On the accurate evaluation and differentiation of the exponential map in flexible multibody dynamics

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EXTENDED ABSTRACT

1 Introduction

The exponential map plays an important role in geometric formulations of flexible multibody systems. In these formulations, the configuration of a mechanical system is represented using finite rotation and translation variables which do not evolve in a vector space but in a Lie group [1, 2, 3, 4]. The exponential map, which represents the fundamental solution of a differential equation on a Lie group, is an important building block for many geometric time integration methods. Furthermore, it can serve for the elaboration of interpolation algorithms and finite difference methods on a Lie group and it can be exploited to construct a set of local coordinates. As pointed out in [5], there is a variety of numerical methods to evaluate the exponential of a matrix. Often, numerical algorithms require not only the exponential map but also its linearization, which is represented by the so-called tangent operator, and higher order derivatives. Therefore, this work addresses the evaluation of the exponential map, the tangent operator and its derivatives, which are useful operators to solve various problems in flexible multibody dynamics.

For specific Lie groups such as the special orthogonal group $SO(3)$, which represents the set of 3D rotations, and the special Euclidean group $SE(3)$, the exponential map and the tangent operator admit a closed form expression. However, these closed form expressions suffer from singularities at the origin. In practice, the analytical formulae should be replaced by their limit value whenever the amplitude is below a given threshold.

Alternatively, the exponential map and the tangent operator can be expressed as series expansions. Interestingly, these series do not suffer from any singularity and they take rather simple and generic expressions for any matrix Lie group such as $SO(3)$ and $SE(3)$. In a practical implementation, the series should be truncated to a finite number of terms, inducing some truncation errors.

In this work, the closed form and the series form are considered. We analyze the influence of round-off errors on the closed form and the influence of truncation errors on the series form and we propose some relevant error estimates for the exponential map, the tangent operator and its higher order derivatives. These theoretical estimates are validated based on numerical experiments. Finally, practical recommendations are made for the accurate and efficient evaluation of these operators.

2 The exponential map and the tangent operator

Let us consider a matrix Lie group G and its Lie algebra $\mathfrak{g}$. The exponential maps takes a matrix $\tilde{\mathbf{x}} \in \mathfrak{g}$ and maps it to a matrix of the Lie group G according to the series expansion

$$\exp(\tilde{\mathbf{x}}) = \sum_{i=0}^{\infty} \frac{1}{i!} \tilde{\mathbf{x}}^i \tag{1}$$

The tangent operator, which defines the linearized expression of the exponential map, is expressed as

$$\mathbf{T}(\mathbf{x}) = \sum_{i=0}^{\infty} \frac{(-1)^i}{(1+i)!} \hat{\mathbf{x}}^i \tag{2}$$

where $\mathbf{x} \in \mathbb{R}^n$ is the vector representation of the matrix $\tilde{\mathbf{x}}$ and $\hat{\mathbf{x}} = \mathrm{ad}_{\mathbf{x}}$ is another matrix formed from the components of $\mathbf{x}$ which is equivalent to the adjoint map. The derivative of the tangent operator can be further developed by differentiation of the above expression. We can show that all higher order derivatives can be implemented using a generic recursive algorithm.

On $SO(3)$, the exponential map also admits a closed form which is equivalent to the Rodrigues formula

$$\exp(\tilde{\mathbf{x}}) = \mathbf{I} + \alpha(\|\mathbf{x}\|)\tilde{\mathbf{x}} + \frac{\beta(\|\mathbf{x}\|)}{2}\tilde{\mathbf{x}}^2 \tag{3}$$

with the functions $\alpha(\theta) = \sin\theta/\theta$ and $\beta(\theta) = 2(1-\cos\theta)/\theta^2$. In this case, $\tilde{\mathbf{x}}$ is a 3×3 skew-symmetric matrix and the exponential map computes a 3×3 rotation matrix. Also, $\hat{\mathbf{x}} = \tilde{\mathbf{x}}$ in this special case and the tangent operator is obtained as

$$\mathbf{T}(\mathbf{x}) = \mathbf{I} - \frac{\beta(\|\mathbf{x}\|)}{2}\tilde{\mathbf{x}} + \frac{1-\alpha(\|\mathbf{x}\|)}{\|\mathbf{x}\|^2}\tilde{\mathbf{x}}^2 \tag{4}$$

The successive derivatives of the tangent operator can be evaluated based on analytical developments, however, the complexity of the mathematical expressions significantly increases at each differentiation step. On $SE(3)$ some analytical expressions are also available but are not detailed here for the sake of conciseness.

3 Numerical implementation and error analysis

The implementation of the series form requires a truncation of Equations (1) and (2) to N terms. The truncation process induces a truncation error whose amplitude can be estimated as

$$Error_{series}(\|\mathbf{x}\|,N) = \frac{1}{N!}\|\mathbf{x}\|^N \tag{5}$$

Based on this error estimate, the value of N can be determined to reach a given level of accuracy at a given amplitude $\|\mathbf{x}\|$. This means that highly accurate expressions can be obtained even for large rotation amplitudes, but at a high computational cost.

On $SO(3)$, the closed form expressions of the exponential map and of the tangent operator suffer from a singularity at the origin. Consequently, their evaluation is affected by increasing round-off errors when the amplitude decreases which can be estimated as

$$Error_{closed}(\|\mathbf{x}\|,s) = c_1\left(\frac{\|\mathbf{x}\|}{\pi}\right)^s \tag{6}$$

where $c_1 = 1.2\times10^{-17}$ for the float64 format and s is the differentiation level: $s=0$ for the exponential map, $s=-1$ for the tangent operator, $s=-2$ for the first derivative of the tangent operator, etc. In a practical implementation, the analytical formula should be replaced by its limit value if $\|\mathbf{x}\| < \varepsilon$ where ε is a threshold. In this way, the error can be brought down to 10^{-16} for the exponential map, $10^{-8.2}$ for the tangent operator and 5×10^{-6} for its first derivative. A deterioration of the accuracy is observed at each differentiation step. Similar observations can be made for the closed form expression of the operators on $SE(3)$.

4 Conclusion

The series form is affected by truncation errors whose influence increases with the rotation or motion amplitude. Nevertheless, provided a suitable choice of the number of terms N, highly accurate expressions can be obtained even for large rotation amplitudes, but at a high computational cost.

The closed form combined with an appropriate threshold at low amplitude leads to an accurate evaluation of the exponential map. The closed form tangent operator is more sensitive to round-off errors. When performing further differentiations, the mathematical expressions becomes particularly complex and the influence of the round-off errors increases progressively.

Based on the analysis, we recommend to use the closed form for the evaluation of the exponential map on $SO(3)$ and $SE(3)$ as it provides a highly accurate expression for a low computational cost. The tangent operator may also be evaluated using the closed form if the tolerance is larger than 10^{-8}. To reach a tighter tolerance, the series expansion should be used, at least at low amplitudes. Regarding the derivatives of the tangent operator, a combination of the series form at low amplitude and of the closed form at high amplitude can be recommended. If the closed form is not available in the code, the series form can always be used with a suitable choice of N.

In Lie group methods, the exponential map is usually exploited locally around the origin to represent motion increments over a time step or relative motions within a finite element. Therefore, if it is crucial to ensure the numerical stability of the evaluation around the origin, the requirements at high amplitude are less critical.

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