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Symmetric Path Fitted Variational Integrators

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Abstract. Recently, the benefits of variational integrators have been combined with efficient high order techniques. On the other hand, a special set of high order methods are the symmetric ones, those who preserve time reversal symmetry and show improved behavior in long term integration. In the present work, we will introduce a systematic way to construct symmetric variational integrators. The idea is to apply the variational principle not in a set of intermediate points but to a set of parameters that characterize a symmetric orbit between starting and ending points. The estimated symmetric orbit may be a polynomial or a general function that sometimes is indicated by the nature of the problem to solve. The results show excellent behavior in long term integration and acceleration of the method when special functions are used.

1. Introduction

It is well known that the dynamics of seemingly unrelated conservative systems in mechanics, physics, biology, and chemistry fit the Hamiltonian formalism ([1]). Included among these are particle, rigid body, ideal fluid, solid, and plasma dynamics. An important property of the Hamiltonian flow or solution to a Hamiltonian system is that it preserves the Hamiltonian and the symplectic form (see, for example, [2]). A key consequence of symplecticity is that the Hamiltonian flow is phase-space volume preserving (Liouville's theorem). Since analytic expressions for the Hamiltonian flow are rarely available, approximations based on discretization of time are used. A numerical integration method which approximates a Hamiltonian flow is called symplectic if it discretely preserves a symplectic 2-form to within numerical round off ([3, 4]) and standard otherwise. By ignoring the Hamiltonian structure, a standard method often introduces spurious dynamics.

Symplectic integrators can be derived by a variety of ways including Hamilton-Jacobi theory, symplectic splitting, and variational integration techniques. Early investigators, guided by Hamilton-Jacobi theory, constructed symplectic integrators from generating functions which approximately solve the Hamilton–Jacobi equation. The symplectic splitting technique is based on the property that symplectic integrators form a group, and thus, the composition of symplectic-preserving maps is also symplectic. The idea is to split the Hamiltonian into terms whose flow can be explicitly solved and then compose these individual flows in such a fashion that the composite flow is consistent and convergent with the Hamiltonian flow being simulated. On the other hand, variational integration techniques determine integrators from a discrete Lagrangian and associated discrete variational principle. The discrete Lagrangian can be designed to inherit the symmetry associated with the action of a Lie group, and hence by a discrete Noether's theorem, these methods can also preserve momentum invariants (for a discussion of the above statements, see [1]).

Variational integration theory derives integrators for mechanical systems from discrete variational principles ([5, 6, 7]). Variational principles have been successfully applied to partial differential equations and to stochastic systems as well. In the general theory, discrete analogs of the Lagrangian, Noether's theorem, the Euler–Lagrange equations, and the Legendre transform can be easily obtained. Moreover, variational integrators can readily incorporate holonomic constraints (via Lagrange multipliers) and non-conservative effects (via their virtual work). The algorithms derived from this discrete principle have been successfully tested in infinite and finite-dimensional conservative, dissipative, smooth and non-smooth mechanical systems.

In general, the accuracy is not the terminus of the application of variational integrators, but rather their ability to discretely preserve essential structure of the continuous system and in computing statistical properties of larger groups of orbits, such as in computing Poincaré sections or the temperature of a system (see, for example. On the other hand, high accuracy can be obtained using special designed methods as it is explained in [5, 6, 7]. In the case of time reversible systems, it has been found that both accuracy and long term behavior is dramatically improved when using methods that are symmetric, which means that they preserve the time reversal symmetry.

In the present work, we will introduce a systematic way to construct symmetric variational integrators. The idea is to apply the variational principle not in a set of intermediate points but to a set of parameters that characterize a symmetric orbit between starting and ending points. The estimated symmetric orbit may be a polynomial or a general function that sometimes is indicated by the nature of the problem to solve. The results show excellent behavior in long term integration and acceleration of the method when special functions are used.

2. Symmetric Path Fitted Methods

2.1. Symmetric Methods

Conservative mechanical systems are reversible in the sense that if we invert the initial direction of the velocity and keep the initial position, the solution trajectory remains the same (only the direction of motion is changed). In general, let ρ be an invertible transformation in the phase space of a system described by the differential equation $\dot{y} = f(y)$. Then, the differential equation and the vector field $f(y)$ are called ρ-reversible if

$$\rho f(y) = -f(\rho y) \tag{1}$$

On the other hand, a map $\Phi(y)$ is called ρ-reversible if

$$\rho \circ \Phi = \Phi^{-1} \circ \rho \tag{2}$$

In the case of a numerical method Φ_h, the condition 2 takes the form

$$\rho \circ \Phi_h = \Phi_{-h} \circ \rho \tag{3}$$

Finally, a method is symmetric if (setting $\rho = -id$, where id is the identity map)

$$\Phi_h = \Phi_{-h}^{-1} \tag{4}$$

or when interchanging y_0 with y_1 and h with $-h$ the resulting method is the same. Symmetric methods have several benefits-in long term integration. One of them is that their order is even (since both the method and the adjoint one must have exactly the same truncation error).

2.2. Path Fitted Variational Integrators

In the case of path fitted variational integrators, we have a parametric estimation of the orbit, and the variational principles applied in order to optimize the values of the free parameters. Thus, considering the Lagrangian of the system

$$L = L(q^i, \dot{q}^i, t), \qquad i = 1, .., n \tag{5}$$

where $2 \cdot n$ is the dimension of the configuration space, we assume that the path between q^i_k at time t_k and q^i_{k+1} at time t_{k+1} can be parametrized as

$$q^i(t) = g^i_k\left(t, q^i_k, x^{i,j}\right)\ ,\ j = 1, 2, \ldots, K \tag{6}$$

where K is the number of free parameters. Moreover, we can assume that the parameter $x^{i,1}$ is the final point of the orbit. Thus, we have the following conditions

$$g^i_k\left(t_k, q^i_k, x^{i,j}_k\right) = q^i_k \tag{7}$$

$$g^i_k\left(t_{k+1}, q^i_k, x^{i,j}_k\right) = x^{i,1}_k \tag{8}$$

As it has been described above, by an appropriate choice of quadrature scheme we can break up the action integral into pieces, which we denote by $S_{d,k}$. Replacing now in the Lagrangian equ. 6, we have

$$S_{d,k} = S_{d,k}\left(q^i_k, x^{i,j}_k\right) \tag{9}$$

The condition in equ. 8 can be obtained using Lagrange multipliers λ^i_k and thus we can redefine the discrete Lagrangian as

$$S_d = \sum_{k=0}^{N-1} S_{d,k}(q^i_k, x^{i,j}_k) - \sum_{k=0}^{N-2}\sum_{i=1}^{n} \lambda^i_k (x^{i,1}_k - q^i_{k+1}) \tag{10}$$

Then by demanding $\delta S_d = 0$ and fixing points at $t = t_0$ and $t = t_N$ we can derive the equations that the unknown variables must follow

$$\begin{aligned} \frac{\partial S_{d,k}}{\partial q^i_k} + \lambda^i_{k-1} &= 0 \\ \frac{\partial S_{d,k}}{\partial x^{i,1}_k} - \lambda^i_k &= 0 \\ \frac{\partial S_{d,k}}{\partial x^{i,J}_k} &= 0, \quad j = 2, 3, \ldots, K \end{aligned} \tag{11}$$

It is easy to verify that the Lagrange multipliers λ^i_k are the momenta p^i_k. Then, the system of K equations

$$\begin{aligned} \frac{\partial S_{d,k}}{\partial q^i_k} + p^i_k &= 0 \\ \frac{\partial S_{d,k}}{\partial x^{i,j}_k} &= 0, \quad j = 2, 3, \ldots, K \end{aligned} \tag{12}$$

is solved to give the K unknowns $x^{i,j}_k$, $j = 1, 2, \ldots, K$. Finally, for the computation of the p^i_{k+1} and q^i_{k+1} we have

$$\begin{aligned} p^i_{k+1} &= \frac{\partial S_{d,k}}{\partial x^{i,1}_k} \\ q^i_{k+1} &= x^{i,1}_k \end{aligned} \tag{13}$$

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2.3. Polynomial fitting
Let $h = t_{k+1} - t_k$. Then we can define the polynomial function

$$g_k^i\left(t, q_k^i, x_k^{i,j}\right) = q_k^i\left(1 - \frac{t}{h}\right) + x_k^{i,1} \cdot \frac{t}{h} + P\left(t, x_k^{i,2}, x_k^{i,3}, \ldots, x_k^{i,K}\right) \tag{14}$$

where $P\left(t, x_k^{i,2}, x_k^{i,3}, \ldots, x_k^{i,K}\right)$ is a polynomial in t which depends on $x_k^{i,2}, x_k^{i,3}, \ldots, x_k^{i,K}$ and is symmetric in the interchange of t with $h - t$. Moreover, $P(0) = P(h) = 0$.

It is easy to verify that interchanging q_k^i with q_{k+1}^i and t with $h - t$ (we assume here that t represents $t - t_k$ so it varies fro 0 to h), the path remains the same and this holds for the resulting method iff $P(t) = P(h - t)$. Setting $t^{(1)} = t$ and $t^{(2)} = h - t$ we can write the polynomial P in 2-variables as $P\left(t^{(1)}, t^{(2)}\right)$. Thus, P must be a symmetric polynomial. In general, let $x_1, \ldots, x_n$ be variables, and denote for $k \geq 1$ by $p_k(x_1, \ldots, x_n)$ the k-th power sum:

$$p_k(x_1, \ldots, x_n) = \sum\nolimits_{i=1}^{n} x_i^k = x_1^k + \cdots + x_n^k, \tag{15}$$

and for $k \geq 0$ denote by $e_k(x_1, \ldots, x_n)$ the elementary symmetric polynomial that is the sum of all distinct products of k distinct variables, so in particular

$$\begin{aligned}
e_0(x_1, \ldots, x_n) &= 1, \\
e_1(x_1, \ldots, x_n) &= x_1 + x_2 + \cdots + x_n, \\
e_2(x_1, \ldots, x_n) &= \sum\nolimits_{i<j} x_i x_j, \\
e_n(x_1, \ldots, x_n) &= x_1 x_2 \cdots x_n, \\
e_k(x_1, \ldots, x_n) &= 0, \quad \text{for } k > n.
\end{aligned}$$

Then, according to the Newton's identities

$$k \cdot e_k(x_1, \ldots, x_n) = \sum_{i=1}^{k} (-1)^{i-1} e_{k-i}(x_1, \ldots, x_n) p_i(x_1, \ldots, x_n), \tag{16}$$

and thus we can write

$$P\left(t, x_k^{i,2}, x_k^{i,3}, \ldots, x_k^{i,K}\right) = \sum_{j=2}^{K+1} x^{i,j}\left(t^j + (h - t)^j\right) \tag{17}$$

with

$$x^{i,K+1} = -\sum_{j=2}^{K} x^{i,j} \tag{18}$$

in order to have $P(0) = 0$.

2.4. Trigonometric fitting
In the case of oscillatory problems, trigonometric or phase fitting can improve dramatically the behavior of the integrators (se, for example, [5, 6]). The analysis is the same as in the polynomial fitting, except that now we are dealing with the phase function. In detail, consider the path

$$q_k^i(t) = A\cos\left(f_k^i(t)\right) + B\sin\left(f_k^i(t)\right) \tag{19}$$

where $f(t)$ is a polynomial similar to that in equ. 14. Thus,

$$f_k^i(t) = f_0^i\left(1 - \frac{t}{h}\right) + f_1^i\frac{t}{h} + \sum_{j=2}^{K+1} f_j^i\left(t^j + (h-t)^j\right) \tag{20}$$

Both constants A, B are calculated be the equations

$$q_k^i(t_k) = q_{k+1}^i$$
$$q_k^i(t_{k+1}) = x_k^{i,1}$$

3. The 2-body problem

We now turn to the study of two objects interacting through a central force. The most famous example of this type, is the Kepler problem (also called the two-body problem) that describes the motion of two bodies which attract each other. In the solar system the gravitational interaction between two bodies leads to the elliptic orbits of planets and the hyperbolic orbits of comets.

If we choose one of the bodies as the center of our coordinate system, the motion will stay in a plane. Denoting the position of the second body by $\mathbf{q} = (q_1, q_2)^T$, the Lagrangian of the system takes the form (assuming masses and gravitational constant equal to 1)

$$L(\mathbf{q}, \dot{\mathbf{q}}, t) = \frac{1}{2}\dot{\mathbf{q}}^T\dot{\mathbf{q}} + \frac{1}{|\mathbf{q}|} \tag{21}$$

The initial conditions are taken

$$\mathbf{q} = (1-\epsilon, 0)^T \ , \ \dot{\mathbf{q}} = \left(0, \sqrt{\frac{1+\epsilon}{1-\epsilon}}\right)^T \tag{22}$$

where ϵ is the eccentricity of the orbit. In the first experiment, we take the eccentricity $\epsilon = 0.5$ and constant step size $h = 0.05$ and plot the relative error in the energy during one period for several number of path parameters K.

In our experiment, we take the eccentricity $\epsilon = 0.95$ and use an adaptive time step control in order to keep the relative error in energy smaller than 10^{-7}. Table 1 shows the number of integration steps needed for one period. The order of approximation is again clearly increases with increasing K as the mean step size needed for the same error in energy increases from $1.8 \cdot 10^{-3}$ for $K = 4$ to 0.1 for $K = 8$.

Table 1. Number of integration steps

S	No of Steps
2	$> 10^4$
3	$> 10^4$
4	3526
5	460
6	421
7	181
8	142

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4. Conclusions

The use of symmetric paths as estimators for trajectories in the construction of variational principles, produces integrators with excellent behavior in energy for long term integration. Moreover, a generalization of the method proposed, can easily applied in order to construct high order methods. The results show that in both stiff problems (like the 2-body one with high eccentricity) and many body one, the symmetric variational integrator can produces accurate and stable solutions. Moreover, the method can be easily adapted in order to use it for the construction of trigonometric fitted or in general function fitting symmetric variational integrators for special problems (like oscillatory ones).

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