Nonlinear Stability of Lie Group Integrators

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EXTENDED ABSTRACT

1 Introduction

In the study of multibody dynamics, one faces inevitably problems like the parameterization of large rotations without singularities, [4]. Lie group integrators that avoid the use of local coordinates are used successfully for this problem class, [1]. Practical experience shows that implicit methods of that type share typically the favourable stability properties of their classical counterparts if applied to stiff systems. This is the reason why the implicit methods are preferred when solving mechanical dynamical systems. Per time step, they usually have higher numerical costs in terms of computation time and efficiency, but they return more precise results independently from the time step size.

In an ongoing research project, we study contractivity of differential equations on Riemannian manifolds [6] using logarithmic matrix norms of a projected system Jacobian. In that way, contractive problems may be analysed by Gronwall estimates [3] and by their counterparts in a time-discrete setting [2] to investigate contractivity of the Lie group integrators.

These analytical investigations are combined with numerical experiments for implicit and explicit Lie group integrators that will be discussed in detail in the present paper. We consider gradient flows on S^2 and TS^2 and observe (as expected) limitations for the time step size of explicit Lie group integrators to guarantee contractivity of the numerical solution. There are no such step size bounds for the implicit Lie-Euler method, that shows contractivity (in terms of the novel analytical setting on the Riemannian manifold) for any time step size.

2 Methodology

Definition 1 (Implicit Lie-Euler). Let $\dot{y} = f(y) := A(y)y$ be a system on the Lie group *G*, where $A(y) \in \mathfrak{g}$, with \mathfrak{g} denoting the corresponding Lie algebra. The implicit Lie-Euler method finds the solution at time $t_{n+1} = t_n + \tau$ as $y_{n+1} = \exp(\tau A(y_{n+1})) \circ y_n$.

We are now interested in the property of contractivity. From classical theory, we know that the implicit Euler is unconditionally contractive for contractive problems in linear spaces. As hypothesis, we formulate the contractivity of the implicit Lie-Euler on S^2 .

Hypothesis 1. Let *d* be the Riemannian distance on S^2 . Let consider the logarithmic norm according to Definition 2 and let $\mu[f'(\xi)] \leq v, \forall \xi$. Then, for any two implicit Lie-Euler solutions \tilde{y}_{n+1}, y_{n+1} starting from \tilde{y}_n and y_n , respectively,

$$d(\tilde{y}_{n+1}, y_{n+1}) \le (1 - \tau \nu)^{-1} d(\tilde{y}_n, y_n), \qquad \forall \tau, \ \tau \nu < 1$$
(1)

The Riemannian distance on the manifold $S^2 \subset \mathbb{R}^3$ is defined by $d(p,q) = 2 \arcsin(||p-q||_2/2)$, where $p, q \in S^2$. In the following numerical tests on TS^2 , the definition of distance is naturally extended by the Sasaki metric, [5].

Definition 2. [Logarithmic norm] Let *A* be a given matrix. The logarithmic norm $\mu[A]$ of *A* is $\mu[A] = \lim_{\Delta \to 0^+} \frac{\|\mathbb{I} + \Delta A\| - 1}{\Delta}$.

In the specific case, we are interested in $\|\cdot\|_g$, where *g* is the metric of the manifold and *G* is the relative metric tensor. Then, we have $\mu[A] = \max\{\lambda | \lambda \text{ is an eigenvalue of } ((GAG^{-1} + A^{\top})/2)\}.$

3 Numerical results

A simple example of a contractive problem on a manifold is the gradient flow. We perform the study both on the unit sphere $S^2 \subset \mathbb{R}^3$ and on its tangent bundle TS^2 . Hypothesis 1 has been formulated only for S^2 , but the numerical examples on TS^2 show the same behaviour and are therefore interesting.

The following systems are obtained based on a function E = E(y), which can be considered an energy function, and its Riemannian gradient. Let \mathfrak{M} be a manifold, $E : \mathfrak{M} \to \mathbb{R}$ a scalar function on the manifold. The dynamical system $\dot{y} = -\operatorname{grad}(E)$ represents the gradient flow on \mathfrak{M} .

On the unit sphere, the given energy function is $E(q) = 1/2q^{\top}Dq$, where $q \in S^2$ and $D \in \mathbb{R}^{3\times 3}$ is a diagonal matrix with two equal entries. The system describing the gradient flow is

$$\dot{q} = -Dq + 2E(q)q \tag{2}$$

When solving the problem on TS^2 , we define $E(q, \omega) = 1/2q^{\top}Dq + 1/2\omega^{\top}\omega$, where $(q, \omega) \in TS^2$, and $D \in \mathbb{R}^{3\times 3}$ has the same properties as in S^2 . After some manipulation, we end up with the system

$$\dot{q} = q \times \left(q \times \frac{\partial E}{\partial q} - q^{\top} \frac{\partial E}{\partial \omega} \right), \qquad \dot{\omega} = \omega \times \left(q \times \frac{\partial E}{\partial q} - q^{\top} \frac{\partial E}{\partial \omega} \right) + q \times \left(q \times \frac{\partial E}{\partial \omega} \right)$$
(3)

Observing the two systems, we can make a parallel to mechanical systems described by ODEs. In particular, if we consider the function *E* as an energy, then we can see it being composed of a potential energy and a kinetic energy. On S^2 , the energy has only the contribution of the potential energy, while in TS^2 , both the potential and the kinetic energy add up for the total energy. The resulting systems are a parallel respectively to a first order ODE and a second order ODE. For that reason, the interest in such simple examples is evident.

In Figure 1, we compare the Riemannian distance between the flow of two solutions. We solve both the problems with an explicit Lie-Euler method and an implicit one for two different initial values. The study is done for increasing values of the time step size. Since the methods are one step methods, we can perform this study over a one step simulation. By deduction, if the property is valid on one step, it will be valid for the entire time interval.



Figure 1: Riemannian distance on the specified manifold.

We observe that the qualitative behaviour of the measure is the same for the problem on S^2 and on TS^2 . In the two tests, the matrix D is the same and the initial values are different, hence the different distance. Nevertheless, the behaviour of the solutions (exact and numerical) looks comparable. In both cases, when the exact solution is contractive, the implicit Lie-Euler is contractive for any size of the time step. On the contrary, the explicit Lie-Euler does not have this property. The numerical solution obtained with the implicit Lie-Euler performs as the exact solution. When the latter is contractive, then the numerical solution is contractive as well. We must notice that the statement is valid only when the logarithmic norm of the symmetric part of the Jacobian is non-positive. Checking this assumption is rather simple in S^2 , and it results in the restriction for the initial conditions. In spherical coordinates, it translates to the restriction on $(\phi(t_0), \theta(t_0))$

$$-\frac{\pi}{2} \le \phi(t_0) \le -\frac{\pi}{4}, \quad \forall \boldsymbol{\theta}(t_0) \in [0, 2\pi]$$
(4)

The numerical test results illustrate contractivity of the implicit Lie-Euler method independently of the time step size. This result allows us to use coarse grid discretisation in time, without losing the desired property.

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