Symmetric Methods on Manifolds

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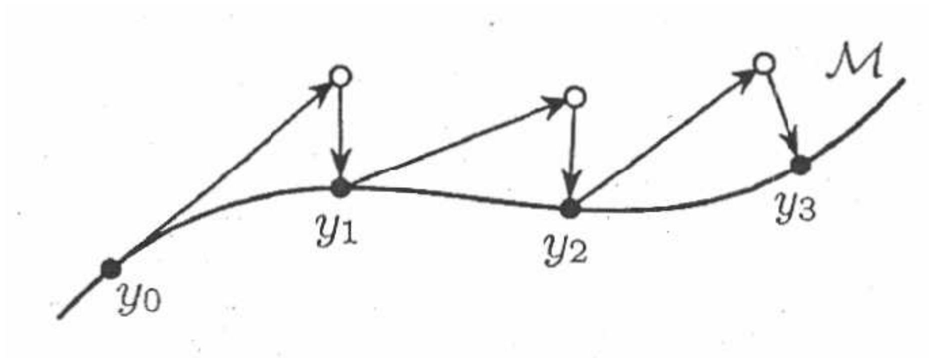
Overview

- **Symmetrize Projection Methods**
- Analyze symmetric projection methods
- Simulation: Solve pendulum equations using symmetric projection methods
- **Symmetrize Local Coordinates methods**
- Find two symmetric Lie group methods

Projection Methods and Symmetry

Standard projection methods are not symmetric, because of asymmetric use of projections.



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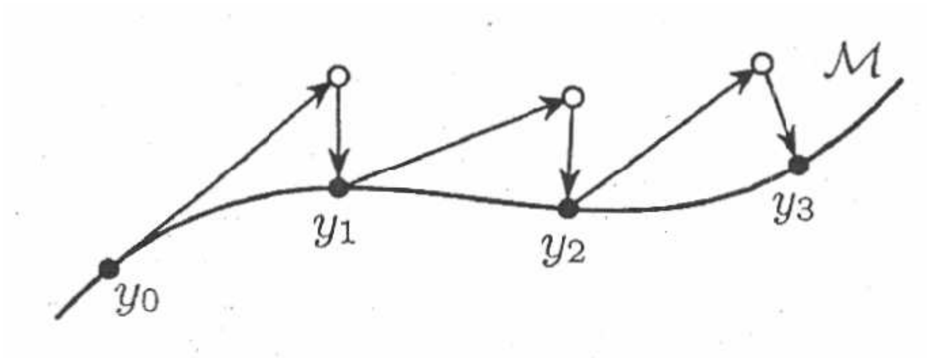

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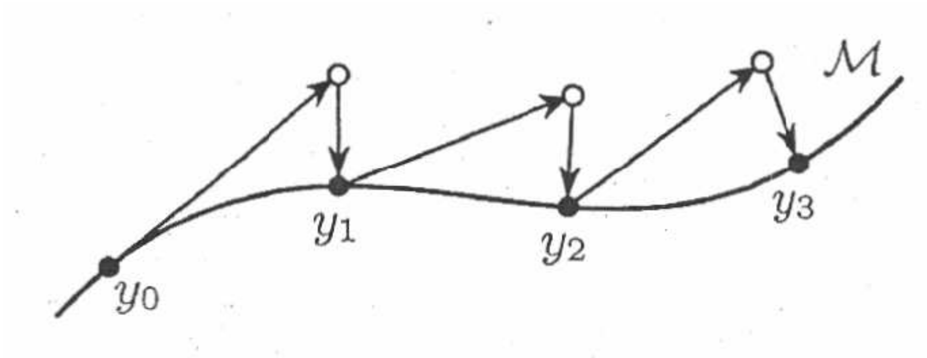
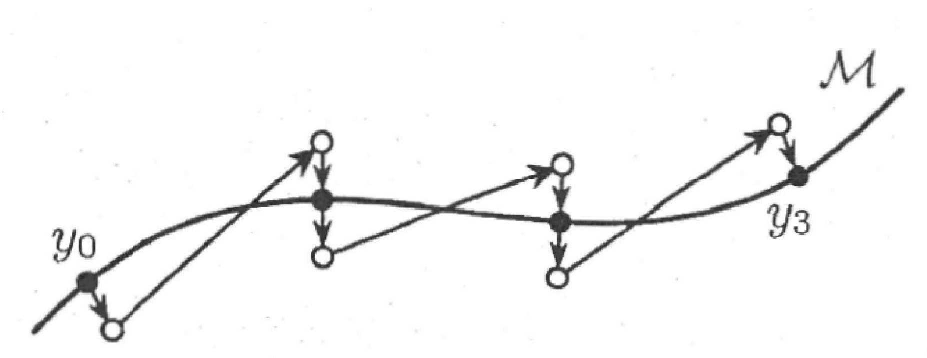


We look for an algorithm using projections that preserves the symmetry of the basic integrator:

Use: “inverse projection” - *symmetric* integration step - projection



Symmetric Projection Methods

If Φ_h is a symmetric method applied to $\dot{y} = f(y)$, define:

Algorithm 1 (Symmetric Projection Method (SPM)) *Assume that $y_n \in \mathcal{M}$. One step $y_n \mapsto y_{n+1}$ is defined as follwos:*

- $\tilde{y}_n = y_n + G(y_n)^T \mu$ *(perturbation step);*
- $\tilde{y}_{n+1} = \Phi_h(\tilde{y}_n)$*;*
- $y_{n+1} = \tilde{y}_{n+1} + G(y_{n+1})^T \mu$ *with* $g(y_{n+1}) = 0$ *(projection step);*

where $G(y) = g'(y)$ and the manifold $\mathcal{M}$ is given by $g(y) = 0$.

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where $G(y) = g'(y)$ and the manifold $\mathcal{M}$ is given by $g(y) = 0$.

Note: μ is determined implicitly by $g(y_{n+1}) = 0$ and

$$\mu_{\text{perturbation}} = \mu_{\text{projection}}.$$

Existence of Numerical Solution

The vector μ and the numerical approximation y_{n+1} are implicitly defined by

$$F(h, y_{n+1}, \mu) = \begin{pmatrix} y_{n+1} - \Phi_h(y_n + G(y_n^T \mu) - G(y_{n+1})^T \mu \\ g(y_{n+1}) \end{pmatrix} = 0.$$

Since $F(0, y_n, 0) = 0$ and since

$$\frac{\partial F}{\partial (y_{n+1}, \mu)}(0, y_n, 0) = \begin{pmatrix} I & -2G(y_n)^T \\ G(y_n) & 0 \end{pmatrix}$$

is invertible (provided that $G(y_n)$ has full rank), an application of the implicit function theorem proves the existence of the numerical solution for sufficiently small step size h.

The implicit function theorem

Theorem 0 (Implicit Function Theorem) *Let $f(x, y)$ be a function from a neighborhood of (a, b) into a neighborhood of $f(a, b)$. Define $f_a(y) := f(a, y)$ and assume that $\mathrm{d}f_a\big|_b$ is an isomorphism.*

Then, there exist neighborhoods U of a and V of $f(a, b)$ and a unique function $\varphi(x, z)$ from $U \times V$ into a neighborhood of b, such that $z = f(x, \varphi(x, z))$. Furthermore

$$\mathrm{d}\varphi = \left(\frac{\partial f}{\partial y}\right)^{-1} \left[\mathrm{d}z - \frac{\partial f}{\partial x}\mathrm{d}x\right].$$

Order of the SPM

For a study of the local error we let $y_n := y(t_n)$ be a value on the exact solution $y(t)$ of

$$\dot{y} = f(y), \qquad f(y) \in T_y\mathcal{M}.$$

If the basic method Φ_h is of order p, i.e., if $y(t_n + h) - \Phi_h(y(t_n))$ $= \mathcal{O}(h^{p+1})$, we have

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Compared to

$$F(h, y_{n+1}, \mu) = 0$$

the implicit function theorem yields

$$y_{n+1} - y(t_{n+1}) = \mathcal{O}(h^{p+1}), \qquad \mu = \mathcal{O}(h^{p+1}).$$

Symmetry of the method

Exchanging $h \longrightarrow -h$ and $y_n \leftrightarrow y_{n+1}$ in the SPM yields

$$\begin{aligned} \tilde{y}_n &= y_{n+1} + G(y_{n+1})^T \mu, \qquad g(y_{n+1}) = 0, \\ \tilde{y}_{n+1} &= \Phi_{-h}(\tilde{y}_n), \\ y_n &= \tilde{y}_{n+1} + G(y_n)^T \mu, \qquad g(y_n) = 0. \end{aligned}$$

Renaming *auxiliary* variables $\mu \longrightarrow -\mu$ and $\tilde{y}_n \leftrightarrow \tilde{y}_{n+1}$ gives

$$\begin{aligned} \tilde{y}_{n+1} &= y_{n+1} - G(y_{n+1})^T \mu, \qquad g(y_{n+1}) = 0, \\ \tilde{y}_n &= \Phi_{-h}(\tilde{y}_{n+1}), \\ y_n &= \tilde{y}_n - G(y_n)^T \mu, \qquad g(y_n) = 0, \end{aligned}$$

which is equivalent to the formulae of the original algorithm provided Φ_h is symmetric.

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We know that for ρ-reversibility, a method Φ_h has to be symmetric and satisfy

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$$\rho G(y)^T = G(\rho y)^T \sigma \qquad \sigma \text{ constant and invertible,}$$

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In many interesting cases,

$$g(\rho y) = \sigma^{-T} g(y)$$

holds, which implies $\rho G(y)^T = G(\rho y)^T \sigma$ if $\rho\rho^T = I$.

Modifications

The perturbation and projection steps can be modified without destroying the symmetry.

For example use a constant projection direction:

$$\tilde{y}_n = y_n + A^T\mu, \qquad y_{n+1} = \tilde{y}_{n+1} + A^T\mu \qquad A \text{ constant.}$$

To guarantee the existence of the numerical solution, $G(y)A^T$ has to be invertible along the solution $y(t)$.

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For ρ-reversibility, A has to satisfy

$$\rho A^T = A^T\sigma$$

for an invertible matrix σ.

Example: The Pendulum

The pendulum equations in Cartesian coordinates are

$$\begin{aligned} \dot{q}_1 &= p_1, & \dot{p}_1 &= -q_1\lambda \\ \dot{q}_2 &= p_2, & \dot{p}_2 &= -1 - q_2\lambda, \end{aligned}$$

with $\lambda = (p^2 - q_2)/q^2$.

- The solution to these equations remains on the manifold

$$\mathcal{M} = \{(q_1, q_2, p_1, p_2) | q^2 = 1, q \cdot p = 0\}.$$

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- The problem is ρ-reversible for both

$$\begin{aligned} \rho(q_1, q_2, p_1, p_2) &= (q_1, q_2, -p_1, -p_2) \quad \text{and} \\ \rho(q_1, q_2, p_1, p_2) &= (-q_1, q_2, p_1, -p_2). \end{aligned}$$

The Pendulum - Projections

Three different ways to project to the Manifold $\mathcal{M}$ were used:

- Orthogonal Projection: $G^T\mu \perp \mathcal{M}$, $G = \begin{pmatrix} 2q_1 & 2q_2 & 0 & 0 \\ p_1 & p_2 & q_1 & q_2 \end{pmatrix}$

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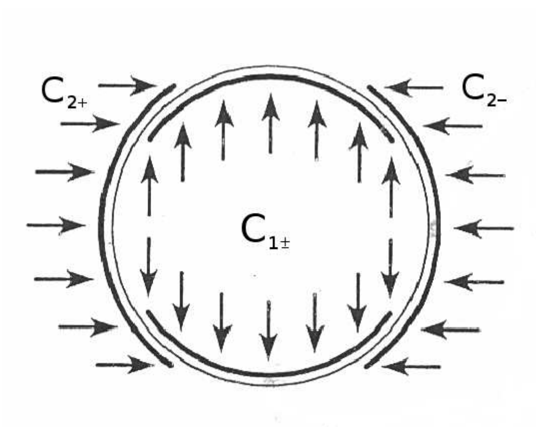
  Coordinate Projection: $C^T\mu$ with

- 

$$C_{1\pm} = \begin{pmatrix} 0 & \pm 2 & 0 & 0 \\ 0 & 0 & 0 & \pm 1 \end{pmatrix}$$

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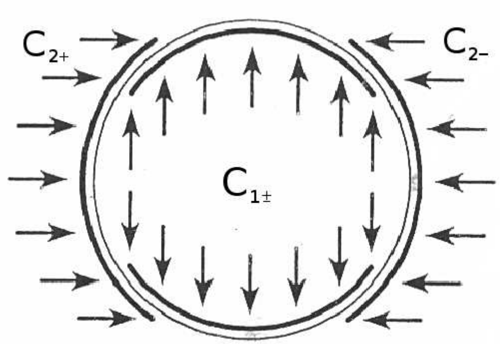
- 

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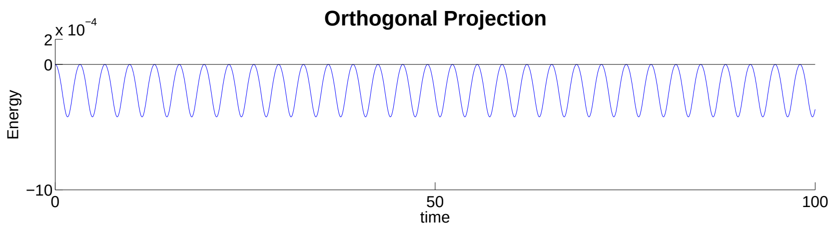
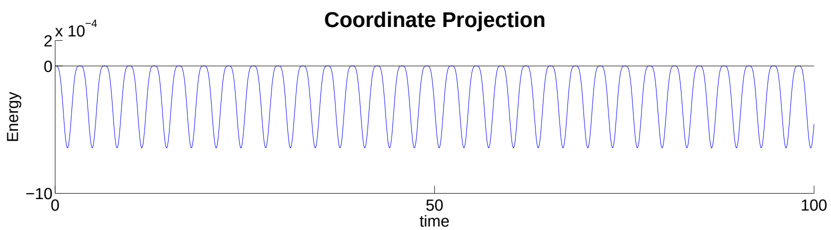
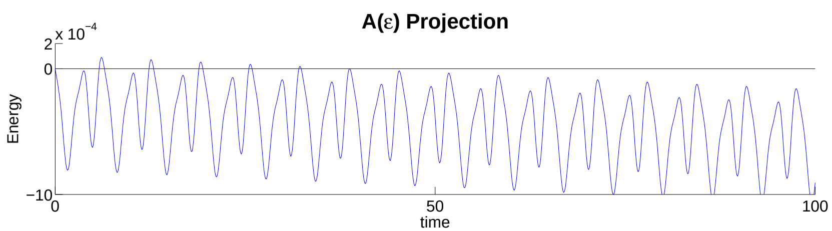
- Projection violating ρ-reversibility: $A = \begin{pmatrix} -\varepsilon & -2 & 0 & 0 \\ -\varepsilon & 0 & 0 & -1 \end{pmatrix}$

The Pendulum - Results

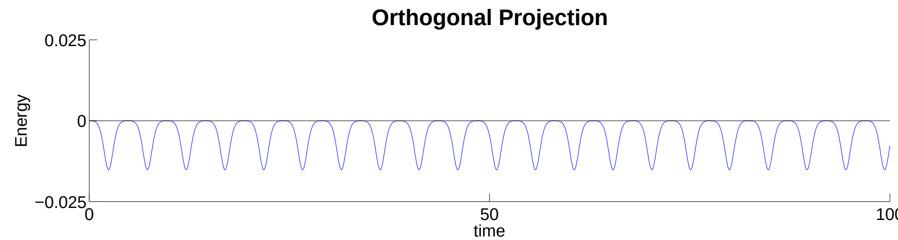
Low Starting Position

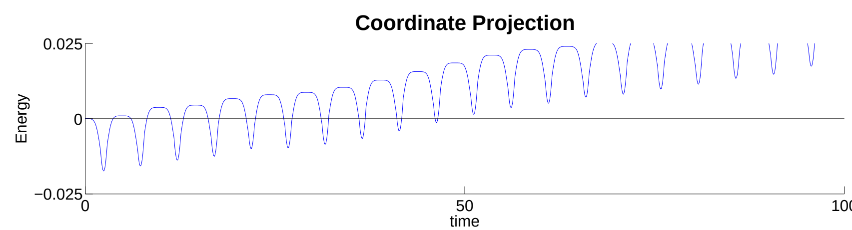






High Starting Position

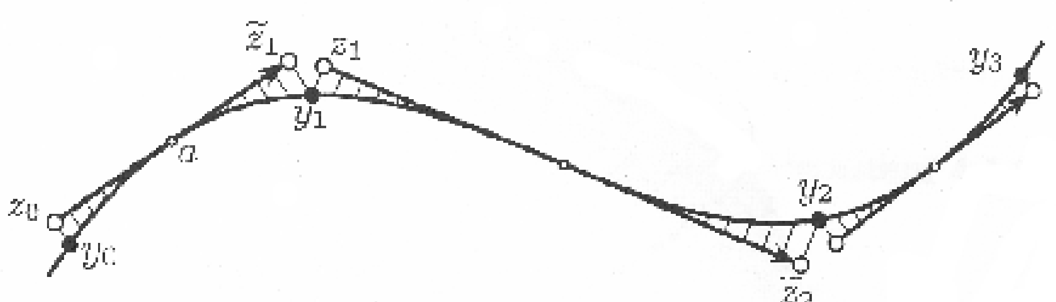




Local Coordinate Methods (LCM)

Algorithm 1 (Symmetric Local Coordinates Approach) *Assume:* $y_n \in \mathcal{M}$ *and* ψ_a *a local parametrization of* $\mathcal{M}$ *with* $\psi_a(0) = a$ *(close to* y_n*).*

- *find* z_n *(close to* 0*) such that* $\psi_a(z_n) = y_n$*;*
- $\tilde{z}_{n+1} = \Phi_h(z_n)$ *(symmetric one-step method applied to* $\dot{z} = \psi'(z)^+ f(\psi(z))$*).*
- $y_{n+1} = \psi_a(\tilde{z}_{n+1})$*;*
- *choose* a *in the parametrization such that* $z_n + \tilde{z}_{n+1} = 0$*.*



Symmetric use of local tangent space parametrization

Reversibility of Symmetric LCM

A symmetric local coordinates method is ρ-reversible, if the parametrization is s.t.:

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If the initial problem is ρ-reversible, this implies σ-reversibility for

$$\dot{z} = \psi'(z)^+ f(\psi(z)).$$

The basic method Φ_h must therefore be σ-reversible.

Symmetric Lie Group Methods

Now, consider

$$\dot{Y} = A(Y)Y, \qquad Y(0) = Y_0,$$

where $A(Y)$ is in the Lie algebra $\mathcal{G}$ whenever Y is in the Lie group G.

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Accidentally, the Lie group method based on the implicit midpoint rule

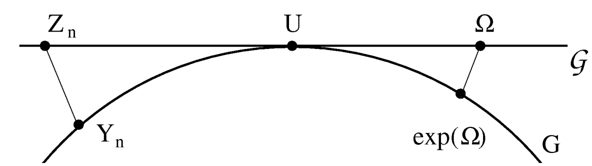
$$Y_{n+1} = \exp(\Omega)Y_n, \qquad \Omega = hA(\exp(\Omega/2)Y_n)$$

is symmetric (exchange $h \leftrightarrow -h$, $Y_n \leftrightarrow Y_{n+1}$ and the auxiliary variable $\Omega \leftrightarrow -\Omega$).

Symmetric Munthe-Kaas Methods

According to the symmetric LCM, we choose a local parametrization

$$\psi_U(\Omega) = \exp(\Omega)U,$$



where $U = \exp(\Theta)Y_n$ plays the role of the midpoint on the manifold.

We put $Z_n = -\Theta$ so that $\psi_U(Z_n) = Y_n$.

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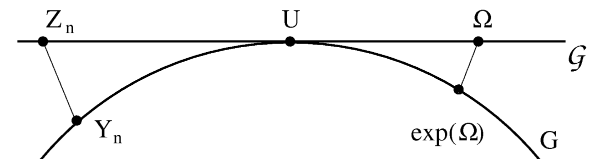

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We put $Z_n = -\Theta$ so that $\psi_U(Z_n) = Y_n$.

Apply any symmetric Runge-Kutta method to the differential equation

$$\dot{\Omega} = A(\psi_U(\Omega)) + \sum_{k=1}^{q} \frac{B_k}{k!} \mathbf{ad}_{\Omega}^{k} \left(A(\psi_U(\Omega)) \right), \qquad \Omega(0) = -\Theta,$$

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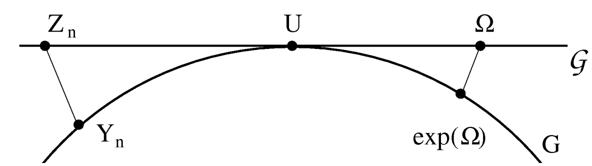

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to obtain $\tilde{Z}_{n+1}$ from Z_n.
Θ is implicitly given by $Z_n + \tilde{Z}_{n+1} = 0$, and the numerical result is

$$Y_{n+1} = \psi_U(\tilde{Z}_{n+1}) = \exp(\tilde{Z}_{n+1}) \exp(\Theta) Y_n = \exp(2\Theta) Y_n.$$

2-stage Gauss on Lie Groups

2-stage Gauss:

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

With the coefficients of the 2-stage Gauss method and with $q = 1$, $B_1 = -\frac{1}{2}$ we thus get:

$$\begin{aligned}
k_1 &= A\left(\exp\left(\underbrace{-\Theta + \frac{h}{4}(k_1+k_2) - h\frac{\sqrt{3}}{6}k_2}_{\Omega_1}\right)U\right) - \frac{1}{2}\Big[\Omega_1, A\big(\exp(\Omega_1)U\big)\Big] \\
k_2 &= A\left(\exp\left(\underbrace{-\Theta + \frac{h}{4}(k_1+k_2) + h\frac{\sqrt{3}}{6}k_1}_{\Omega_2}\right)U\right) - \frac{1}{2}\Big[\Omega_2, A\big(\exp(\Omega_2)U\big)\Big] \\
\Theta &= -\Theta + \frac{h}{2}\left(k_1+k_2\right).
\end{aligned}$$

2-stage Gauss on Lie Groups

With

$$2\Theta = \frac{h}{2}(k_1 + k_2) \Rightarrow \Omega_1 = -h\frac{\sqrt{3}}{6}k_2,\ \Omega_2 = h\frac{\sqrt{3}}{6}k_1$$

and $A_i := A(\exp(\Omega_i)U)$ we can rewrite this as

$$\begin{aligned}
\Omega_1 &= -h\frac{\sqrt{3}}{6}\left(A_2 - \frac{1}{2}[\Omega_2, A_2]\right)\\
\Omega_2 &= h\frac{\sqrt{3}}{6}\left(A_1 - \frac{1}{2}[\Omega_1, A_1]\right)\\
Y_{n+1} &= \exp(2\Theta)Y_n\\
&= \exp\left(\frac{h}{2}(A_1 + A_2) - \frac{h}{4}([\Omega_1, A_1] + [\Omega_2, A_2])\right)Y_n.
\end{aligned}$$

2-stage Gauss on Lie Groups

Neglecting terms of size $\mathcal{O}(h^4)$ in Y_{n+1} gives

$$\begin{aligned}
\Omega_1 &= -h\frac{\sqrt{3}}{6}A_2 + \frac{h^2}{24}[A_1, A_2] \\
\Omega_2 &= h\frac{\sqrt{3}}{6}A_1 - \frac{h^2}{24}[A_1, A_2] \\
Y_{n+1} &= \exp\left(\frac{h}{2}(A_1 + A_2) - h^2\frac{\sqrt{3}}{12}[A_1, A_2]\right)Y_n.
\end{aligned}$$

This method is symmetric and therefore still of order 4 (orders of symmetric methods are even).

Reversibility of 2-stage Gauss

For any linear invertible transformation ρ, the parametrization $\psi_U(\Omega) = \exp(\Omega)U$ satisfies

$$\rho\psi_U(\Omega) = \rho \exp(\Omega)U = \exp(\rho\Omega\rho^{-1})\rho U = \psi_{\rho U}(\sigma\Omega)$$

with $\sigma\Omega = \rho\Omega\rho^{-1}$.

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with $\sigma\Omega = \rho\Omega\rho^{-1}$.

If the initial problem is ρ-reversible, i.e. $\rho A(Y) = -A(\rho Y)\rho$, then

$$\dot{\Omega} = A(\psi_U(\Omega)) + \sum_{k+1}^{q} \frac{B_k}{k!}\mathbf{ad}_\Omega^k\left(A(\psi_U(\Omega))\right), \qquad \Omega(0) = -\Theta$$

is σ-reversible for all truncation indices q.

Summary

- symmetric projection methods
  - have the same order as basic integrator
  - are ρ-reversible if the basic method is ρ-reversible and $\rho G(y)^T = G(\rho y)^T \sigma$ for some invertible σ.
- symmetric local coord. methods
  - (have the same order as basic integrator)
  - are ρ-reversible if $\rho \psi_a(z) = \psi_{\rho a}(\sigma z)$ for some invertible σ and if the basic method is σ -reversible.
- symmetric Lie group methods can be obtained by symmetrizing Munte-Kaas methods. Examples:
  - 2^{nd} order: implicit midpoint rule as basic integrator
  - 4^{th} order: 2-stage Gauss as basic integrator