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Multi-step numerical methods derived using discrete Lagrangian integrators

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Abstract. On the basis of the variational integrators theory, we initially examine the possibility of deriving multi-step numerical methods. Then, we propose an integration technique that approximates the action integral within one time interval by using appropriate expressions for the relevant configurations and velocities. These approximations depend on a specific number of known configurations defined at previous time nodes. Multi-step numerical methods can finally be deduced, by defining, as usually, the Lagrange function as a weighted sum over the discrete Lagrangians corresponding to each of the curve segments and using the discrete Euler-Lagrange equations.

1. Introduction and motivation

Numerical integration of ordinary differential equations with oscillatory solutions has been the subject of intensive research in the past few decades. Special cases of such ordinary differential equations are often met in real problems, such as the N-body problem. For highly oscillatory problems, standard nonspecialized methods may require a huge number of steps to track the oscillations. One of the possible ways to obtain a more efficient integration process, is to construct numerical methods with an increased algebraic order, even though the implementation of high algebraic order meets several difficulties [1].

On the other hand, variational integrators are relatively new tools to model dynamical systems. In particular, they constitute an alternative to continuous ordinary differential equations to simulate mechanical systems. They can be considered as a class of integrators [1, 2] that preserve (or nearly preserve, depending on the particular integrator) fundamental physical observables like energy and momentum [3, 4, 5]. They have traditionally been used to study conservative systems (e.g., celestial mechanics), but modern variational integrators also include forcing and dissipation. In fact, the results with external forcing often have better accuracy than those of classical methods.

In the present contribution, a new way to derive multi-step numerical methods is investigated. Based on the variational integration schemes, the proposed technique approximates the action integral within one time interval by using expressions for configurations and velocities that depend on a specific number of known configurations at previous time nodes. By defining the Lagrange function as a weighted sum over the discrete Lagrangians corresponding to the each of the curve segments and using the discrete Euler-Lagrange equations, multi-step numerical methods can be defined. The application of these methods may be tested in several numerical problems.

2. Discrete mechanics and variational integrators

When discretizing a mechanical system, whose continuous Lagrangian is defined as $L : TQ \to R$, on the time interval $[0, T]$, a finite number of time nodes $0 = t_0 < ... < t_N = T$ derives the sequence of configurations $q_0, ..., q_N$, where $q_k \approx q(t_k)$ for $N \in \mathbb{N}$. The discrete Lagrange function $L_d : Q \times Q \to \mathbb{R}$ can be defined by the approximation of the action integral along the curve segment between q_k and q_{k+1}, i.e. $L_d(q_k, q_{k+1}) \approx \int_{t_k}^{t_{k+1}} L(q, \dot{q})dt$. The discrete action sum corresponding to the above discrete Lagrangians then reads

$$S_d(q_0, ..., q_N) = \sum_{k=0}^{N-1} L_d(q_k, q_{k+1}) \approx \int_0^T L(q, \dot{q})dt \tag{1}$$

Applying Hamilton's actions principle, $\delta S_d(q_0, ..., q_N) = 0$, by requiring the endpoints to be fixed, i.e. $\delta q_0 = \delta q_N = 0$, discrete Euler-Lagrange equations are obtained as

$$D_2 L_d(q_{k-1}, q_k) + D_1 L_d(q_k, q_{k+1}) = 0, \qquad k = 1, ..., N-1 \tag{2}$$

where $D_1 L_d$ and $D_2 L_d$ denote the partial derivatives of L_d with respect to the first and second arguments, see e.g. [4].

3. Deriving multi-step methods from discrete Lagrangian integrators

Following the steps of [4, 5, 6] to derive multi-step numerical schemes using variational integrators, we use intermediate configuration $q^j \in [q_k, q_{k+1}]$ at time $t^j \in [t_k, t_{k+1}]$ for $j = 0, ..., S$ ($S \in \mathbb{N}$) by expressing $t^j = t_k + C^j h$ for $C^j \in [0, 1]$ such that $C^0 = 0, C^S = 1$ for $h = t_{k+1} - t_k$. Under these assumptions the general expression for q^j can then be written as

$$q^j = f_{k-\sigma}(t^j)q_{k-\sigma} + ... + f_{k+1+\sigma}(t^j)q_{k+1+\sigma}, \qquad \sigma \in \mathbb{N} \tag{3}$$

where $2\sigma + 2$ represents the number of configuration points needed for the above approximation and

$$\begin{array}{c} f_{k-\sigma}(t^j) = 0, \quad \text{for} \quad j = 0, j = S \quad \text{and} \quad \sigma \neq 0 \\ f_k(t_k) = f_{k+1}(t_{k+1}) = 1, \quad f_k(t_{k+1}) = f_{k+1}(t_k) = 1 \end{array} \tag{4}$$

The velocity obtained for the above expression of the intermediate point can be written as

$$\dot{q}^j = \dot{f}_{k-\sigma}(t^j)q_{k-\sigma} + ... + \dot{f}_{k+1+\sigma}(t^j)q_{k+1+\sigma}, \qquad \sigma \in \mathbb{N} \tag{5}$$

($\dot{f}$ denotes, as usually, time derivative). It is worth notting that the phase-fitted discrete Lagrangian integrators of Ref. [6] are a special case of the above expressions for $\sigma = 0$ and

$$f_k(t^j) = \frac{\sin\left(u - \frac{t^j - t_k}{h}u\right)}{\sin u}, \qquad f_{k+1}(t^j) = \frac{\sin\left(\frac{t^j - t_k}{h}u\right)}{\sin u} \tag{6}$$

($u \in \mathbb{R} - \{k\pi, k \in \mathbb{Z}\}$). It is now clear that the latter functions satisfy the assumptions of Eqs. 4. For these functions the expressions for intermediate points are

$$\begin{aligned} q^j &= \frac{\sin\left(u - \frac{t^j - t_k}{h}u\right)}{\sin u} q_k + \frac{\sin\left(\frac{t^j - t_k}{h}u\right)}{\sin u} q_{k+1} \\ \dot{q}^j &= \frac{1}{h}\left[- \frac{u\cos\left(u - \frac{t^j - t_k}{h}u\right)}{\sin u} q_k - \frac{u\cos\left(\frac{t^j - t_k}{h}u\right)}{\sin u} q_{k+1} \right] \end{aligned} \tag{7}$$

4. Numerical schemes derived using Catmull-Rom splines

Following the above assumptions, we employ the cubic Hermitian spline interpolation on a single unit interval to obtain points $q^j \in [q_k, q_{k+1}]$ from a linear combination of the form [7]

$$q^j = a_1 q_k + a_2 p_k + a_3 q_{k+1} + a_4 p_{k+1} \tag{8}$$

where

$$\begin{aligned} a_1 &= 2(c^j)^3 - 3(c^j)^2 + 1, \qquad a_2 = (c^j)^3 - 2(c^j)^2 + c^j, \\ a_3 &= -2(c^j)^3 + 3(c^j)^2, \qquad a_4 = (c^j)^3 - (c^j)^2. \end{aligned} \tag{9}$$

If we chose the tangents to be given by $p_k = (q_{k+1} - q_{k-1})(2h)^{-1}$, a Catmull-Rom spline interpolation of the interval can be obtained as [7]

$$q^j = f_{k-1} q_{k-1} + f_k q_k + f_{k+1} q_{k+1} + f_{k+2} q_{k+2} \tag{10}$$

where

$$\begin{aligned} f_{k-1} &= -\frac{a_2}{2h}, \qquad f_k = a_1 - \frac{a_4}{2h}, \\ f_{k+1} &= \frac{a_2}{2h} + a_3, \qquad f_{k+2} = \frac{a_4}{2h}. \end{aligned} \tag{11}$$

Using the latter expression for q^j the discrete Lagrangian is of the same form, i.e. it depends only on the endpoints $[q_k, q_{k+1}]$. From Eq. (10) the expression for $\dot{q}^j$ can be functional cast in the form

$$\dot{q}^j = \dot{f}_{k-1} q_{k-1} + \dot{f}_k q_k + \dot{f}_{k+1} q_{k+1} + \dot{f}_{k+2} q_{k+2} \tag{12}$$

where

$$\begin{aligned} \dot{f}_{k-1} &= \frac{-3(c^j)^2 + 4c^j - 1}{2h^2}, \qquad \dot{f}_k = \frac{12(c^j)^2 h - 12c^j h - 3(c^j)^2 - 2(c^j)}{2h^2}, \\ \dot{f}_{k+1} &= \frac{3(c^j)^2 - 4c^j - 12(c^j)^2 h + 12c^j h + 1}{2h^2}, \qquad \dot{f}_{k+2} = \frac{3(c^j)^2 - 2c^j}{2h^2}. \end{aligned} \tag{13}$$

By combining Eqs. (10) and (12), with Eqs. (9) and (9) the discrete Lagrangian reads

$$L_d(q_{k-1}, q_k, q_{k+1}, q_{k+2}) \approx h \sum_{j=1}^{S} W_j L(q(t_k + c^j h), \dot{q}(t_k + c^j h)). \tag{14}$$

Using the Hamilton's principle we can now compute the variations of the action sum S providing that the boundary points q_0,q_1,q_2 and q_{N-2},q_{N-1},q_N are kept fixed. Furthermore, by demanding the variations of the action to be zero for any choice of δq_k with $\delta q_0 = \delta q_1 = \delta q_2 = \delta q_N = \delta q_{N+1} = \delta q_{N+2} = 0$, we obtain

$$\begin{aligned} D_1 L_d(q_k, q_{k+1}, q_{k+2}, q_{k+3}, h) &+ D_2 L_d(q_{k-1}, q_k, q_{k+1}, q_{k+2}, h) + \\ D_3 L_d(q_{k-2}, q_{k-1}, q_k, q_{k+1}, h) &+ D_4 L_d(q_{k-3}, q_{k-2}, q_{k-1}, q_k, h) = 0 \end{aligned} \tag{15}$$

The latter equations are the discrete Euller-Lagrange equations stemming from the discrete Lagrangian Eq. (14) and must hold for each value of k.

We can now use the expressions (10) and (12) to derive the discrete Lagrangian of Eq. (14) for some specific physical problems. For the resulting Lagrangian, the discrete Euller–Lagrange equations of (15) will be used.

5. Simple harmonic oscillator

We first consider the simple harmonic oscillator described by the Lagrangian

$$L = \frac{1}{2}\dot{q}^2 - \frac{1}{2}\omega q^2 \tag{16}$$

The interpolation technique of Eqs. (10) defines the discrete Lagrangian

$$L_d(q_{k-1}, q_k, q_{k+1}, q_{k+2}, h) = \frac{h}{2}\left[\sum_{j=0}^{S} W_j\left(\dot{q}^j\right)^2 - \omega^2 \sum_{j=0}^{S} W_j\left(q^j\right)^2\right] \tag{17}$$

Subsequently the discrete Euler-Lagrange equations (15) give the variational integrator (see Ref. [4])

$$P_1 q_{k+3} + P_2 q_{k+2} + P_3 q_{k+1} + P_4 q_k + P_3 q_{k-1} + P_2 q_{k-2} + P_1 q_{k-3} = 0 \tag{18}$$

where

$$\begin{aligned}
P_1 &= \sum_{j=0}^{S} W_j\left(\dot{f}_{k-1}\dot{f}_{k+2} - \omega^2 f_{k-1} f_{k+1}\right) \\
P_2 &= \sum_{j=0}^{S} W_j\left[\dot{f}_{k-1}\dot{f}_{k+1} + \dot{f}_k\dot{f}_{k+1} - \omega^2(f_{k-1}f_{k+1} + f_k f_{k+1})\right] \\
P_3 &= \sum_{j=0}^{S} W_j\left[\dot{f}_{k-1}\dot{f}_k + \dot{f}_k\dot{f}_{k+1} + \dot{f}_{k+1}\dot{f}_{k+2} - \omega^2(f_{k-1}f_k + f_k f_{k+1} + f_{k+1}f_{k+2})\right] \\
P_4 &= \sum_{j=0}^{S} W_j\left[\dot{f}_{k-1}^2 + \dot{f}_k^2 + \dot{f}_{k+1}^2 + \dot{f}_{k+2}^2 - \omega^2(f_{k-1}^2 + f_k^2 + f_{k+1}^2 + f_{k+2}^2)\right]
\end{aligned} \tag{19}$$

For the above integrator since the first six points must be known, any numerical scheme can be used as starting method.

6. Summary and conclussions

In the present we have investigated the possibility of deriving multi-step numerical schemes by combining variational integrators theory and spline interpolation techniques. A special case of the proposed technique, that uses Catmull-Rom spline interpolationhas been derived for the numerical solution of physical problems with oscillating solution.

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