbb{T}_k$.

The coefficients α_τ are also recursive functions of previous α_{τ^i}, that is, $\alpha_\tau = r\left(\alpha_{\tau^1}, \alpha_{\tau^2}, ..., \alpha_{\tau^m}\right)$. From (5.3),

$$\alpha_\tau = \frac{B_p}{p!} \prod_{i=1}^{p} \alpha_{\tau^i}.$$

We can also see this relation at the level of the trees. Given a tree $\tau \in \mathbb{T}_k$, in order to find α_τ, we look at the tree



(5.11)

Since integration is linear, and commutation is bilinear, reading from the top down we can see that the coefficients build up as $(1 \cdot \alpha_{\tau^p})$ after the commutation of $\int H_{\tau^p}$ with A, then $(1 \cdot \alpha_{\tau^p} \cdot \alpha_{\tau^{p-1}})$ following commutation of $\int H_{\tau^{p-1}}$ with $\left[\int H_{\tau^p}, A\right]$, ..., and finally $(1 \cdot \alpha_{\tau^p} \cdot \alpha_{\tau^{p-1}} \cdot ... \cdot \alpha_{\tau^2} \cdot \alpha_{\tau^1})$. The coefficient $\frac{B_p}{p!}$ appears in (5.3), from H_τ which contains exactly p commutations of previous trees. It is valuable to point out that $B_{2l+1} = 0$ for $l \in \mathbb{N}$; many coefficients α_τ end up zero.

5.5 Determination of order for the terms H_τ.

Knowledge of the structure of the elements τ in the indexing set helps us determine the order in time for each H_τ that appear in Iserles Magnus'expansion [18].

Definition 16 *Let* $\{Y_p(t)\}_{p\in\mathbb{N}}$ *be a sequence of matrix functions of time such that* $Y_p(t) \longrightarrow Y(t)$ *for all* t *in an interval around* 0. *We say that the approximation* $Y_p(t)$ *to* $Y(t)$ *is of* order q in time *if* $\frac{\|Y(t)-Y_p(t)\|}{t^{q+1}} \longrightarrow c$ *for* $0 < c < \infty$ *as* $t \rightarrow 0^+$.
For expressions $f(t)$ *continuous in* t *which satisfy* $\lim_{t\rightarrow 0^+} \frac{\|f(t)\|}{t^q} = c$ *where* $0 < c < \infty$, *we use* $O(t^q)$ *to represent* $f(t)$.

In expression (5.2), k indexes the number of integrals. But remember that for $\tau \in \mathbb{T}_k$, H_τ appears in (5.1), the expression for $D_t\Omega$. This means that for $\tau \in \mathbb{T}_k$, H_τ is a k-integral.

We have the following

Lemma 17 *For* $\tau \in \mathbb{T}_0, H_\tau = A$ *is at least an order 0 in time approximation to* $D_t\Omega$.

Proof. From (4.9), the first two terms of the Maclaurin series expansion for Ω are

$$\begin{aligned}
\Omega(t) &= \Omega(0) + D_t\Omega(0)(t-0) + O(t^2) \\
&= \mathbf{0} + \left(\sum_{k=0}^{\infty} B_k \frac{ad^k_{\Omega(0)}(A(0))}{k!}\right)(t) + O(t^2) \\
&= A(0)\,t + O(t^2)
\end{aligned}$$

This gives us that

$$\|D_t\Omega - A(0)\| = O(t)$$

Since A is continuous, $A = A(0) + O(t)$.
Now, $\lim_{t\rightarrow 0^+} \frac{\|D_t\Omega - A\|}{t} = \lim_{t\rightarrow 0^+} \frac{\|D_t\Omega - A(0) + O(t)\|}{t} = \lim_{t\rightarrow 0^+} \frac{\|D_t\Omega - A(0)\|}{t} + \frac{O(t)}{t} = \lim_{t\rightarrow 0^+} \frac{O(t)}{t}$, which if $\lim_{t\rightarrow 0^+} \frac{O(t)}{t} \neq 0$, then A is an order 0 in time approximation to Ω, else if $\lim_{t\rightarrow 0^+} \frac{O(t)}{t} = 0$, then A is a greater order in time approximation to Ω. ■

It can be shown that if $\tau^k \in \mathbb{T}_k$ and $\tau^j \in \mathbb{T}_j$, then $H_\tau = \left[\int H_{\tau^k}, H_{\tau^j}\right]$ is at least of order $k + j + 1$ in time. But we can do better.

An important contribution that Iserles [4] has made to Magnus' expansion is the recognition of order in time for each term H_τ. Specifically, we can reorganize the indexing sets $\mathbb{T}_k$ arranged according to k number of integrals, into indexing sets $\mathbb{F}_k$ (forests) arranged according to minimum order k in time.

Definition 18 *The indexing set (or forest) $\mathbb{F}_k \subset \bigcup_{p=0}^{\infty} \mathbb{T}_p$ contains all τ such that*

$$\lim_{t\to 0^+} \frac{\left\| D_t\Omega - \sum\limits_{\left(\tau' \in \bigcup_{p=0}^{\infty} \mathbb{T}_p - \{\tau\}\right)} \alpha_{\tau'} H_{\tau'} \right\|}{t^k} = c \textit{ for } 0 < c < \infty.$$

Essentially this definition means that $\tau \in \mathbb{F}_k$ iff H_τ contributes an expression to the approximation of $D_t\Omega$ which is $O(t^k)$.

We find the sets $\mathbb{F}_k$ by letting $\mathbb{F}_0 = \left\{ \bullet \right\}$, then finding $\mathbb{F}_k$ for $k \geq 1$ through application of the following theorem.

Theorem 19 $\mathbb{T}_1 \subset \mathbb{F}_2$. *Furthermore, in a neighborhood of $t = 0$, for $\tau \in \mathbb{F}_k$, $H_\tau = h_\tau t^k + O(t^{k+1})$ where h_τ is a fixed matrix. If $\tau^i \in \mathbb{F}_{k^i}, \tau^j \in \mathbb{F}_{k^j}$, then $H_\tau = \left[\int H_{\tau^i}, H_{\tau^j}\right]$ is of order $k^i + k^j + 1$ in time except when $\tau^i = \tau^j$; then $H_\tau = \left[\int H_{\tau^i}, H_{\tau^j}\right]$ is of order $k^i + k^j + 2$ in time.*

Proof. For $\tau \in \mathbb{T}_1$,

$$\begin{aligned} H_\tau &= \left[\int A, A\right] \\ &= \left[\int_0^t A(0) + \int_0^t O(\xi)\ , A(0) + O(t)\right] \\ &= \left[\int_0^t A(0)\ , A(0)\right] + \left[\int_0^t A(0)\ , O(t)\right] + \left[\int_0^t O(\xi)\ , A(0)\right] + \left[\int_0^t O(\xi)\ , O(t)\right] \\ &= [A(0)t\ , O(t)] + \left[O(t^2)\ , A(0)\right] + O(t^3) \end{aligned}$$

So, $\lim\limits_{t\to 0^+} \frac{\|H_\tau\|}{t^0} = \mathbf{0}$, and

$$\begin{aligned} \lim_{t\to 0^+} \frac{\|H_\tau\|}{t} &= \lim_{t\to 0^+} \frac{\|[A(0)t\ , O(t)] + [O(t^2)\ , A(0)] + O(t^3)\|}{t} \\ &= \lim_{t\to 0^+} \left\|[A(0)\ , O(t)] + [O(t)\ , A(0)] + O(t^2)\right\| \\ &= \mathbf{0} \end{aligned}$$

Following the same line, $\lim_{t\to 0^+} \frac{\|H_\tau\|}{t^2} = c$, where $0 < c < \infty$. Which means that for $\tau \in \mathbb{T}_1$, $H_\tau = O(t^2)$. So, $\tau \in \mathbb{F}_2$.

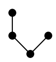
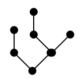
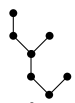
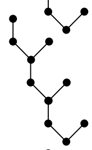
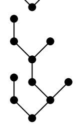
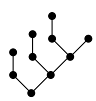
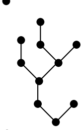
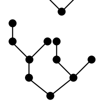
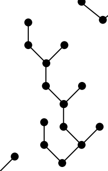
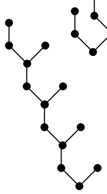
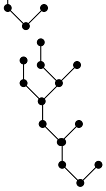
Suppose, for $\tau \in \mathbb{F}_n, n \in \{1, 2, \ldots, p-1\}$ $\quad H_\tau = h_n t^n + O(t^{n+1})$. Then for $\tau \in \mathbb{F}_m$, $H_\tau = \left[\int H_{\tau^i},\ H_{\tau^j}\right]$, where $\tau^i \in \mathbb{F}_{k^i}, \tau^j \in \mathbb{F}_{k^j}$ $\quad k^i, k^j \le p-1$. By the multilinearity of the Lie commutator,

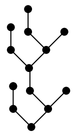
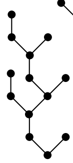
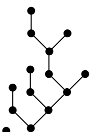
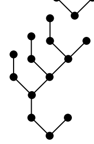
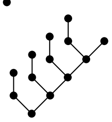
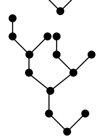
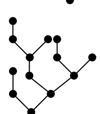
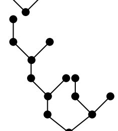
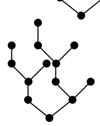
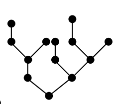
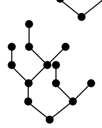
$$\begin{aligned}
H_\tau &= \left[\int H_{\tau^i}, H_{\tau^j}\right] \\
&= \left[\int \left(h_{\tau^i} t^{k^i} + O(t^{k^i+1})\right), h_{\tau^j} t^{k^j} + O(t^{k^j+1})\right] \\
&= \left[h_{\tau^i} \frac{t^{k^i+1}}{k^i+1} + O\left(t^{k^i+2}\right),\ h_{\tau^j} t^{k^j} + O\left(t^{k^j+1}\right)\right] \\
&= \left[h_{\tau^i} \frac{t^{k^i+1}}{i+1},\ h_{\tau^j} t^{k^j}\right] + O\left(t^{k^j+k^i+2}\right) \\
&= [h_{\tau^i},\ h_{\tau^j}] \frac{t^{k^j+k^i+1}}{i+1} + O\left(t^{k^j+k^i+2}\right)
\end{aligned}$$

Letting $m = k^i + k^j + 1$, $\;H_\tau = [h_{\tau^i},\ h_{\tau^j}] \frac{t^{k^j+k^i+1}}{i+1} + O\left(t^{k^j+k^i+2}\right) = h_\tau t^m + O\left(t^{k^j+k^i+2}\right)$, so $\tau \in \mathbb{F}_m$.

Now if $\tau^i = \tau^j$, then $[h_{\tau^i},\ h_{\tau^j}] = \mathbf{0}$, giving us H_τ of order $k^i + k^j + 2$ in time. ■

5.6 Table of trees (up to $\mathbb{T}_4$), the containing forest(s), and coefficients.

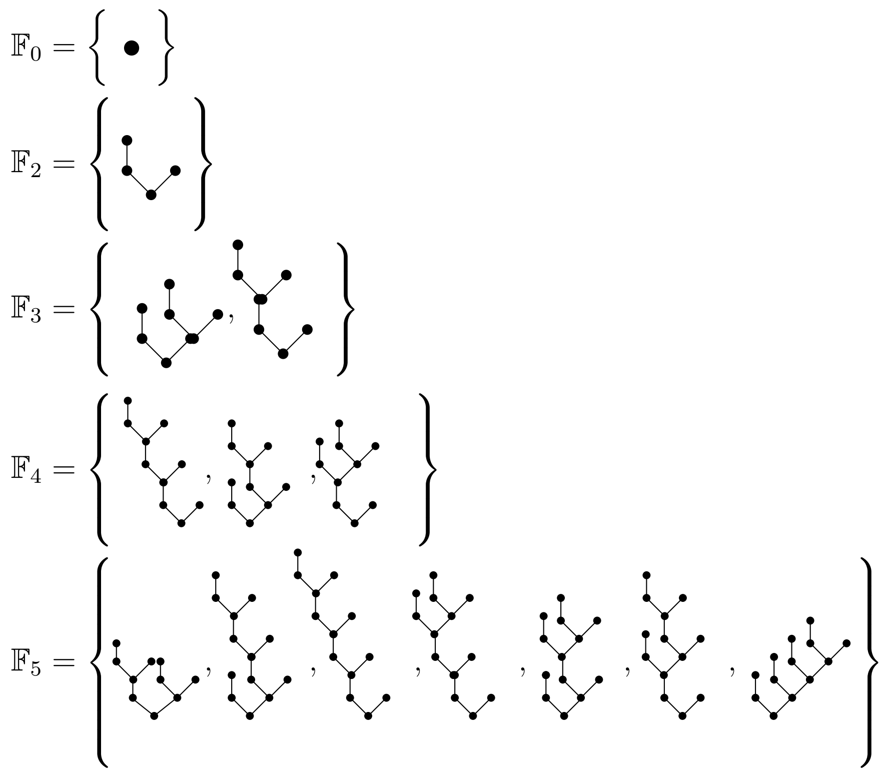
Tree τ	H_τ	*Forest*	α_τ
	A	$\mathbb{T}_0; \mathbb{F}_0$	$\frac{B_0}{0!} = 1$
	$\left[\int_{t_0}^t A, A\right]$	$\mathbb{T}_1; \mathbb{F}_2$	$\frac{B_1}{1!} = -\frac{1}{2}$
	$\left[\int_{t_0}^t A, \left[\int_{t_0}^t A, A\right]\right]$	$\mathbb{T}_2; \mathbb{F}_3$	$\frac{B_2}{2!} = \frac{1}{12}$
	$\left[\int_{t_0}^t \left[\int_{t_0}^t A, A\right], A\right]$	$\mathbb{T}_2; \mathbb{F}_3$	$\frac{B_1}{1!}\frac{B_1}{1!} = \frac{1}{4}$
	$\left[\int_{t_0}^t \left[\int_{t_0}^t \left[\int_{t_0}^t A, A\right], A\right], A\right]$	$\mathbb{T}_3; \mathbb{F}_4$	$\frac{B_1}{1!}\frac{B_1}{1!}\frac{B_1}{1!} = -\frac{1}{8}$
	$\left[\int_{t_0}^t A, \left[\int_{t_0}^t \left[\int_{t_0}^t A, A\right], A\right]\right]$	$\mathbb{T}_3; \mathbb{F}_4$	$\frac{B_1}{1!}\frac{B_2}{2!} = -\frac{1}{24}$
	$\left[\int_{t_0}^t A, \left[\int_{t_0}^t A, \left[\int_{t_0}^t A, A\right]\right]\right]$	$\mathbb{T}_3; \mathbb{F}_4$	$\frac{B_1}{1!}\frac{B_1}{1!}\frac{B_1}{1!}\frac{B_3}{3!} = 0$
	$\left[\int_{t_0}^t \left[\int_{t_0}^t A, \left[\int_{t_0}^t A, A\right]\right], A\right]$	$\mathbb{T}_3; \mathbb{F}_4$	$\frac{B_2}{2!}\frac{B_1}{1!} = -\frac{1}{24}$
	$\left[\int_{t_0}^t \left[\int_{t_0}^t A, A\right], \left[\int_{t_0}^t A, A\right]\right]$	$\mathbb{T}_3; \mathbb{F}_5$	$\frac{B_1}{1!}\frac{B_2}{2!} = -\frac{1}{24}$
	$\left[\int_{t_0}^t A, \left[\int_{t_0}^t \left[\int_{t_0}^t \left[\int_{t_0}^t A, A\right], A\right], A\right]\right]$	$\mathbb{T}_4; \mathbb{F}_5$	$\frac{B_2}{2!}\frac{B_1}{1!}\frac{B_1}{1!} = \frac{1}{48}$
	$\left[\int_{t_0}^t \left[\int_{t_0}^t \left[\int_{t_0}^t \left[\int_{t_0}^t A, A\right], A\right], A\right], A\right]$	$\mathbb{T}_4; \mathbb{F}_5$	$\frac{B_1}{1!}\frac{B_1}{1!}\frac{B_1}{1!}\frac{B_1}{1!} = \frac{1}{16}$
	$\left[\int_{t_0}^t \left[\int_{t_0}^t \left[\int_{t_0}^t A, \left[\int_{t_0}^t A, A\right]\right], A\right], A\right]$	$\mathbb{T}_4; \mathbb{F}_5$	$\frac{B_1}{1!}\frac{B_1}{1!}\frac{B_2}{2!} = \frac{1}{48}$

Tree τ	H_τ	*Forest*	α_τ
	$\left[\int_{t_0}^t A, \left[\int_{t_0}^t \left[\int_{t_0}^t A, \left[\int_{t_0}^t A, A\right]\right], A\right]\right]$	$\mathbb{T}_4; \mathbb{F}_5$	$\frac{B_2}{2!}\frac{B_2}{2!} = \frac{1}{144}$
	$\left[\int_{t_0}^t \left[\int_{t_0}^t A, \left[\int_{t_0}^t \left[\int_{t_0}^t A, A\right], A\right]\right], A\right]$	$\mathbb{T}_4; \mathbb{F}_5$	$\frac{B_1}{1!}\frac{B_1}{1!}\frac{B_2}{2!} = \frac{1}{48}$
	$\left[\int_{t_0}^t A, \left[\int_{t_0}^t A, \left[\int_{t_0}^t \left[\int_{t_0}^t A, A\right], A\right]\right]\right]$	$\mathbb{T}_4; \mathbb{F}_5$	$\frac{B_3}{3!}\frac{B_1}{1!} = 0$
	$\left[\int_{t_0}^t \left[\int_{t_0}^t A, \left[\int_{t_0}^t A, \left[\int_{t_0}^t A, A\right]\right]\right], A\right]$	$\mathbb{T}_4; \mathbb{F}_5$	$\frac{B_1}{1!}\frac{B_3}{3!} = 0$
	$\left[\int_{t_0}^t A, \left[\int_{t_0}^t A, \left[\int_{t_0}^t A, \left[\int_{t_0}^t A, A\right]\right]\right]\right]$	$\mathbb{T}_4; \mathbb{F}_5$	$\frac{B_4}{4!} = -\frac{1}{720}$
	$\left[\int_{t_0}^t \left[\int_{t_0}^t \left[\int_{t_0}^t A, A\right], \left[\int_{t_0}^t A, A\right]\right], A\right]$	$\mathbb{T}_4; \mathbb{F}_6$	$\frac{B_1}{1!}\frac{B_1}{1!}\frac{B_2}{2!} = \frac{1}{48}$
	$\left[\int_{t_0}^t A, \left[\int_{t_0}^t \left[\int_{t_0}^t A, A\right], \left[\int_{t_0}^t A, A\right]\right]\right]$	$\mathbb{T}_4; \mathbb{F}_6$	$\frac{B_3}{3!}\frac{B_1}{1!} = 0$
	$\left[\int_{t_0}^t \left[\int_{t_0}^t \left[\int_{t_0}^t A, A\right], A\right], \left[\int_{t_0}^t A, A\right]\right]$	$\mathbb{T}_4; \mathbb{F}_6$	$\frac{B_2}{2!}\frac{B_1}{1!}\frac{B_1}{1!} = \frac{1}{48}$
	$\left[\int_{t_0}^t \left[\int_{t_0}^t A, A\right], \left[\int_{t_0}^t \left[\int_{t_0}^t A, A\right], A\right]\right]$	$\mathbb{T}_4; \mathbb{F}_6$	$\frac{B_2}{2!}\frac{B_1}{1!}\frac{B_1}{1!} = \frac{1}{48}$
	$\left[\int_{t_0}^t \left[\int_{t_0}^t A, A\right], \left[\int_{t_0}^t A, \left[\int_{t_0}^t A, A\right]\right]\right]$	$\mathbb{T}_4; \mathbb{F}_6$	$\frac{B_3}{3!}\frac{B_1}{1!} = 0$
	$\left[\int_{t_0}^t \left[\int_{t_0}^t A, \left[\int_{t_0}^t A, A\right]\right], \left[\int_{t_0}^t A, A\right]\right]$	$\mathbb{T}_4; \mathbb{F}_6$	$\frac{B_2}{2!}\frac{B_2}{2!} = \frac{1}{144}$

(Recall that the functions H_τ appear in the expression for $D_t\Omega$ in (5.3).)

5.7 The algorithm

Collecting terms from the forests $\mathbb{T}_k$ into forests $\mathbb{F}_p$ according to *pth* order in time as specified by Theorem 19 shown in Table 2, and ignoring those with coefficient zero, it turns out that we have a computationally efficient expression for the *index sets of* $D_t\Omega$ in (5.3). Specifically these index sets are given by



(Table 3)

So equation (5.3) becomes instead

$$D_t\Omega = \sum_{k=0}^{\infty}\left(\sum_{\tau\in\mathbb{F}_k}\alpha_\tau H_\tau\right) \tag{5.12}$$

where k indexes the forest of trees according to order in time and H_τ are the functions indexed by τ. Now in order to solve Hausdorff's equation (5.1), all we need to do is integrate the expression (5.12). This gives us

$$\Omega = \sum_{k=0}^{\infty}\left(\sum_{\tau\in\mathbb{F}_k}\alpha_\tau \int H_\tau\right) \tag{5.13}$$

as the solution. For an approximation of order in time t^{m+1}, we can truncate the solution at m to give us

$$\Omega_m = \sum_{k=0}^{m} \left(\sum_{\tau \in \mathbb{F}_k} \alpha_\tau \int H_\tau \right). \tag{5.14}$$

In order to build an order m in time approximation Ω_m,

1. Build the forests $\mathbb{T}_k$ up to the desired order in time (which is a little more than necessary, but sufficient).
2. Construct the coefficients α_τ according to $\alpha_\tau = \frac{B_p}{p!} \prod_{i=1}^{p} \alpha_{\tau^i}$.
3. Determine the order in time for the terms H_τ.
4. Collect the terms into the new indexing forests $\mathbb{F}_k$.
5. Write down the expression for Ω_m, taking advantage of the recursive nature of each H_τ.

This provides us with a means to compute Magnus' expansion to the desired order.

5.8 Summary

What Iserles has done is to take the work of Wilhelm Magnus and extend it to a form amenable to computation. Given a differential equation of the form (3.1) , with fundamental solution $e^\Omega = \Phi$, the expression for Magnus' expansion, using Iserles reordering is (5.13).

We now address the questions which naturally arise:

1. For what values of t does $\Omega_m(t)$ converge to $\Omega(t)$ as $m \to \infty$?
2. If Ω_m converges, how close is Ω_m to Ω for a given m?
3. For what values of t is $e^{\Omega(t)} = \Phi(t)$?
4. Exactly how close is e^{Ω_m} to Φ for a given m?

6 Estimates for Convergence of Magnus' Expansion

Given an arbitrary power series of a real variable, the first question that should come to mind is: for what values of the real variable does the power series converge? For Magnus' expansion, this is a difficult question. The first result regarding the convergence of Magnus' expansion is little more than an exercise in brute force norm estimates for absolute convergence. The second convergence estimate relies on a more subtle rewriting of Magnus' expansion using step functions.

The Brute - Force Approach.

We start with Hausdorff's equation, (4.9), and the expansion of the solution is given as

$$\Omega = \sum_{k=1}^{\infty} \Gamma_k \tag{6.1}$$

where Γ_k is the sum of elements from the set $\mathbb{T}_k$.

Substituting (6.1) into (4.9), much the same as in the previous chapter, we get

$$D_t \left(\sum_{k=1}^{\infty} \Gamma_k \right) = \sum_{m=0}^{\infty} \frac{B_m}{m!} ad^m_{\left(\sum_{k=0}^{\infty} \Gamma_k \right)} (A)$$

Collecting terms on the right according to the number of commutators (or equivalently, the number of integrals) and integrating, we find that Magnus' expansion accepts the form

$$\begin{aligned} \Gamma_1 (t) &= \int_0^t A(\xi)\, d\xi \\ \Gamma_n (t) &= \sum_{j=1}^{n-1} \frac{B_j}{j!} \int_0^t S_n^{(j)} (\xi)\, d\xi \end{aligned} \tag{6.2}$$

where

$$\begin{aligned} S_n^{(j)} &= \sum_{m=1}^{n-j} ad_{\Gamma_m}\left(S_{n-m}^{(j-1)}\right) \text{ for } 2 \leq j \leq n-1 \\ S_n^{(1)} &= ad_{\Gamma_{n-1}}(A) \quad S_n^{(n-1)} = ad_{\Gamma_1}^{n-1}(A) \end{aligned} \tag{6.3}$$

Insert (6.2) into (6.3). This gives us the expressions

$$\begin{aligned} S_n^{(j)}(t) &= \left[\int_0^t A(\xi)\,d\xi, S_{n-1}^{(j-1)}(t)\right] + \sum_{m=2}^{n-j}\left[\left\{\sum_{k=1}^{m-1}\frac{B_k}{k!}\int_0^t S_m^{(k)}(\xi)\,d\xi\right\}, S_{n-m}^{(j-1)}(t)\right] \\ S_n^{(1)} &= \left[\left\{\sum_{j=1}^{n-2}\frac{B_j}{j!}\int_0^t S_{n-1}^{(j)}(\xi)\,d\xi\right\}, A\right] \quad S_n^{(n-1)} = ad^{n-1}_{\left\{\int_0^t A(\xi)d\xi\right\}}(A) \end{aligned}$$

After substituting these expressions for the S_i's into (6.2), then substituting (6.2) into (6.1), and taking the norm of (6.1), [23] states the convergence of Magnus' expansion as:

> a numerical application of the D'Alembert criterion of convergence [ratio test] directly leads (up to numerical precision) to

$$f(t) = \int_0^t \|A(\xi)\|\,d\xi \leq 1.086869 \tag{6.4}$$

The Step Function Approach.

A second approach by PC Moan and JA Oteo [22] is an effort to expand the radius of convergence beyond the previous estimate. This time, they use the solution to (4.2) in the form

$$\Omega(t) = \sum_{n=1}^{\infty}\Gamma_n(t) = \sum_{n=1}^{\infty}\int_0^t \cdots \int_0^t L_n(t_n,\ldots,t_1)\,A(t_n)\cdots A(t_1)\,dt_n\cdots dt_1$$

where

$$L_n\left(t_n,\ldots,t_1\right)=\frac{\Theta_n!\left(n-1-\Theta_n\right)!}{n!}\left(-1\right)^{\left(n-1-\Theta_n\right)!}$$

with $\Theta_n=\theta_{n-1,n-2}+\ldots+\theta_{2,1}$ and $\theta_{a,b}=1$ if $t_a>t_b$ and 0 otherwise.

By using this expression, they are able to bypass the commutator structure of Magnus' expansion. Yet, the commutator structure can be recovered if desired, but will be avoided here.

The L_∞-norm is applied to the Γ_n, giving

$$\left\|\Gamma_n\left(t\right)\right\|_\infty\leq\left(\left\|A\right\|_\infty\right)^n\int_0^t\cdots\int_0^t\left|L_n\left(t_n,\ldots,t_1\right)\right|dt_n\cdots dt_1$$

They observe that L_n is constant on all sections of the $n-cube$ $\left[0,t\right]^n$ corresponding to constant $\Theta_n=k$. So a calculation of the fraction of the volume of $\left[0,1\right]^n$ for a given k $\left(V_n^k\right)$ gives us the bound

$$\left\|\Gamma_n\left(t\right)\right\|_\infty\leq\left(t\cdot\left\|A\right\|_\infty\right)^n\sum_{k=0}^{n-1}V_n^k\frac{k!\left(n-1-k\right)!}{n!}$$

A bound on the expression for $\sum\limits_{k=0}^{n-1}V_n^k\frac{k!(n-1-k)!}{n!}$ is derived and is

$$\sum_{k=0}^{n-1}V_n^k\frac{k!\left(n-1-k\right)!}{n!}\leq 2^{-(n-1)}$$

so that a full bound on the convergence of $\Omega\left(t\right)$ is

$$\left\|\Omega\left(t\right)\right\|_\infty\leq\sum_{n=1}^{\infty}\left(t\cdot\left\|A\left(t\right)\right\|_\infty\right)^n2^{-(n-1)}$$

And D'Alembert's criteria requires that

$$t\cdot\left\|A\right\|_\infty<2\tag{6.5}$$

Neither (6.4) nor (6.5) is (strictly) stronger. In fact, a couple of examples will demonstrate the incomparability of the two.

Example 20 *Let* $A(t) = \begin{pmatrix} 0 & 1 \\ f(t) & 0 \end{pmatrix}$

Consider $f(t) = \cos^2(b \cdot t)$ *so that* $\|A(t)\| \sim |\cos(b \cdot t)|$. *Notice that* (6.5) *gives us a radius of convergence of* $t \sim 2$; *yet* (6.4) *gives us a radius of convergence of* $t \sim b$.

Consider $f(t) = \begin{cases} (\epsilon+1)^2 & , t_1 \leq t \leq t_2 \\ \epsilon^2 & , \textit{otherwise} \end{cases}$ *so that* $\|A(t)\| \sim \begin{cases} \epsilon+1 & , t_1 \leq t \leq t_2 \\ \epsilon & , \textit{otherwise} \end{cases}$
Notice that (6.5) *gives us a radius of convergence of* $t \sim t_1$; *yet* (6.4) *gives us a radius of convergence of* $t \sim \frac{1}{\epsilon}$.

Notice that neither (6.4) nor (6.5) consider whether A is commutative, in which Magnus' expansion would yield an exact solution for all time. We can see that both estimates (6.4) and (6.5) for the radius of convergence are unsatisfactory.

7 Examples

In an effort to provide motivation for studying questions of convergence, as well as to display the nice properties of the Magnus' expansion approach, a few numerical implementations are provided. These examples provide us with some evidence for what convergence results might be possible.

7.1 The Mathieu Example

Let's consider for a first numerical example[1] the ODE system known as the Mathieu equation. The Mathieu equation arises as a model of a cyclic stiffness in a spring-mass system. In unitless form, it is the second order differential equation of period 2π with the initial conditions

$$D_t^{(2)} y(t) + (a + b\cos(t))\, y(t) = 0,\ y(0) = y_0,\ D_t y(0) = y_1$$

This equation can be written as the first order system

$$D_t \Phi(t) + \begin{pmatrix} 0 & 1 \\ a + b\cos(t) & 0 \end{pmatrix} \Phi(t) = \mathbf{0}, \quad \Phi(0) = I \tag{7.1}$$

For example, Iserles' order 4 in time version of Magnus' expansion (5.14) is

$$\begin{aligned}
\Omega_4(t) \;=\;& \int_0^t \begin{pmatrix} 0 & 1 \\ -a - b\cos(\xi_1) & 0 \end{pmatrix} d\xi_1 + \\
& -\frac{1}{2}\int_0^t \int_0^{\xi_1} b\left(\cos(\xi_2) - \cos(\xi_1)\right) \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} d\xi_2 d\xi_1 + \\
& \frac{1}{12}\int_0^t \int_0^{\xi_1} \int_0^{\xi_1} 2b\left(\cos(\xi_2) - \cos(\xi_1)\right) \begin{pmatrix} 0 & 1 \\ -a - b\cos(\xi_3) & 0 \end{pmatrix} d\xi_3 d\xi_2 d\xi_1 + \\
& \frac{1}{4}\int_0^t \int_0^{\xi_1} \int_0^{\xi_2} 2b\left(\cos(\xi_2) - \cos(\xi_1)\right) \begin{pmatrix} 0 & 1 \\ -a - b\cos(\xi_3) & 0 \end{pmatrix} d\xi_3 d\xi_2 d\xi_1
\end{aligned}$$

[1] The computer code in Mathematica® used for these examples is given in the appendix (E).

For the numerical computations below, we have used the order 6 and order 8 Magnus' expansion as indicated.

Taking advantage of Mathematica's built-in Mathieu functions, we can create an exact fundamental solution which we compare Magnus' solution to. These built-in Mathieu functions are well understood. [2].

Using this, we have a solution to compare to the Magnus solution. For this comparison, we have two alternatives:

1. entrywise examination of the matrices, or

2. an operator norm examination.

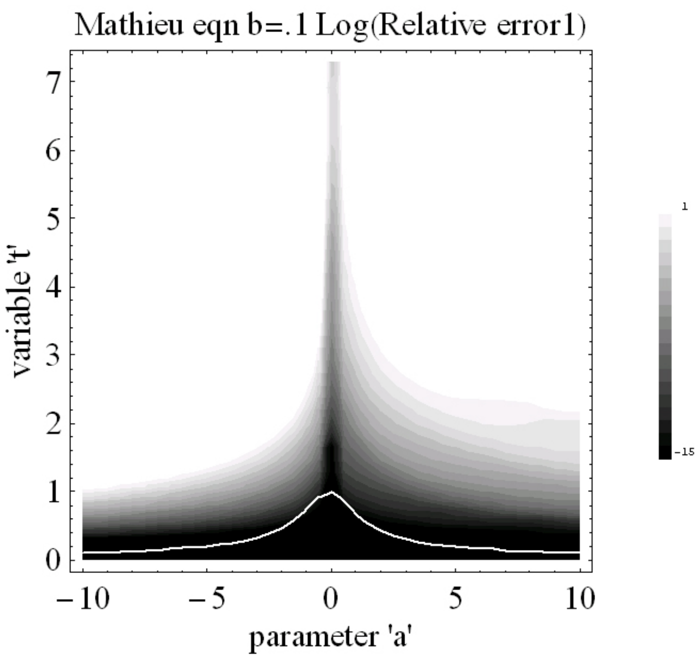
Our choice is to use the Frobenius norm

$$\|A\|_F = \sqrt{Trace(A \cdot A^{\dagger})}.$$

From the order 8 approximation, the relative error $\left\|\left(e^{\Omega_8(t)} - \Phi\right) \cdot \Phi^{-1}\right\|_F$ can be found by computing the solution Ψ to the adjoint equation, also a Mathieu equation, and computing

$$\left\|\left(e^{\Omega_8(t)} - \Phi\right) \cdot \Phi^{-1}\right\|_F = \left\|e^{\Omega_8(t)} \cdot \Psi^T - I\right\|_F$$

Using this relative error with the order 8 in time Magnus' expansion and the adjoint solution found using built-in Mathieu functions, the relative error as an analytic function of time dependent on the parameters a and b was found. Setting b to the value $b = .1$, we produce in the picture below, a contour plot of the logarithm of the relative error. The lighter line in the shape of a bell curve is an estimate of the convergence for $\Omega(t)$ as given by (6.4).



The black region corresponds to the error on the order of $e^{-15} \sim 10^{-7}$ which increases to the white region with an error of order 1.

Example 21 *A reasonable case to consider is where the ODE is commutative. Mathieu's equation* (7.1) *is an example when there is no driving force, that is, when* $b = 0$:

$$D_t\Phi\left(t\right) + \begin{pmatrix} 0 & 1 \\ a & 0 \end{pmatrix} \Phi\left(t\right) = \mathbf{0} \quad \Phi\left(0\right) = I$$

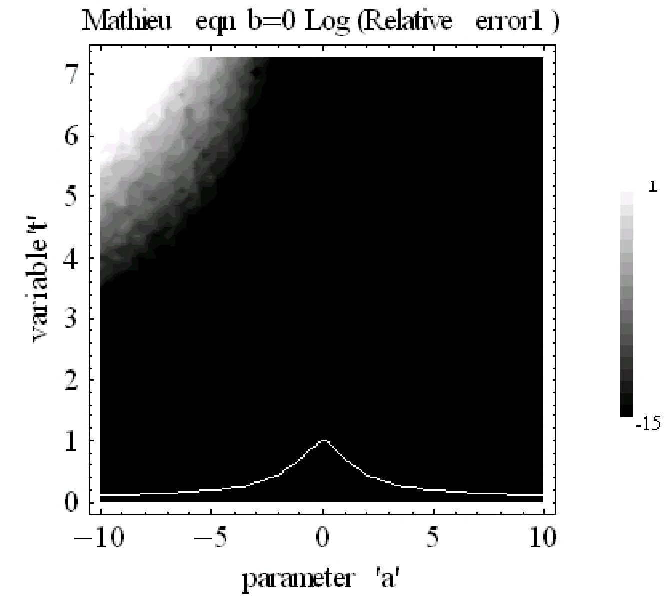
Magnus' expansion is

$$\Omega\left(t\right) = \int_0^t \begin{pmatrix} 0 & 1 \\ -a & 0 \end{pmatrix} d\xi_1,$$

exactly, *for all orders in time. So, provided our parameter dependent fundamental solution is correct, we expect the fundamental solution found from exponentiating Magnus' expansion should be*

$$\Phi(t) = e^{\int_0^t \begin{pmatrix} 0 & 1 \\ -a & 0 \end{pmatrix} d\xi} = \begin{pmatrix} \cos\left(\sqrt{a}t\right) & \frac{\sin\left(\sqrt{a}t\right)}{\sqrt{a}} \\ -\sqrt{a}\sin\left(\sqrt{a}t\right) & \cos\left(\sqrt{a}t\right) \end{pmatrix}$$

The contour plot of our relative error produced this picture:



There are two features of this plot that we should note. First, the black region for convergence extends well beyond the analytic estimate for the radius of convergence. And second, we have a large discrepancy between the built-in solution and the Magnus' approximation where a is negative for large t. The fact that we have convergence beyond the analytic estimate is expected, as suggested in section (6). As for the discrepancy in the solution, we neglected the fact that for negative a, the solution Φ has the appearance

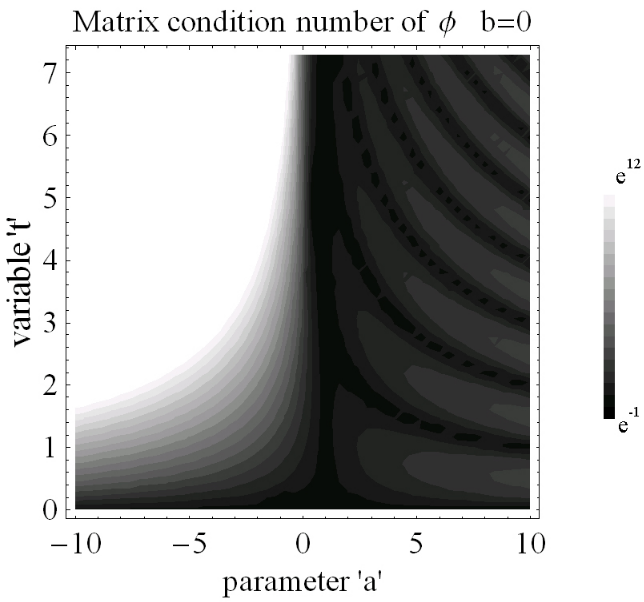
$$\Phi(t) = \begin{pmatrix} \cosh\left(\sqrt{|a|}t\right) & -\frac{\sinh\left(\sqrt{|a|}t\right)}{\sqrt{|a|}} \\ \sqrt{|a|}\sinh\left(\sqrt{|a|}t\right) & \cosh\left(\sqrt{|a|}t\right) \end{pmatrix}$$

What this means is that when t is fairly large, $\frac{\cosh\left(\sqrt{|a|}t\right)}{\sinh\left(\sqrt{|a|}t\right)} \sim \frac{\frac{1}{2}e^{\sqrt{|a|}t}}{\frac{1}{2}e^{\sqrt{|a|}t}} = 1$, so that for $a < 0$,

$$\Phi(t) \sim \frac{1}{2}e^{\sqrt{|a|}t} \begin{pmatrix} 1 & -\frac{1}{\sqrt{|a|}} \\ \sqrt{|a|} & 1 \end{pmatrix} \text{ and } \Phi^{-1}(t) \sim 2e^{-\sqrt{|a|}t} \begin{pmatrix} 1 & -\sqrt{|a|} \\ \frac{1}{\sqrt{|a|}} & 1 \end{pmatrix}$$

Noticing this, we can see that $\|\Phi(t)\|_\infty \sim e^{\sqrt{|a|}t}\left(1+\sqrt{|a|}\right)$ and $\|\Phi^{-1}(t)\|_\infty \sim e^{-\sqrt{|a|}t}\left(1+\sqrt{|a|}\right)$. Essentially, the point is that the solution matrices have a wide range of eigenvalues and are ill-conditioned. For example, the matrix $\begin{pmatrix} 10^5 & 0 \\ 0 & 10^{-5} \end{pmatrix}$ has the inverse $\begin{pmatrix} 10^{-5} & 0 \\ 0 & 10^5 \end{pmatrix}$, yet the dominant term is 10^5, so either matrix appears to be $10^5 \begin{pmatrix} 10^{-10} & 0 \\ 0 & 1 \end{pmatrix} \sim 10^5 \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$ a singular matrix. This is an example of a <u>stiff</u> system. For our system, the condition number $\sim \left(1+\sqrt{|a|}\right)^2$. And any condition number $\gg$1 tells us that having an ill-conditioned matrix will result in something like having a system with fewer eigenvalues than the dimension of the vector space that the matrix operates on. What this means for us is that any computation done with any of $\Phi(t)$, ϕ, or Ψ will not be accurate since only the largest eigenvalues of the system dominate and determine what the solution will appear like, independent of the 'true' solution.

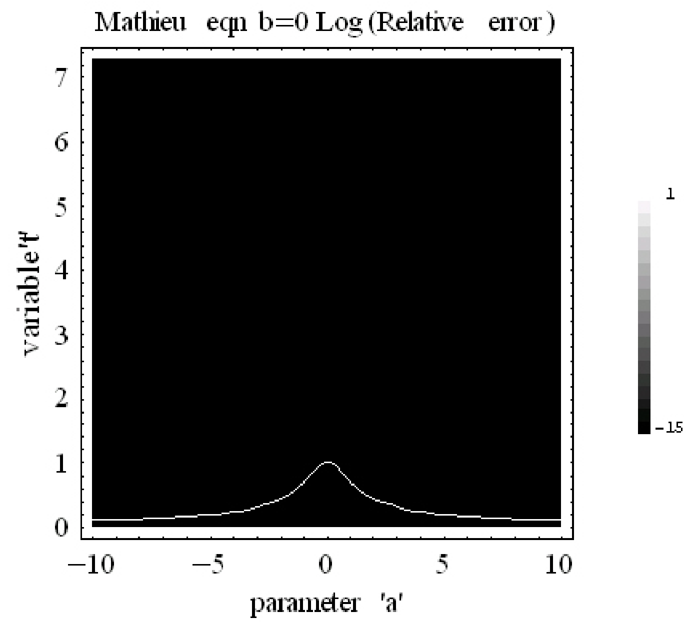
In the following picture, we show a plot of the condition number ($= \|\Phi(t)\|\,\|\Phi^{-1}(t)\|$) of the solution found from built-in Mathieu functions. Note the huge values of the condition number in the region $a < 0, t > 0$.



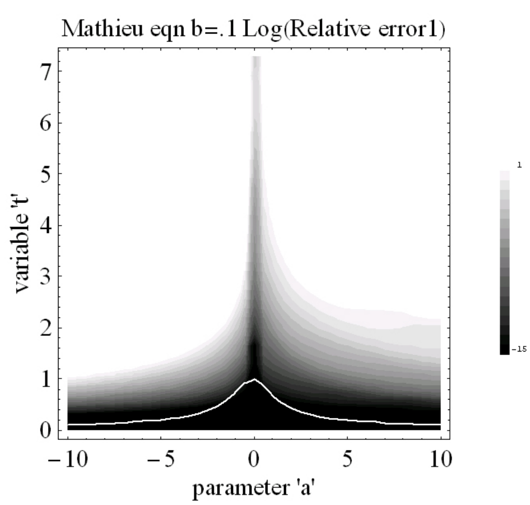
In order to work around having ill-conditioned matrices, it required the use of a different relative error. The second relative error that was calculated is

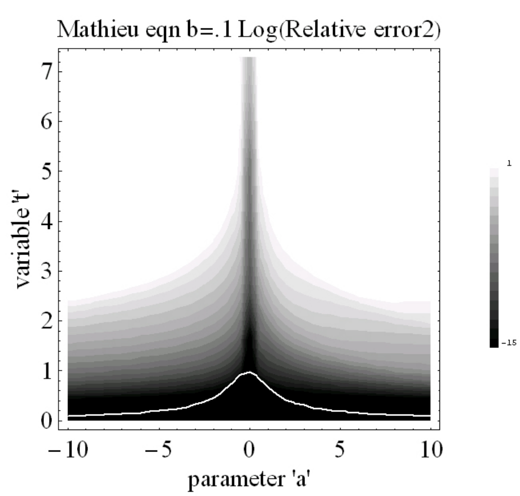
$$\text{Relative error 2} = \frac{\left\|\left(e^{\Omega_8(t)} - \Phi\right)\right\|_F}{\|\Phi\|_F}$$

Using this second relative error, we produced the plot



Notice that the order of magnitude for $a < 0$ is correct. This confirms that in the commutative case, we have a correct solution. For a matter of comparison, with $b = 0.1$, we place side by side the contour plots of the relative error of Magnus' approximation using the two different relative errors.





7.2 A Non-commutative Example

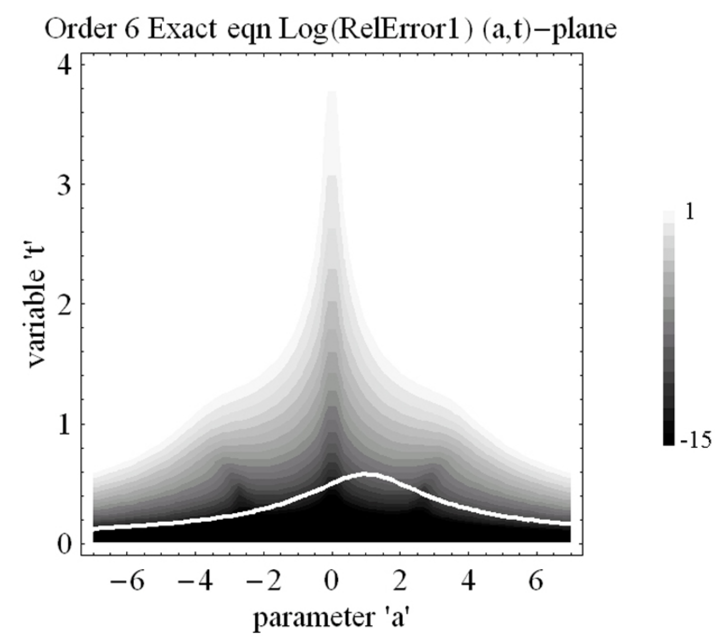
For a second example, we chose a 2×2 coupled system defined by the equation

$$D_t\Phi(t) + \begin{pmatrix} 1 - a\cos^2(t) & -1 + a\cos(t)\sin(t) \\ 1 + a\cos(t)\sin(t) & 1 - a\sin^2(t) \end{pmatrix} \Phi(t) \quad \Phi(0) = I \qquad (7.2)$$

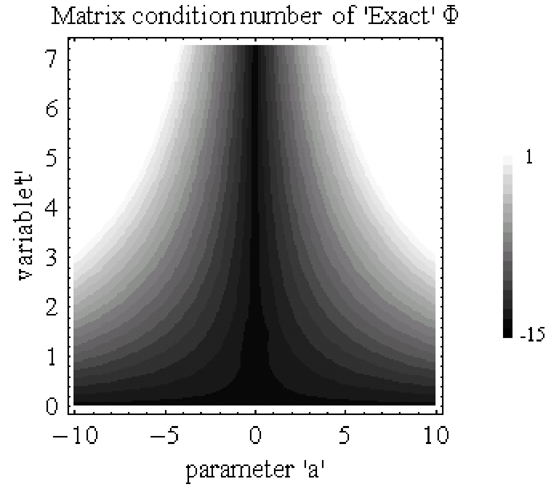
This example was chosen because it has a known 'exact' solution

$$\Phi(t) = \begin{pmatrix} e^{(a-1)t}\cos(t) & e^{-t}\sin(t) \\ -e^{(a-1)t}\sin(t) & e^{-t}\cos(t) \end{pmatrix}$$

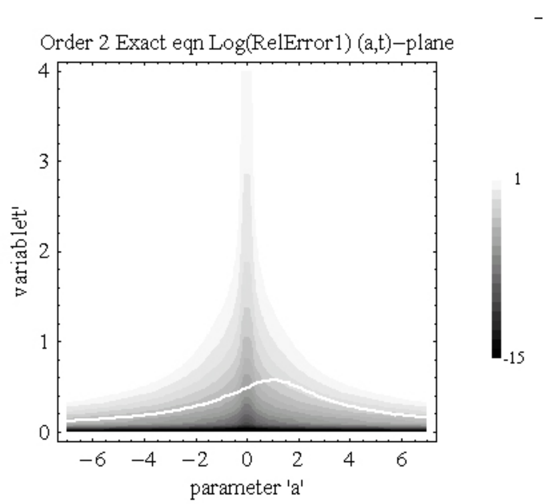
Note that $\begin{pmatrix} -1 + a\cos^2(t) & 1 - a\cos(t)\sin(t) \\ -1 - a\cos(t)\sin(t) & -1 + a\sin^2(t) \end{pmatrix}$ is a noncommutative matrix function, except for the parameter value $a = 0$. The order 6 in time Magnus' approximation, $e^{\Omega_6(t)}$, with the first relative error $\left(Relative\ error = \left\|\left(e^{\Omega_6(t)} - \Phi\right) \cdot \Phi^{-1}\right\|_F\right)$ produces the contour plot

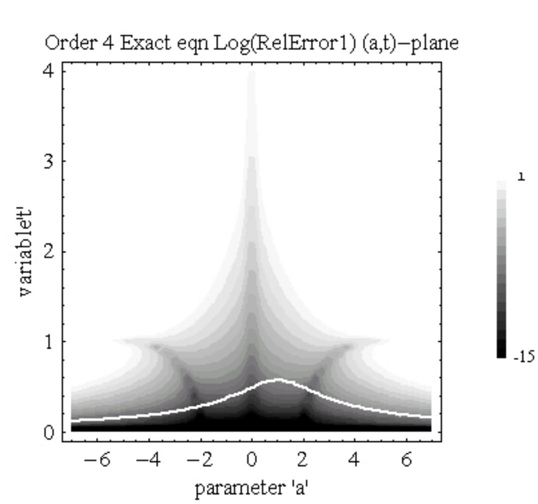


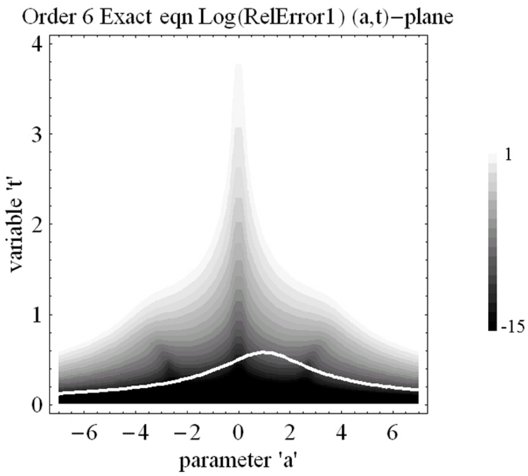
Again, the lighter line marks the analytic estimate of (6.4) for the radius of convergence of Magnus' expansion. In order to verify that the solution is close in the region we plotted, we produced a contour plot of the condition number of $\Phi(t)$.

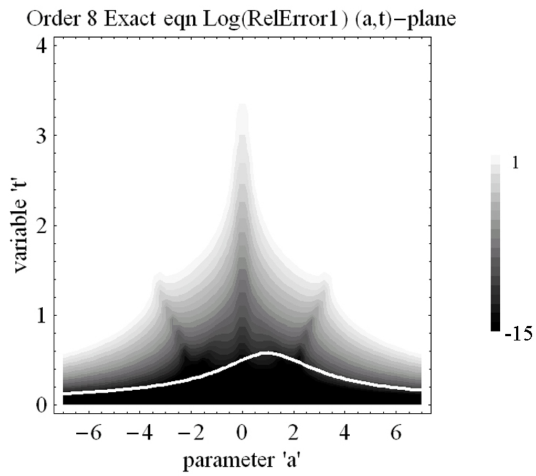


From these, we have every reason to believe that our solution is close in the region $-7 < a < 7$, $0 < t < 2\pi + 1$. To make a point about the convergence estimate of Magnus' expansion, included below are plots from the order 2 in time Magnus expansion to the order 8 in time Magnus' expansion.









Notice the growth of the black region (convergent area) from one plot to the next. This illustrates the rough convergence of Magnus' expansion as the order in time grows for this example.

7.3 A Frenet Example

Recall the Frenet relations from differential geometry [10]

$$\begin{aligned} D_s \overrightarrow{\mathbf{T}}(s) &= \kappa(s)\, \overrightarrow{\mathbf{N}}(s) \\ D_s \overrightarrow{\mathbf{N}}(s) &= -\kappa(s)\, \overrightarrow{\mathbf{T}}(s) - \tau(s)\, \overrightarrow{\mathbf{B}}(s) \\ D_s \overrightarrow{\mathbf{B}}(s) &= \tau(s)\, \overrightarrow{\mathbf{N}}(s) \end{aligned}$$

where $\overrightarrow{\mathbf{T}}(s)$, $\overrightarrow{\mathbf{N}}(s)$, and $\overrightarrow{\mathbf{B}}(s)$ are the tangent, normal, and binormal unit vectors of an orthogonal frame[2] on the curve $\alpha(s) \in \mathbb{R}^3$ parametrized by the arclength s and $\kappa(s)$, $\tau(s)$ are the curvature and torsion of $\alpha(s)$. Each unit vector has three scalar components, meaning that for a fixed number s, $\overrightarrow{\mathbf{T}}(s) = \{T_1(s), T_2(s), T_3(s)\}$, likewise $\overrightarrow{\mathbf{N}}(s)$, and $\overrightarrow{\mathbf{B}}(s)$. For emphasis,

$$D_s \overrightarrow{\mathbf{T}}(s) = \kappa(s)\, \overrightarrow{\mathbf{N}}(s) = \{\kappa(s) N_1(s), \kappa(s) N_2(s), \kappa(s) N_3(s)\}$$

[2]Notice that since these are all orthogonal unit vectors, we are dealing with some subset of the Lie group SO(3).

. Looking closely, this is a first order, linear ODE in the form

$$D_s \begin{pmatrix} T_1(s) & T_2(s) & T_3(s) \\ N_1(s) & N_2(s) & N_3(s) \\ B_1(s) & B_2(s) & B_3(s) \end{pmatrix} + \begin{pmatrix} 0 & -\kappa(s) & 0 \\ \kappa(s) & 0 & -\tau(s) \\ 0 & \tau(s) & 0 \end{pmatrix} \begin{pmatrix} T_1(s) & T_2(s) & T_3(s) \\ N_1(s) & N_2(s) & N_3(s) \\ B_1(s) & B_2(s) & B_3(s) \end{pmatrix} = \mathbf{0} \tag{7.3}$$

Using this, we can construct an example in the matrix algebra $M_3(\mathbb{R})$.

In order to construct a non-trivial example, to which we know the exact solution, we started with the curve $\alpha(t) = (\cos(t), \sin(t), f(t))$, with $f(t)$ a yet-to-be-determined function. First, we parametrize the curve α with respect to arclength. Arclength, $s(t)$, is given by

$$s(t) = \int_0^t \sqrt{1 + (D_\theta f(\theta))^2}\, d\theta$$

The trick we need to utilize is this: $1 + (D_\theta f(\theta))^2$ needs to be a 'perfect square,' e.g. $1 + (D_\theta f(\theta))^2 = (g(\theta))^2$ where $g(\theta)$ is a 'nice' function. Let $D_\theta f(\theta) = \sinh(\theta)$. This allows us to integrate the arclength for a non-trivial example . This gives us the arclength for $\alpha(t)$ as

$$\begin{aligned} s(t) &= \int_0^t \sqrt{1 + (\sinh(\theta))^2}\, d\theta \\ &= \int_0^t \cosh(\theta)\, d\theta = \sinh(t) \end{aligned}$$

We also need $f(t)$, given by $D_\theta f(\theta) = \sinh(\theta)$. Integrating this separable differential equation yields $f(t) = \cosh(t) + constant$. Parametrizing the curve α by arclength gives us

$$\begin{aligned} \alpha(s) &= \left(\cos\left(\sinh^{-1}(s)\right), \sin\left(\sinh^{-1}(s)\right), \cosh\left(\sin h^{-1}(s)\right)\right) \\ &= \left(\cos\left(\sinh^{-1}(s)\right), \sin\left(\sin h^{-1}(s)\right), \sqrt{1+s^2}\right) \end{aligned}$$

Now for the tangent, normal and binormal unit vectors, we use the definitions $\overrightarrow{\mathbf{T}}(s) = D_s\alpha(s)$, $\overrightarrow{\mathbf{N}}(s) = \frac{D_s^{(2)}\alpha(s)}{\left\| D_s^{(2)}\alpha(s) \right\|}$, and $\overrightarrow{\mathbf{B}}(s) = \overrightarrow{\mathbf{T}}(s) \times \overrightarrow{\mathbf{N}}(s)$.

[2] Exercise: A second non-trivial example is $\alpha(s) = (\cos(s), \sin(s), Ln(\cosh(s)))$; again, some form of a helix. Note that the derivation and any Magnus' results are nearly the same as for this non-trivial example.

The expressions for the curvature and torsion are found by the definitions $\kappa(s) = \left\| D_s \overrightarrow{\mathbf{T}}(s) \right\|$, and $\tau(s) = -\overrightarrow{\mathbf{N}}(s) \cdot D_s \overrightarrow{\mathbf{B}}(s)$. These yield

$$\begin{aligned} \kappa(s) &= \frac{\sqrt{2}}{1+s^2} \\ \tau(s) &= \frac{s}{1+s^2} \end{aligned}$$

These give us

$$D_s \begin{pmatrix} -\overrightarrow{\mathbf{T}}(s)- \\ -\overrightarrow{\mathbf{N}}(s)- \\ -\overrightarrow{\mathbf{B}}(s)- \end{pmatrix} + \begin{pmatrix} 0 & -\frac{\sqrt{2}}{1+s^2} & 0 \\ \frac{\sqrt{2}}{1+s^2} & 0 & -\frac{s}{1+s^2} \\ 0 & \frac{s}{1+s^2} & 0 \end{pmatrix} \begin{pmatrix} -\overrightarrow{\mathbf{T}}(s)- \\ -\overrightarrow{\mathbf{N}}(s)- \\ -\overrightarrow{\mathbf{B}}(s)- \end{pmatrix} \tag{7.4}$$

with $\begin{pmatrix} -\overrightarrow{\mathbf{T}}(s)- \\ -\overrightarrow{\mathbf{N}}(s)- \\ -\overrightarrow{\mathbf{B}}(s)- \end{pmatrix}$ the row vectors from 7.3.

We normalize the ODE 7.4 by finding $\left.\begin{pmatrix} -\overrightarrow{\mathbf{T}}(s)- \\ -\overrightarrow{\mathbf{N}}(s)- \\ -\overrightarrow{\mathbf{B}}(s)- \end{pmatrix}\right|_{s=0} = \begin{pmatrix} 0 & 1 & 0 \\ -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \end{pmatrix}$.

Notice that it's <u>not</u> I, yet it is invertible. Let $\begin{pmatrix} -\overrightarrow{\mathbf{T}}(s)- \\ -\overrightarrow{\mathbf{N}}(s)- \\ -\overrightarrow{\mathbf{B}}(s)- \end{pmatrix} = \Phi(s) \cdot \begin{pmatrix} 0 & 1 & 0 \\ -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \end{pmatrix}$ where $\Phi(0) = I$. From this we have the ODE

$$D_s \Phi(s) + \begin{pmatrix} 0 & -\frac{\sqrt{2}}{1+s^2} & 0 \\ \frac{\sqrt{2}}{1+s^2} & 0 & -\frac{s}{1+s^2} \\ 0 & \frac{s}{1+s^2} & 0 \end{pmatrix} \Phi(s), \ \Phi(0) = I \tag{7.5}$$

Note that with this ODE, we have a known fundamental solution

$$\Phi(s) = \begin{pmatrix} -\overrightarrow{\mathbf{T}}(s)- \\ -\overrightarrow{\mathbf{N}}(s)- \\ -\overrightarrow{\mathbf{B}}(s)- \end{pmatrix} \cdot \begin{pmatrix} 0 & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 1 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}$$

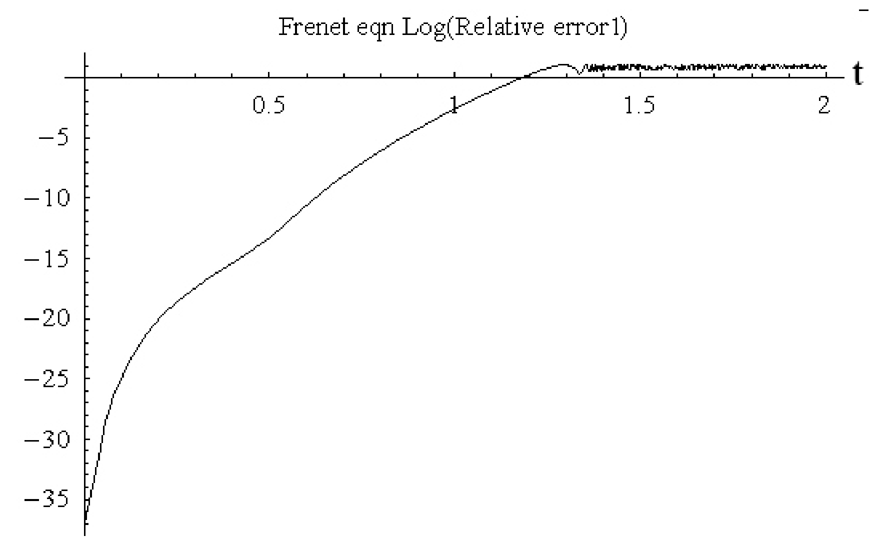
And, $\Phi(s) \in SO(3)$, so the adjoint solution $\Psi(s) = \Phi(s)$. Note also that this is because the matrix A which defines the ODE is skew-symmetric, hence the adjoint equation takes the form

$$D_t \Psi = -A^T \Psi = A\Psi$$

which is simply the Frenet ODE.

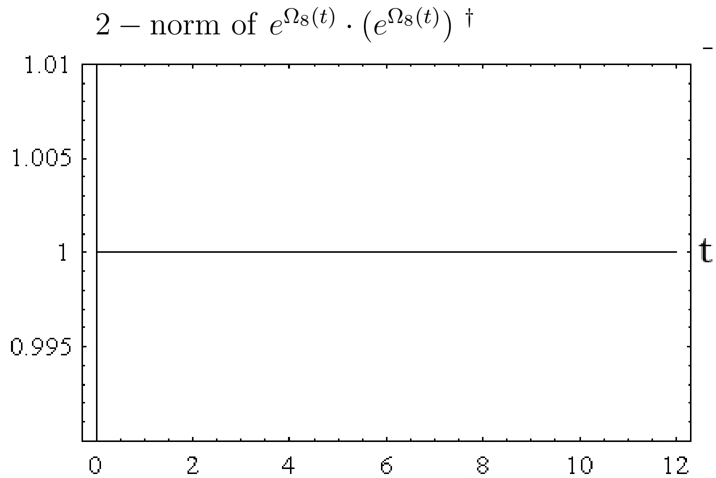
Magnus' Expansion for the Frenet example.

Now that we have the Frenet example built, we can apply Magnus' expansion to it. Magnus' expansion applied to the Frenet system (7.5) produces the relative error

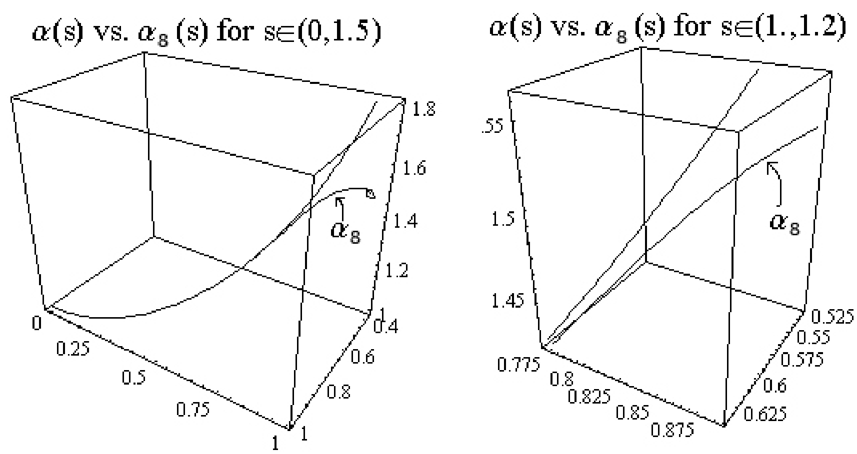


Note the magnitude of the error for $t < 0.5$. The relative error is less than $e^{-10} = O(10^{-5})$. From the analytic estimate (6.4) for the convergence of Magnus' expansion, the bound on convergence is $t < .5857$. Numerically we are close in norm, hinting that we might possibly have convergence beyond $t = .5857$.

With this example, we can demonstrate a significant property of geometric integration. In essence, since $\Phi(s) \in SO(3)$, and Magnus' expansion $\Omega_m(t) \in so(3), \forall m \in \mathbb{Z}, \forall t \in \mathbb{R}$, we have Magnus' approximation $\mathsf{e}^{\Omega_m(t)} \in SO(3), \forall m \in \mathbb{Z}, \forall t \in \mathbb{R}$, meaning that $\mathsf{e}^{\Omega_m(t)}$ is *orthonormal for all* m *and* t. Here is a picture of the L_1 norm of $\mathsf{e}^{\Omega_8(t)} \cdot \left(\mathsf{e}^{\Omega_8(t)}\right)^{\dagger}$, where † denotes the conjugate transpose.



Next is a picture of the Magnus' curve $\alpha_8(s)$ vs. the analytic curve $\alpha(s) = \left(\cos\left(\sinh^{-1}(s)\right), \sin\left(\sinh^{-1}(s)\right), \sqrt{1+s^2}\right)$. The construction is unique up to translation in $\mathbb{R}^3$ (due to the fact that Magnus' approximation only finds $\alpha'(s)$). We show the solution $\alpha_8(s)$ up to the point of rapid divergence from $\alpha(s)$, and in a neighborhood of the rapid divergence from $\alpha(s)$.



8 Conclusions

We are unable to satisfactorily answer the following questions in general:

1. For what values of t does $\Omega_m(t)$ converge to $\Omega(t)$ as $m \to \infty$?

2. If Ω_m converges, how close is Ω_m to Ω for a given m?

3. For what values of t is $e^{\Omega(t)} = \Phi(t)$, the fundamental solution to (3.1)?

4. Exactly how close is e^{Ω_m} to Φ for a given m?

Note that (3) is a distinct question from 1, though if Ω_m, Ω are close, then e^{Ω_m}, e^{Ω} are close by continuity of the exponential. For question (2), it is known that if $\int_0^t \|A\| < 1.086869$, then $e^{\Omega_m} \to \Phi$ as $m \to \infty$, [23] although this is very unsatisfying since it doesn't take commutativity into account.

Besides these questions listed above, the collection of open questions discussed here are the follow up questions that I would like to see answered.

Cauchyness of Ω_m in the tangent space.

Since $\Omega_m(t) = \sum_{n=1}^{m} \Gamma_m(t)$, provided we are in the neighborhood $[0, t)$ such that $\int_0^t \|A\| < 1.086869$, exactly what is the bound $\epsilon_m \in \mathbb{R}$, so that $\|\Omega(t) - \Omega_m(t)\| < \epsilon_m$? And can it be found from $\|\Gamma_{m+1}(t)\|$? Does some function of this bound correspond to $\left\|\Phi(t) - e^{\Omega_m(t)}\right\| < f(\epsilon_m)$?

Special cases.

Consider the special cases of:

1. equation (1.1) with $A(t) = \begin{pmatrix} 0 & 1 \\ f(t) & k \end{pmatrix}$, or even $A(t) = \begin{pmatrix} 0 & 1 \\ f(t) & 0 \end{pmatrix}$ where $f(t)$ is an integrable function and k is a constant.

2. equation (1.1) with $A(t) = \begin{pmatrix} 0 & \kappa(t) & 0 \\ -\kappa(t) & 0 & \tau(t) \\ 0 & -\tau(t) & 0 \end{pmatrix}$, where $\tau(t)$ and $\kappa(t)$ are integrable functions (the curvature and torsion of a curve in 3-space).

Magnus' expansion in both of these cases gives rise to a series the terms of which are made up of linearly indepenent matrices u_1, u_2, and u_3.

Numerical applications.

If $A(t) = A(t+T)$ for all t, is there a good numerical algorithm for finding a high-order (in the parameters) numerical approximation to $\Omega(t_0 + T)$ where T is the principal period of the system?

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A Euler's method & Taylor series methods for approximating solutions of differential equations

---

A.1 Euler's method

Let's start with equation (3.1). A simple Eulerian approach would be to approximate $D_t\Phi(t)$ by $\frac{\Phi(t+h)-\Phi(t)}{h}$ for some small h. This yields an iterative time step equation of

$$\Phi(t+h) = (I + hA(t))\,\Phi(t)$$

and, with the initial condition $\Phi(t_0) = I$, over n steps gives us the approximation

$$\begin{aligned}
\Phi(t) &\approx (I + hA(t_0))\,(I + hA(t_0+h))\,(I + hA(t_0+2h))\cdots(I + hA(t_0+nh)) \\
&= \prod_{k=0}^{n} (I + hA(t_0+kh))
\end{aligned}$$

where $t - t_0 = nh$.

A.2 Taylor series methods

Another method of approximation for a fundamental solution is through the use of Taylor series. Again, considering an equation of the form (3.1), suppose we try approximating the fundamental solution by truncating the Taylor series expansion, using the differential relation (3.1). Let's try

$$\Phi(t) = \sum_{j=0}^{\infty} a_j \frac{(t-t_0)^j}{j!}$$

Note that each a_j is an $n \times n$ matrix.

Then we have from equation (3.1),

$$\sum_{j=0}^{\infty} a_{j+1} \frac{(t-t_0)^j}{j!} = A(t) \sum_{j=0}^{\infty} a_j \frac{(t-t_0)^j}{j!} \quad a_0 = I$$

Suppose we also have $A(t)$ analytic in some neighborhood of t_0. Then we can Taylor expand $A(t)$ as $A(t) = \sum_{k=0}^{\infty} b_k \frac{(t-t_0)^k}{k!}$. This gives us the equation

$$\begin{aligned} \sum_{j=0}^{\infty} a_{j+1} \frac{(t-t_0)^j}{j!} &= \sum_{j=0}^{\infty} \sum_{k=0}^{\infty} b_k a_j \frac{(t-t_0)^{k+j}}{k!j!} \quad a_0 = I \\ &= \sum_{j=0}^{\infty} \sum_{k=0}^{j} \binom{j}{k} b_{j-k} a_k \frac{(t-t_0)^j}{j!} \end{aligned}$$

The relation of the coefficients is

$$a_{j+1} = \sum_{k=0}^{j} \binom{j}{k} b_{j-k} a_k$$

Our approximate solution is the polynomial

$$\Phi_m(t) = \sum_{j=0}^{m} \sum_{k=0}^{j} \binom{j}{k} b_{j-k} a_k \frac{(t-t_0)^j}{j!}$$

A.3 Examples

Let's apply each of the three methods to the following ODE:

$$D_t \Phi(t) = \begin{pmatrix} 0 & 1 \\ -t & 0 \end{pmatrix} \Phi(t) \quad \Phi(0) = I$$

For each of these methods, we evaluate the approximate solution $\tilde{\Phi}(t)$ at the time $t = 1$. Each approximate solution is compared to a solution $\Phi(t)$ computed from Airy functions and evaluated at time $t = 1$. The Airy function solution is

$$\Phi(1) = \begin{pmatrix} 0.83881 & 0.91863 \\ -0.46735 & 0.68034 \end{pmatrix}.$$

Euler's method.

Using a stepsize of $\frac{1}{100}$, the approximate solution is

$$\tilde{\Phi}(1) = \begin{pmatrix} 0.83859 & 0.92853 \\ -0.47272 & 0.67509 \end{pmatrix}$$

which has a relative error of 0.01299. More significantly, the determinant of $\tilde{\Phi}(1)$ is 1.005, indicating that the solution is no longer in the Lie group SL(2), while the true solution can be shown to be in SL(2).

Taylor series method.

Using a Taylor series out to t^8, the approximate solution is

$$\tilde{\Phi}(t) = \begin{pmatrix} 1 - \frac{t^3}{6} - \frac{t^6}{180} & t - \frac{t^4}{12} - \frac{t^7}{504} \\ -\frac{t^2}{2} - \frac{t^5}{30} + \frac{t^8}{1440} & 1 - \frac{t^3}{3} - \frac{t^6}{72} \end{pmatrix}$$

Evaluated at $t = 1$,

$$\tilde{\Phi}(t) = \begin{pmatrix} 0.83889 & 0.91863 \\ -0.46736 & 0.68056 \end{pmatrix}$$

which is much closer to the solution $\Phi(1)$ than the Euler method.

Picard iterative methods.

Starting the iteration with $\tilde{\Phi}_0(t) = I$ and following five iterations,

$$\tilde{\Phi}(t) = \begin{pmatrix} 1 - \frac{t^3}{6} - \frac{t^6}{180} & t - \frac{t^4}{12} - \frac{t^7}{504} \\ -\frac{t^2}{2} - \frac{t^5}{30} + \frac{t^8}{1440} & 1 - \frac{t^3}{3} - \frac{t^6}{72} \end{pmatrix}$$

equal to the Taylor series out to t^8.

Though these methods are numerically close, they still retain certain problems. As pointed out for the Euler method, all three of these methods are geometrically flawed; none lie on the manifold the solution evolves on.

B Magnus' expansion as an integrating factor

What we would like to show here is why we can re-write the ODE

$$D_t x\left(t\right) + A\left(t\right) x\left(t\right) = \mathbf{0} \quad x(0) = x_0 \tag{B.1}$$

as

$$\begin{aligned} D_t\left(e^{\Omega(t)} x\left(t\right)\right) &= \mathbf{0} \\ &\Rightarrow \quad x\left(t\right) = e^{\Omega(t)} e^{-\Omega(t_0)} x\left(t_0\right) \end{aligned}$$

analogous to the scalar equation (2.2) with the solution (2.3).

Let $x(t) = \Phi(t)x(t_0)$ where $\Phi(t)$ is the fundamental solution to (B.1) so that (B.1) becomes

$$D_t \Phi\left(t\right) x_0 + A\left(t\right) \Phi\left(t\right) x_0 = \mathbf{0} \quad \Phi(0) = \mathbf{I}$$

Provided there exists an "$n \times n''$ matrix function $\Omega\left(t\right)$, such that $D_t\left(\Phi\right) = e^{-\Omega(t)} A\left(t\right)$, we can multiply on the left by $e^{-\Omega(t)}$ (the integrating factor) and re-write the ODE as

$$\left(e^{-\Omega(t)}\right)\left(D_t x\left(t\right) + A\left(t\right) x\left(t\right)\right) = e^{-\Omega(t)} D_t x\left(t\right) + e^{-\Omega(t)} A\left(t\right) x\left(t\right) = \mathbf{0}$$

Since there exists an $\Omega(t)$ such that $D_t\left(\Phi\right) = e^{-\Omega(t)} A\left(t\right)$ (using uniqueness and existence of a solution to Hausdorff's equation (4.9)), we can re-write (B.1) as

$$D_t\left(e^{-\Omega(t)} \Phi\left(t\right) x_0\right) = \mathbf{0}$$

This exact differential integrates to $e^{-\Omega(t)} \Phi\left(t\right) x_0 - e^{-\Omega(t_0)} \Phi\left(t_0\right) x_0 = \mathbf{0}$. By definition of a fundamental solution,$\Phi(t_0) = \mathbf{0}$ and $e^{-\Omega(t)}$ is invertible, giving us

$$\Phi\left(t\right) x_0 = x(t) = e^{\Omega(t)} e^{-\Omega(t_0)} x_0$$

Note that this also implies that $\Phi(t) = e^{\Omega(t)}e^{-\Omega(t_0)}$.

C Proof of proposition 4

Proof. Let $D_t\Phi = A\Phi$, $\Phi(t_0) = I$, for $A(t)$ such that $A(\xi)A(\zeta) = A(\zeta)A(\xi)$, $\forall \zeta, \xi \in \mathbb{R}$. Magnus' expansion is

$$\begin{aligned}\Omega(t) &= \int_{t_0}^{t} A(\zeta_1)d\zeta_1 - \frac{1}{2}\int_{t_0}^{t}\int_{t_0}^{\zeta_1}\left[A(\zeta_2), A(\zeta_1)\right]d\zeta_2 d\zeta_1 \\ &+\frac{1}{4}\int_{t_0}^{t}\int_{t_0}^{\zeta_1}\int_{t_0}^{\zeta_2}\left[\left[A(\zeta_3), A(\zeta_2)\right], A(\zeta_1)\right]d\zeta_3 d\zeta_2 d\zeta_1 \\ &+\frac{1}{12}\int_{t_0}^{t}\int_{t_0}^{\zeta_1}\int_{t_0}^{\zeta_1}\left[A(\zeta_3), \left[A(\zeta_2), A(\zeta_1)\right]\right]d\zeta_3 d\zeta_2 d\zeta_1 + ...\end{aligned}$$

But since $A(\xi)A(\zeta) = A(\zeta)A(\xi)$, the only term that remains is the one that contains no Lie commutators, that is $\Omega(t) = \displaystyle\int_{t_0}^{t} A(\zeta_1)d\zeta_1$ so $\Phi(t) = e^{\int_{t_0}^{t} A(\xi)d\xi}$. ■

D Proof regarding existence of a solution $y = e^{\Omega}$

In section 4.2, it was shown that for the existence of a solution $\Phi(t) = e^{\Omega}$ to (1.1), the spectrum $\sigma(ad_{\Omega})$ must not contain a λ such that $\lambda \in \{2\pi in\}$, for $n \in \mathbb{Z} - \{0\}$. Here is the relationship between the eigenvalues of the ad_{Ω} operator and the matrix Ω.

Theorem 22 *Let Ω be an $n \times n$ matrix. Then ad_{Ω} is diagonalizable iff Ω is diagonalizable.*

Proof. First, suppose Ω is diagonalizable, $\sigma(\Omega) = \{\nu_i\}_{i \le n}$, and $\Omega = \begin{pmatrix} \nu_1 & 0 & \cdots & 0 \\ 0 & \nu_2 & & \vdots \\ \vdots & & \ddots & \vdots \\ 0 & \cdots & \cdots & \nu_n \end{pmatrix}$. Take a 'unit' matrix, $U_{i,j}$, an $n \times n$ matrix filled entirely with zeros except for a one in the $i'th$ row and $j'th$ column. So $U_{i,j} = \begin{pmatrix} 0 & 0 & \cdots & 0 \\ \vdots & & & \vdots \\ \vdots & 1 & & \vdots \\ 0 & \cdots & \cdots & 0 \end{pmatrix}$, where the 1 is in the $i, j'th$ place. Now notice that $ad_{\Omega}(U_{i,j}) = \begin{pmatrix} 0 & 0 & \cdots & 0 \\ \vdots & & & \vdots \\ \vdots & \nu_i - \nu_j & & \vdots \\ 0 & \cdots & \cdots & 0 \end{pmatrix} = (\nu_i - \nu_j) \begin{pmatrix} 0 & 0 & \cdots & 0 \\ \vdots & & & \vdots \\ \vdots & 1 & & \vdots \\ 0 & \cdots & \cdots & 0 \end{pmatrix}$, so that $(ad_{\Omega} - (\nu_i - \nu_j) I) U_{i,j} = 0$. The set $\{U_{i,j}\}$

forms a basis in which ad_Ω is diagonal with entries the differences of elements of $\sigma(\Omega)$.

Conversely, suppose ad_Ω is diagonalizable for $\Omega \in M_n$. This means that there exists a basis $\{U_i\}_{1\leq i\leq n^2}$ of M_n such that $ad_\Omega(U_i) = \alpha_i U_i$ for $\alpha_i \in \mathbb{R}$. So $\Omega U_i - U_i\Omega = \alpha_i U_i$.

Let $\alpha_i = \beta_i - \lambda_q$ for some $\lambda_q \in \sigma(\Omega)$.

Then

$$\Omega U_i - U_i\Omega = \beta_i U_i - \lambda_q U_i,$$

and

$$\Omega U_i - \beta_i U_i = U_i\Omega - \lambda_q U_i$$

which gives

$$(\Omega - \beta_i I)U_i = U_i(\Omega - \lambda_q I) \tag{D.1}$$

Take $V \in \mathbb{C}^n$ such that $\Omega V = \lambda_q V$. Multiply on the right of both sides of (D.1) by V. This yields

$$\begin{aligned}(\Omega - \beta_i I)U_i V &= U_i(\Omega - \lambda_q I)V \\ &= \mathbf{0}\end{aligned}$$

So either $U_i V = \mathbf{0}$ or $(\beta_i;\ U_i V)$ form an (eigenvalue ; eigenvector) pair.

If $U_i V = \mathbf{0}$, then there exists at least one nonzero row of U_i which is orthogonal to V for each $i \in \{1, 2, \ldots, n^2\}$.

Since $V \in \mathbb{C}^n$, there are at most $n-1$ linearly independent vectors which are orthogonal to V; meaning there are at most $n-1$ linearly independent U_i which satisfy $U_i V = \mathbf{0}$.

Since there are at most n linearly independent $V \in \mathbb{C}^n$, we must have <u>at most</u> $n(n-1)$ linearly independent U_i which satisfy $U_i V = \mathbf{0}$.

This means that there must be <u>at least</u> n linearly independent $U_i V \neq \mathbf{0}$ for $1 \leq i \leq n^2$ and $V \in \mathbb{C}^n$.

$\Rightarrow$ There exists at least n linearly independent $(\beta_i;\ U_iV)$ (eigenvalue ; eigenvector) pairs. Hence, Ω is diagonalizable. ■

Now let us remove the assumption that Ω is diagonalizable.

Corollary 23 *Suppose Ω is an $n \times n$ matrix, $\{\nu_i\} = \sigma(\Omega)$, and let $\lambda \in \sigma(ad_\Omega)$. Then $\lambda = \nu_m - \nu_l$ for some $\nu_m, \nu_l \in \{\nu_i\}$.*

Proof. Let Ω be an $n \times n$ matrix operator, $\{\nu_i\}_{i \leq n} = \sigma(\Omega)$, and let $\lambda \in \sigma(ad_\Omega)$. What we're looking for is λ as a function of $\sigma(\Omega)$ such that $Det(ad_\Omega - \lambda I) = 0$.

From the proof of the previous theorem, when Ω is diagonalizable, we have that for $\lambda \in \sigma(ad_\Omega)$, $\lambda = \nu_m - \nu_l$ for some $\nu_m, \nu_l \in \sigma(\Omega)$.

Now suppose Ω is not diagonalizable. We know that Ω has a unique Jordan canonical form, unique up to the order of the elements on the diagonal. Without any loss of generality, we can assume Ω is in Jordan canonical form. Let's write $\Omega = \Omega_S + \Omega_N$ where Ω_S is the matrix of diagonal entries of Ω, and Ω_N is an upper triangular nilpotent matrix of all entries on the diagonal zero. Since the Lie commutator is bilinear, $ad_{A+B} = ad_A + ad_B$, hence

$$ad_\Omega = ad_{\Omega_S + \Omega_N} = ad_{\Omega_S} + ad_{\Omega_N}$$

for which ad_{Ω_S} is diagonalizable by (22), and ad_{Ω_N} is nilpotent.

Let $P(\lambda)$ be the characteristic polynomial of ad_{Ω_S}. Recall that $P(ad_{\Omega_S}) = 0$, by the Cayley-Hamilton theorem. Now the key point to notice is that $P(\lambda) = Det(ad_{\Omega_S} - \lambda I)$ and, that

$$\begin{aligned} P(ad_\Omega) &= Det(ad_{\Omega_S} - ad_\Omega \circ I) \\ &= Det(ad_{\Omega_S} - ad_\Omega) \\ &= Det(-ad_{\Omega_N}) \\ &= 0 \end{aligned}$$

since ad_{Ω_N} is nilpotent.

So ad_Ω satisfies the characteristic polynomial for ad_{Ω_S}, hence the eigenvalues of ad_Ω are precisely the eigenvalues of ad_{Ω_S}; i.e. for $\lambda \in \sigma(ad_\Omega)$, $\lambda = \nu_m - \nu_l$ for some $\nu_m, \nu_l \in \sigma(\Omega)$. $\blacksquare$

E Computer Program

The program given below estimates the fundamental solution to (3.1). The first thing that should be done is to define $A(t)$, the matrix valued function of t. This is done by setting

- A[t_] := $\begin{pmatrix} f_{1,1}(t) & \cdots & f_{1,n}(t) \\ \vdots & \ddots & \vdots \\ f_{n,1}(t) & \cdots & f_{n,n}(t) \end{pmatrix}$

We also must define the Lie commutator. This is one line of code defining a function to multiply and subtract matrices.

- Comm[A_, B_] := Simplify[A.B - B.A]

The next seven lines of code defined the first seven Baker-Hausdorff functionals according to their order as specified by Iserles' work. First, the root functional of order t,

- $\omega_1[t\_] := \int_0^t A(s)ds$

Then the functional of order t^3,

- $\omega_2[t\_] := \int_0^t \text{Comm}[\omega_1(s),\, A(s)]ds$

These next five functionals give us an approximation of order t^5,

- $\omega_3[t\_] := \int_0^t \text{Comm}[\omega_1(s),\, \text{Comm}[\omega_1(s),\, A(s)]]ds$
- $\omega_4[t\_] := \int_0^t \text{Comm}[\omega_2(s),\, A(s)]ds$
- $\omega_5[t\_] := \int_0^t \text{Comm}[\omega_1(s),\, \text{Comm}[\omega_2(s),\, A(s)]]ds$
- $\omega_6[t\_] := \int_0^t \text{Comm}[\omega_3(s),\, A(s)]ds$

- $\omega_7[t\_] := \int_0^t \text{Comm}[\omega_4(s),\, A(s)]ds$

Next, we define the approximate solution to (1.2) as

- $\Omega[T\_] := \text{Simplify}[\omega_1[T]$ - $\frac{\omega_2[T]}{2} + \frac{\omega_3[T]}{12} + \frac{\omega_4[T]}{4}$ - $\frac{\omega_5[T]}{24}$ - $\frac{\omega_6[T]}{24}$ - $\frac{\omega_7[T]}{8}]$

In order to find the fundamental solution, that is, the solution $\Phi(t)$ for (3.1), we need to exponentiate $\Omega[t]$. Mathematica calculates the exact numerical exponential of a matrix by Jordan decomposition methods. Specifically, the line is,

- $\Phi_M = \text{MatrixExp}[\Omega[T]]$

Now, at this point in the code, it is helpful to enter various functions and values that will be useful when trying to verify the accuracy of the solution. One value that helps is in setting a name to the identity matrix the size of the system (the simplest cases considered are of size 2×2). Here it's referred to as

- ID = IdentityMatrix[2]

A necessary part, though seemingly unrelated section of the code is the definition of a norm for a given matrix. With a given norm, we have the ability to associate a non-negative real number with a given matrix, in some sense giving the 'size' or 'distance from zero' for a specified input. The simplest norm to use and to compute with is the Frobenius norm given by

- $\text{norm}_F[\text{rr}\_] := (\text{Tr}[\text{rr.Transpose}[\text{rr}]])^{\frac{1}{2}}$

Following the creation and construction of Φ and Ψ^T, the analytic fundamental and adjoint fundamental solutions respectively, we are able to calculate the relative error for the approximate fundamental solution Φ_M. Our two choices to calculate the relative error are:

- Method 1) Relative error = $\left\|\frac{\Phi_M - \Phi}{\Phi}\right\| = \left\|\Phi_M \Psi^T - I\right\| = \text{norm}_F\left[\Phi_M \Psi^T - I\right]$
- Method 2) Relative error = $\frac{\|\Phi_M - \Phi\|}{\|\Phi\|} = \frac{\text{norm}_F[\Phi_M - \Phi]}{\text{norm}_F[\Phi]}$

In the examples of section (7), we note where we used which relative error.

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