

Family of higher order exponential variational integrators for split potential systems

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Abstract. In the present work, we derive a family of higher order exponential variational integrators for the numerical integration of systems containing slow and fast potential forces. To increase the order of variational integrators, first the discrete Lagrangian in a time interval is defined as a weighted sum of the evaluation of the continuous Lagrangian at intermediate time nodes while expressions for configurations and velocities are obtained using interpolating functions that can depend on free parameters. Secondly, in order to choose those parameters appropriately, exponential integration techniques are embedded. When the potential can be split into a fast and a slow component, we use different quadrature rules for the approximation of the different parts in the discrete action. Finally, we study the behavior of this family of integrators in numerical tests.

1. Introduction

In many Hamiltonian systems, the potential part of the corresponding energy function is composed of different parts with strongly varying dynamics. As an example, in classical molecular dynamics, the potential energy includes contributions of several types of atomic interaction. These interactions lead to extremely stiff potentials which force the solution of the equations of motion to oscillate on a very small time scale [1].

Following [1, 2, 3], in order to derive numerical integration schemes for these systems, we split their potential energy into a fast and a slow component. For the resulting Hamilton function, we derive a family of higher order exponential variational integrators that use different quadrature rules in the discrete action corresponding to the different potentials.

2. Review of variational integrators using interpolation techniques

For the derivation of high order variational integrators, we need to recall discrete variational calculus [4]. A discrete Lagrangian is a map $L_d : Q \times Q \rightarrow \mathbb{R}$ which may be considered as an approximation of a continuous action with Lagrangian $L : TQ \rightarrow \mathbb{R}$, i.e. $L_d(q_k, q_{k+1}) \approx \int_{t_k}^{t_{k+1}} L(q, \dot{q}) dt$. The action sum $S_d : Q^{N+1} \rightarrow \mathbb{R}$, $N \in \mathbb{N}$ corresponding to the Lagrangian L_d is defined as $S_d(\gamma_d) = \sum_{k=0}^{N-1} L_d(q_k, q_{k+1})$, with $\gamma_d = (q_0, \dots, q_N)$ representing the discrete trajectory. The discrete Hamilton principle states that a motion γ_d of the discrete mechanical system extremizes the action sum, i.e. $\delta S_d = 0$. By differentiation and rearrangement of the terms and having in mind that both q_0 and q_N are fixed, the discrete Euler-Lagrange equations (DEL) are obtained [4]

$$D_2 L_d(q_{k-1}, q_k) + D_1 L_d(q_k, q_{k+1}) = 0, \quad k = 1, \dots, N-1 \quad (1)$$

where the notation $D_i L_d$ indicates the slot derivative with respect to the i -th argument of L_d .



The definition of the discrete conjugate momentum at time steps k and $k + 1$ reads $p_k = -D_1 L_d(q_k, q_{k+1})$, $p_{k+1} = D_2 L_d(q_k, q_{k+1})$, $k = 0, \dots, N - 1$. The latter equations, also known as position-momentum form of a variational integrator, can be used when an initial condition (q_0, p_0) is known, to obtain (q_1, p_1) .

To construct high order methods, we approximate the action integral along the curve segment between q_k and q_{k+1} using a discrete Lagrangian that depends only on the end points. We obtain expressions for configurations q_k^j and velocities \dot{q}_k^j for $j = 0, \dots, S-1$, $S \in \mathbb{N}$ at time $t_k^j \in [t_k, t_{k+1}]$ by expressing $t_k^j = t_k + C_k^j h$ for $C_k^j \in [0, 1]$ such that $C_k^0 = 0$, $C_k^{S-1} = 1$ using

$$q_k^j = g_1(t_k^j)q_k + g_2(t_k^j)q_{k+1}, \quad \dot{q}_k^j = \dot{g}_1(t_k^j)q_k + \dot{g}_2(t_k^j)q_{k+1}, \quad (2)$$

where $h \in \mathbb{R}$ is the time step. We choose functions

$$g_1(t_k^j) = \sin\left(u - \frac{t_k^j - t_k}{h}u\right) (\sin u)^{-1}, \quad g_2(t_k^j) = \sin\left(\frac{t_k^j - t_k}{h}u\right) (\sin u)^{-1}, \quad (3)$$

to represent the oscillatory behavior of the solution, see [5, 6]. For continuity, $g_1(t_{k+1}) = g_2(t_k) = 0$ and $g_1(t_k) = g_2(t_{k+1}) = 1$ is required.

For any choice of interpolation used, we define the discrete Lagrangian by the weighted sum $L_d(q_k, q_{k+1}) = h \sum_{j=0}^{S-1} w^j L(q_k^j, \dot{q}_k^j)$, where it can be easily proved that for maximal algebraic order $\sum_{j=0}^{S-1} w^j (C_k^j)^m = \frac{1}{m+1}$, where $m = 0, 1, \dots, S-1$ and $k = 0, 1, \dots, N-1$ see [5, 6].

Applying the above interpolation technique with the trigonometric expressions (3), following the phase lag analysis of [5, 6], the parameter u can be chosen as $u = \omega h$. For problems that include a constant and known domain frequency ω (such as the harmonic oscillator) the parameter u can be easily computed. For the solution of orbital problems of the general N -body problem, where no unique frequency is given, a new parameter u must be defined by estimating the frequency of the motion of any moving point mass [6].

3. Exponential integrators

We now consider the Hamiltonian systems

$$\ddot{q} + \Omega q = g(q), \quad g(q) = -\nabla U(q), \quad (4)$$

where Ω is a diagonal matrix and $U(q)$ is a smooth potential function. We are interested in the long time behavior of numerical solutions when ωh is not small.

Since $q_{k+1} - 2 \cos(h\omega)q_k + q_{k-1} = 0$ is an exact discretisation of (4), see [10, 11, 12], we can consider the numerical scheme

$$q_{k+1} - 2 \cos(h\omega)q_k + q_{k-1} = h^2 \psi(\omega h) g(\phi(\omega h)q_k), \quad (5)$$

where the functions $\psi(\omega h)$ and $\phi(\omega h)$ are even, real-valued functions satisfying $\psi(0) = \phi(0) = 1$, see [1]. The resulting methods using the latter numerical scheme are known as exponential integrators (for some examples of those integrators see [1, 7, 8, 9]).

3.1. Exponential high order variational integrators

If we now use the phase fitted variational integrator in (4), the discrete Euler-Lagrange equations (1) read

$$q_{k+1} + \Lambda(u, \omega, h, S)q_k + q_{k-1} = h^2 \Psi(\omega h) g(\Phi(\omega h)q_k), \quad (6)$$

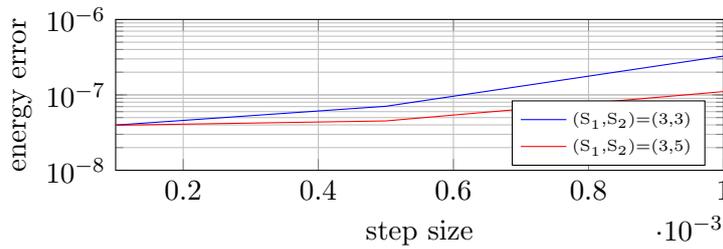


Figure 1: Modified satellite solar system. Global error for the energy error using the proposed family of exponential methods (red line) for $S_1 = 3$, $S_2 = 5$ and the ones that use $S = 3$ (blue line).

where

$$\Lambda(u, \omega, h, S) = \frac{\sum_{j=0}^{S-1} w^j \left[\dot{g}_1(t_k^j)^2 + \dot{g}_2(t_k^j)^2 - \omega^2 (g_1(t_k^j)^2 + g_2(t_k^j)^2) \right]}{\sum_{j=0}^{S-1} w^j \left[\dot{g}_1(t_k^j) \dot{g}_2(t_k^j) - \omega^2 g_1(t_k^j) g_2(t_k^j) \right]}. \tag{7}$$

Exponentially fitted methods using phase fitted variational integrators can be derived when

$$\Lambda(u, \omega, h, S) = -2 \cos(\omega h). \tag{8}$$

holds. Thus, phase fitted variational integrators using trigonometric interpolation can be considered as exponential integrators.

4. Family of higher order exponential variational integrators for split potential systems

We focus in the derivation of a family of exponential high order variational integrators for systems containing slow and fast potentials as described in Section 1. Following [1, 2], we split the potential energy of the Lagrangian to fast and slow terms, i.e.

$$L(q, \dot{q}) = T(\dot{q}) - V^f(q) - V^s(q), \tag{9}$$

where $T(\dot{q}) = \frac{1}{2} \dot{q}^T M \dot{q}$ is the kinetic energy of the system (M is a constant mass matrix). In order to use different quadrature rules to approximate the contribution of each potential to the action, we use different numbers of intermediate points for each potential. Denoting the numbers of intermediate points for the slow and the fast potential by S_1 and S_2 respectively, we restrict ourselves to choices that $S_1 < S_2$ (the choice $S_1 = S_2$ creates the exponential integrators of Section 2).

Following Section 2 (see also [5, 6]) the discrete Lagrangian corresponding to (9) is

$$L_d^{S_1, S_2}(q_k, q_{k+1}) = h \left[\sum_{j=0}^{S_1-1} w_1^j \left[T(\dot{q}(t_k^j)) - V^s(q(t_k^j)) \right] - \sum_{j=0}^{S_2-1} w_2^j V^f(q(t_k^j)) \right], \tag{10}$$

where intermediate positions and velocities are given in (2) and (3), for $S = S_1$ and $S = S_2$ respectively.

5. Satellite solar system

As a numerical example, we choose the modified solar system with two planets (with masses $m_1 = 1$ and $m_2 = m_3 = 10^{-2}$) and a satellite ($m_4 = 10^{-4}$) which moves rapidly around the mass m_2 , see [1]. Considering initial configurations $q_1 = (0, 0)$, $q_2 = (1, 0)$, $q_3 = (4, 0)$, $q_4 = (1.01, 0)$ and initial velocities $\dot{q}_1 = (0, 0)$, $\dot{q}_2 = (0, 1)$, $\dot{q}_3 = (0, 0.5)$, $\dot{q}_4 = (0, 0)$, the motion of the two planets is nearly circular with periods close to 2π and 14π , respectively [1]. The problem is then described by the Lagrange function

$$L(q, \dot{q}) = \frac{1}{2} \sum_{i=1}^4 m_i \dot{q}_i^2 - V^f(q) - V^s(q), \quad (11)$$

where

$$V^s(q) = \sum_{i < j, (i,j) \neq (2,4)}^4 \frac{m_i m_j}{\|q_i - q_j\|}, \quad V^f(q) = \frac{m_2 m_4}{\|q_2 - q_4\|}. \quad (12)$$

Figure 1 shows the comparison of errors in total energy of the system at $t = 1$ for time steps $h \in \{10^{-4}, 5 \cdot 10^{-4}, 10^{-3}\}$ for the proposed family of exponential methods (red line) for $S_1 = 3$, $S_2 = 5$ and the ones that use $S = 3$ (blue line), see [6]. In that, it is clear that for all the step sizes that are tested, the smallest energy errors are obtained when using the splitting technique of Section 4.

6. Conclusions

A family of higher order exponential variational integrators for the numerical integration of systems containing slow and fast potential forces is presented. For these methods, the discrete Lagrangian in any time interval is defined as a weighted sum of the evaluation of the continuous Lagrangian at intermediate time nodes. In order to use different quadrature rules for the different potential terms, a splitting of their potential energy into a fast and a slow component is addressed, and different numbers of intermediate points for each potential is used. Preliminary numerical results for the case of the modified solar system, show better behavior of the proposed simulation technique, when compared to the one derived without potential energy splitting.

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