Advancement Talk

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Outline

1. Classical Mechanics
2. Numerical Example
3. Discrete Mechanics
4. Taylor Variational Integrator
5. Discrete Hamiltonian Variational Integrators

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Lagrangian Dynamical System

Lagrangian System

The **Configuration Space** is a differentiable manifold, Q.
The **State Space** is the corresponding tangent bundle, TQ, with local coordinates $(q, \dot{q})$.
The **Lagrangian** function, $L : TQ \to \mathbb{R}$ is a differentiable function.
Together Q and L define a **Lagrangian system**.

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Dynamics of the Lagrangian system

$\mathcal{C}(Q) = \{q : [0, T] \to Q | q \text{ is a } C^2 \text{ curve } \}$ is the **path space**.
$q \in \mathcal{C}(Q)$ where $\dot{q}(t) \in T_{q(t)}Q$, is called a **motion** in the Lagrangian system, if q extremizes the **action** functional,

$$\mathbf{S}(q) = \int_0^T L(q(t), \dot{q}(t))dt$$

Theorem

A motion, q, satisfies the **Euler − Lagrange** *equations,*

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}} - \frac{\partial L}{\partial q} = 0.$$

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Proof

$$\begin{aligned} 0 &= \delta \mathbf{S} \\ &= \delta \int_0^T L(q, \dot{q}) dt \\ &= \int_0^T \delta L(q, \dot{q}) dt \\ &= \int_0^T \frac{\partial L}{\partial q}\delta q + \frac{\partial L}{\partial \dot{q}}\delta \dot{q} dt \end{aligned}$$

Proof, cont'd

$$= \int_0^T \left(\frac{\partial L}{\partial q} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}}\right)\delta q dt$$

The last line comes from integration by parts, where we have constrained our variations to vanish on the boundary. Finally, the fudamental theorem of the calculus of variations implies,

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}} - \frac{\partial L}{\partial q} = 0.$$

Legendre Transform

Definition

Given a Lagrangian system, define the fiber derivative $\mathbb{F}L : TQ \to T^*Q$ by,

$$\mathbb{F}L(v) \cdot w = \frac{d}{ds}|_{s=0} L(v + sw),$$

where $v, w \in T_q Q$.

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where $v, w \in T_q Q$.

Legendre Transform

$\mathbb{F}L$ is called the **Legendre Transform**. For a finite dimensional configuration manifold,

$$\mathbb{F}L : (q, \dot{q}) \to (q, \frac{\partial L}{\partial \dot{q}}) = (q, p).$$

Definition

The generalized **momentum** coordinates, $p \in T^*Q$, are defined by,

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Hamiltonian

Assuming $\mathbb{F}L$ is a diffeomorphism, define the **Hamiltonian** $H : T^*Q \to \mathbb{R}$ as,

$$H(q,p) = p\dot{q} - L(q,\dot{q})|_{p=\frac{\partial L}{\partial \dot{q}}}.$$

Hamilton's Equations

Definition

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$$\dot{q} = \frac{\partial H}{\partial p}$$

$$\dot{p} = -\frac{\partial H}{\partial q}$$

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Theorem

Hamilton's equations are equivalent to the Euler-Lagrange equations.

Sketch of the Proof

$$\begin{aligned} 0 &= \dot{p} + \frac{\partial H}{\partial q} \\ &= \frac{d}{dt} p + \frac{\partial H}{\partial q} \end{aligned}$$

Noting $p = \frac{\partial L}{\partial \dot{q}}$ by defintion, and $\frac{\partial H}{\partial q} = -\frac{\partial L}{\partial q}$ implies,

$$0 = \frac{d}{dt} \frac{\partial L}{\partial \dot{q}} - \frac{\partial L}{\partial q}.$$

Conservation of Energy

Theorem

Given a Lagrangian, $L(q, \dot{q})$, that is not explicitly a function of time, then the Hamiltonian is an invariant of the flow.

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Proof

$$\begin{aligned}\frac{dH}{dt} &= \frac{\partial H}{\partial q}\frac{dq}{dt} + \frac{\partial H}{\partial p}\frac{dp}{dt} \\ &= -\dot{p}\dot{q} + \dot{q}\dot{p} \\ &= 0\end{aligned}$$

Can we build a numerical method that takes into account the underlying (geometric)structure of the dynamical system?

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Simple Pendulum

Consider a pendulum consisting of a ball with unit mass attached to a rod of unit length, where for simplicity we assume the rod has negligible weight. The pendulum's configuration manifold is S^1. The Lagrangian will be of the form L=T-U, where T is the kinetic energy and U is the potential energy of the system. We will parametrize the manifold by θ the angle between the rod and the negative y-axis.

$$L(\theta, \dot{\theta}) = \frac{1}{2}\dot{\theta}^2 + 9.8sin(\theta)$$

The corresponding Hamiltonian will then be the total energy of the system, which will remain constant.

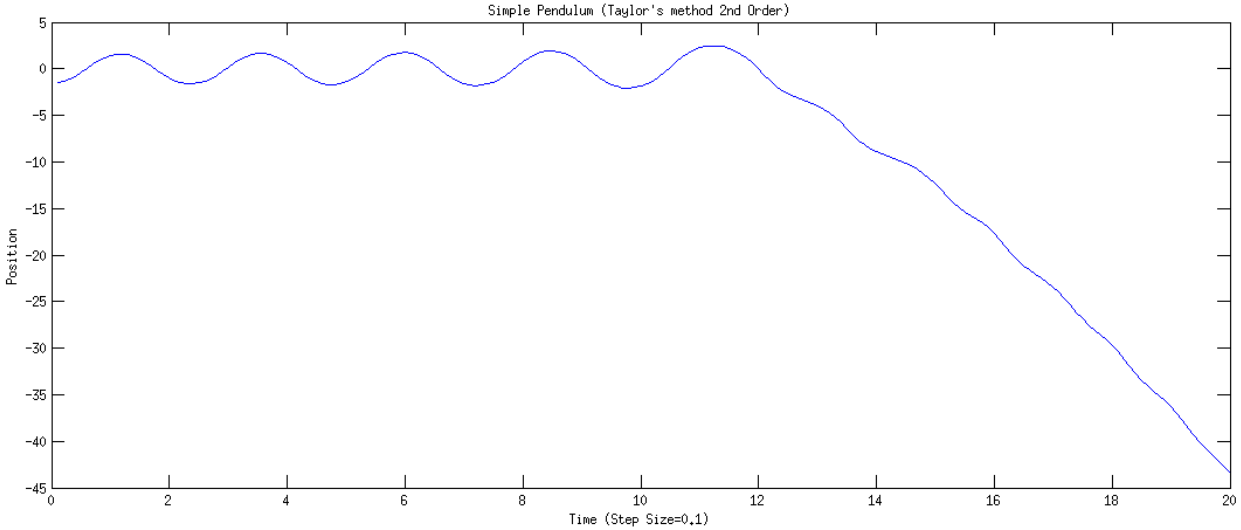
Simple Pendulum

The corresponding Euler-Lagrange equation is,

$$\ddot{\theta} = -9.8 sin(\theta)$$

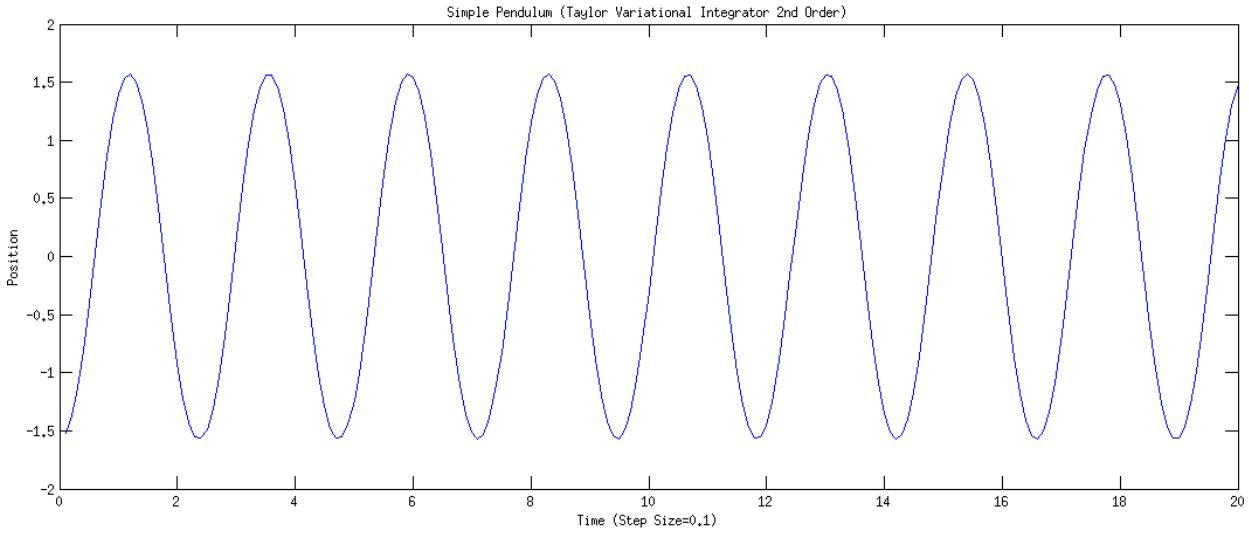
Simple Pendulum

Taylor's Method 2nd Order h=0.1



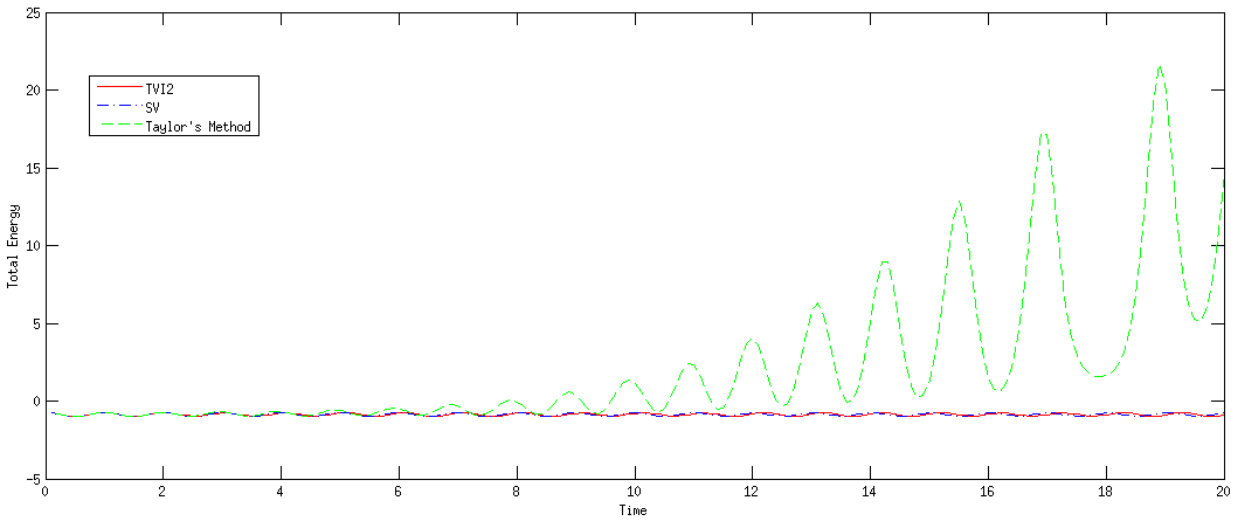
Simple Pendulum

Taylor Variational Integrator 2nd Order(TVI2) h=0.1

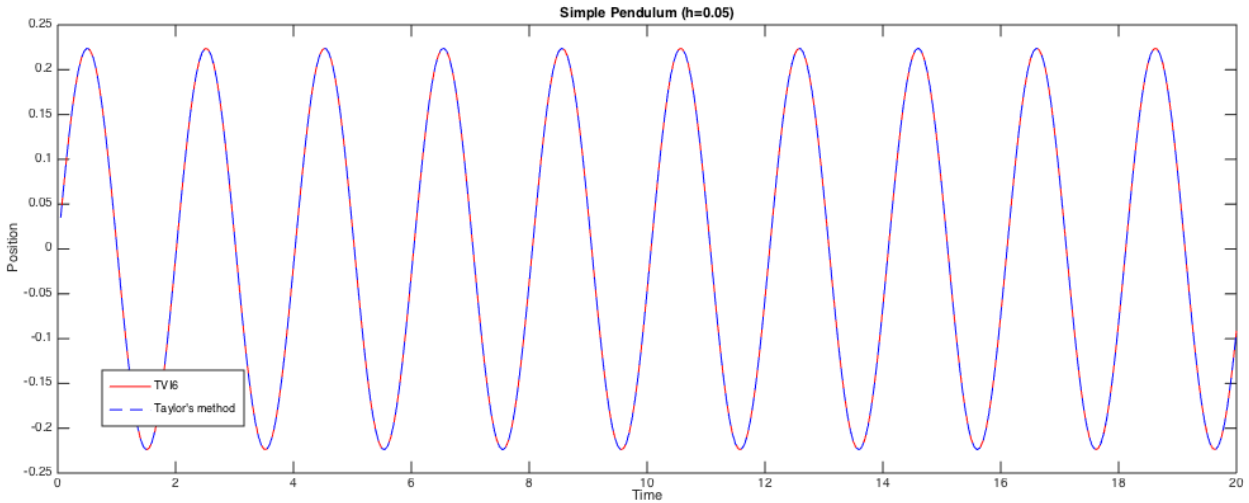


Simple Pendulum

Total Energy for Taylor's Method 2nd Order and TVI2 h=0.1



Taylor's Method 6th Order h=0.05 and TVI6



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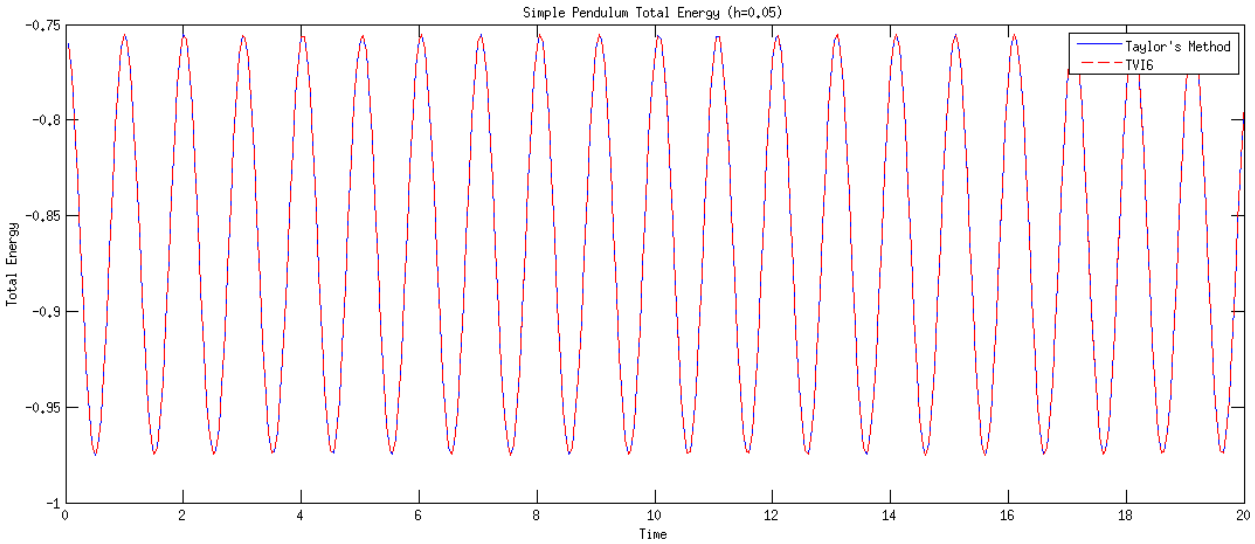

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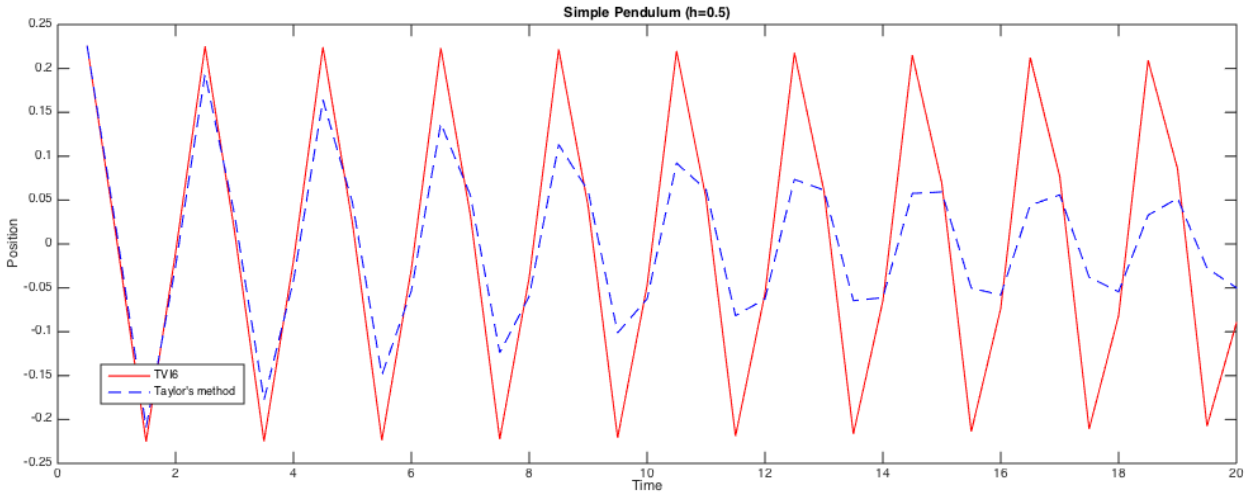

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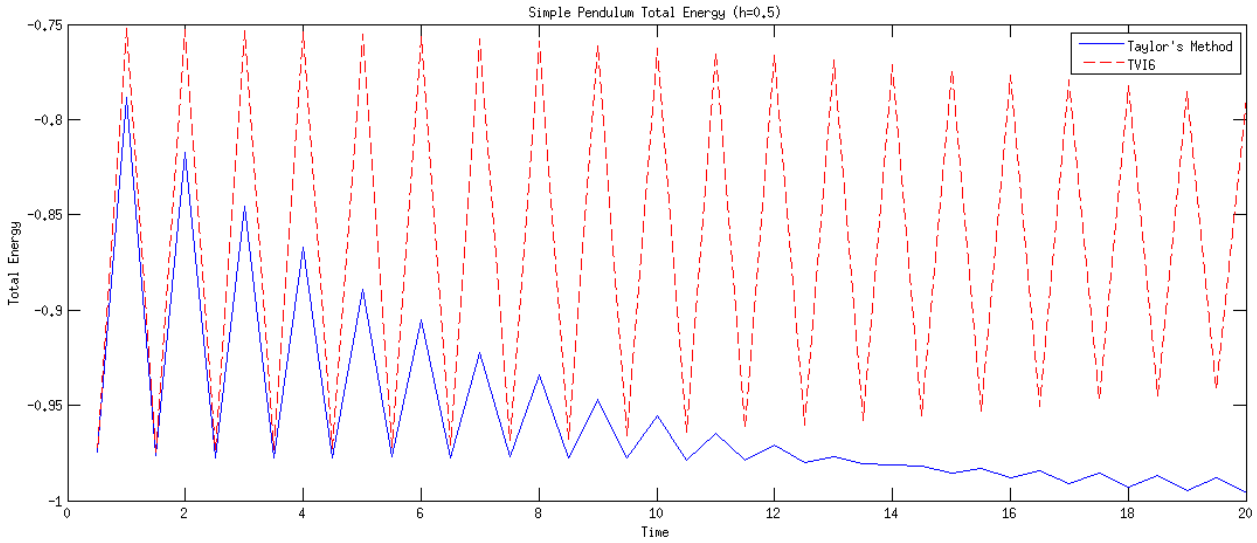

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Discrete Mechanics

Discrete Lagrangian System

Q configuration manifold.

$Q \times Q$ is the **discrete State Space**.

$L_d : Q \times Q \to \mathbb{R}$ is the **discrete Lagrangian** function.

Definition

Given an increasing sequence of times $\{t_k = kh | k = 0, \ldots, N\} \subset \mathbb{R}$ define the **discrete Path Space** to be,

$$\mathcal{C}_d(Q) = \{q_d : \{t_k\}_{k=0}^{N} \to Q\}$$

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Definition

The **discrete Action Sum**, $\mathbb{S}_d : \mathcal{C}_d(Q) \to \mathbb{R}$ is defined as,

$$\mathbb{S}_d(q_0, q_1, \ldots, q_N) = \sum_{i=0}^{N-1} L_d(q_i, q_{i+1}).$$

discrete Hamilton's Principle

$q \in \mathcal{C}_d(Q)$ is called a **Discrete Motion** if it satisfies,

$$\delta \mathbb{S}_d = 0$$

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Theorem

Discrete motion's satisfy the **discrete Euler − Lagrange** equations,

$$D_2 L_d(q_{k-1}, q_k) + D_1 L_d(q_k, q_{k+1}) = 0.$$

discrete Hamiltonian map

The discrete Euler-Lagrange equations are equivalent to the **implicit discrete Euler − Lagrange** equations,

$$p_k = -D_1 L_d(q_k, q_{k+1}),$$

$$p_{k+1} = D_2 L_d(q_k, q_{k+1}).$$

This defines the **discrete Hamiltonian map**,

$$\tilde{F}_{L_d} : (q_k, p_k) \mapsto (q_{k+1}, p_{k+1})$$

Discrete Legendre Tranforms

Define the **discrete Legendre transforms**, $\mathbb{F}^{\pm}L_d : Q \times Q \to T^*Q$, as,

$$\mathbb{F}^{+}L_d : (q_0, q_1) \mapsto (q_1, p_1) = (q_1, D_2 L_d(q_0, q_1)),$$

$$\mathbb{F}^{-}L_d : (q_0, q_1) \mapsto (q_0, p_0) = (q_0, -D_1 L_d(q_0, q_1)).$$

The discrete Hamiltonian map is given by, $\tilde{F}_{L_d} = \mathbb{F}^{+}L_d \circ (\mathbb{F}^{-}L_d)^{-1}$.
The discrete Lagrangian map is given by, $F_{L_d} = (\mathbb{F}^{-}L_d)^{-1} \circ \mathbb{F}^{+}L_d$.
This leads to the following commutative diagram.

$$
\begin{tikzcd}
 & (q_k, p_k) \arrow[rr, "\tilde{F}_{L_d}"] & & (q_{k+1}, p_{k+1}) & \\
(q_{k-1}, q_k) \arrow[ur, "\mathbb{F}^+ L_d"] \arrow[rr, "F_{L_d}"'] & & (q_k, q_{k+1}) \arrow[ul, "\mathbb{F}^- L_d"'] \arrow[ur, "\mathbb{F}^+ L_d"] \arrow[rr, "F_{L_d}"'] & & (q_{k+1}, q_{k+2}) \arrow[ul, "\mathbb{F}^- L_d"']
\end{tikzcd}
$$

Connecting the discrete to the continuous

Now that we have both a discrete and continuous mechanical system, how do we connect the two?

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Exact Discrete Lagrangian

$$L_d^E(q_0, q_1; h) = \int_0^h L(q_{01}(t), \dot{q}_{01}(t))dt,$$

where $q_{01}(0) = q_0$, $q_{01}(h) = q_1$, and q_{01} satisfies the Euler-Lagrange equations on the interval $(0, h)$.

Variational Error Analysis

Theorem (Marsden and West, 2001)

If a discrete Lagrangian, $L_d : Q \times Q \to \mathbb{R}$, approximates the exact discrete Lagrangian, $L_d^E : Q \times Q \to \mathbb{R}$ to order r, i.e.,

$$L_d(q_0, q_1; h) = L_d^E(q_0, q_1; h) + \mathcal{O}(h^{r+1}),$$

then the discrete Hamiltonian map, $\tilde{F}_{L_d} : (q_k, p_k) \mapsto (q_{k+1}, p_{k+1})$, viewed as a one-step method, is order r accurate.

How do we construct the discrete Lagrangian?

- The variational form of the exact discrete Lagrangian is $L_d^E(q0, q1; h) = \underset{q \in C^2([0,h],Q), q(0)=q_0, q(h)=q_1}{ext} \int_0^h L(q(t), \dot{q}(t))dt$, which leads naturally to Galerkin methods. Pick a finite dimensional subspace and a numerical quadrature method to build the discrete Lagrangian.(Leok, Shingel)

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- The type-I generating function form of the exact discrete Lagrangian is $L_d^E(q0, q1; h) = \int_0^h L(q_{01}(t), \dot{q}_{01}(t))dt$, where $q_{01}(0) = q_0$, $q_{01}(h) = q_1$, and q_{01} satisfies the Euler-Lagrange equation in $(0, h)$. Pick a one-step method, apply the shooting method to the Euler-Lagrange BVP, and use a quadrature rule to generate the discrete Lagrangian.(Leok, Shingel)

- Prolongate the Euler-Lagrange vector field, and then apply a collocation method using Hermite interpolating polynomials to approximate values of q and $\dot{q}$ satisfying the Euler-Lagrange BVP. Combing these with a quadrature rule yields a discrete Lagrangian.(Leok, Shingel)

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- Prolongate the Euler-Lagrange vector field, and use this to construct Taylor's method. Find the initial velocity by solving an inverse problem, and then apply a quadrature rule to create a discrete Lagrangian.

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- Step 1: Given the Euer-Lagrange BVP, use a $r - th$ order Taylor's method on TQ to solve for an approximation to v_0 implicitly defined by $q_1 = \pi_Q \circ \Phi_h(q_0, v_0)$.

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- Step 2: Combine $\tilde{v}_0$ with the $r - th$ order Taylor's method to generate the quadrature points to define our discrete Lagrangian.
- Step 3: Apply the implicit Euler-Lagrange equations to the discrete Lagrangian to generate the one-step method.

$$p_k = -D_1 L_d(q_k, q_{k+1}),$$
$$p_{k+1} = D_2 L_d(q_k, q_{k+1}).$$

- The discrete Hamiltonian map, $\tilde{F}_{L_d} : (q_k, p_k) \mapsto (q_{k+1}, p_{k+1})$, viewed as a one-step method, will be initialized with some $(q_0, p_0) \in T^*Q$.

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- $(q_0, q_1) = (\mathbb{F}^- L_d)^{-1}(q_0, p_0)$ yields the initial values for the discrete Lagrangian map, whose values also provide the boundary conditions for the Euler-lagrange BVP.

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- $(q_0, q_1) = (\mathbb{F}^- L_d)^{-1}(q_0, p_0)$ yields the initial values for the discrete Lagrangian map, whose values also provide the boundary conditions for the Euler-lagrange BVP.
- Combining the discrete Legendre transform with the continuous Legendre transform provides a connection between the Euler-Lagrange BVP and the Euler-Lagrange IVP via,

$$(q_0, q_1) = (\mathbb{F}^- L_d)^{-1} \circ \mathbb{F}L(q_0, v_0).$$

The flow of the Euler-Lagrange IVP,$\Phi_t : TQ \to TQ$ combined with the canonical projection onto the configuration manifold,$\pi_Q : TQ \to Q$, gives an explicit connection to the Euler-Lagrange BVP.

$$(q_0, q_1) = (q_0, \pi_Q \circ \Phi_h(q_0, v_0)),$$

$$
\begin{tikzcd}
(q_0, v_0) \arrow[rr, "\Phi_h"] \arrow[d, "\mathbb{F}L"'] & & (q_1, v_1) \arrow[d, "\mathbb{F}L"] \\
(q_0, p_0) \arrow[rr, "\tilde{F}_{L_d^E}"] & & (q_1, p_1) \\
& (q_0, q_1) \arrow[ul, "\mathbb{F}^- L_d^E"] \arrow[ur, "\mathbb{F}^+ L_d^E"'] &
\end{tikzcd}
$$

Euler-Lagrange Boudary Value Problem

Given an Euler–Lagrange equation of the form,

$$\ddot{q}(t) = f(q(t), \dot{q}(t), t),$$

we denote the exact solution of the Euler–Lagrange boundary-value problem with boundary conditions (q_0, q_1) by $(q(t), v(t))$.

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- We seek an estimate of the true initial velocity, v_0, for the corresponding Euler–Lagrange initial-value problem, with order of accuracy r. Let us denote this estimate by $\tilde{v}_0$.

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- We seek an estimate of the true initial velocity, v_0, for the corresponding Euler–Lagrange initial-value problem, with order of accuracy r. Let us denote this estimate by $\tilde{v}_0$.
- Combining $\tilde{v}_0$ with the prolongation of the Euler-Lagrange vector field will allow us to construct Taylor's method up to the desired order.

Theorem

A r-order Taylor's method,

$$\Psi_h(q_0, v_0) = \left(\sum_{k=0}^{r} \frac{h^k}{k!} q^{(k)}(0), \sum_{k=1}^{r+1} \frac{h^{k-1}}{(k-1)!} q^{(k)}(0) \right),$$

with initial conditions $(q_0, \tilde{v}_0)$, where $\tilde{v}_0$ is an order r approximation to the true intial velocity v_0, has order of accuracy r for the Euler–Lagrange boundary-value problem with boundary conditions (q_0, q_1).

Proof

- Denote the solution to the Euler-Lagrange BVP with boundary conditions (q_0, q_1) by $(q(t), v(t))$ for $t \in [0, h]$.

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- Denote the solution to the Euler-Lagrange BVP with boundary conditions (q_0, q_1) by $(q(t), v(t))$ for $t \in [0, h]$.
- Then $(q(t), v(t))$ is also a solution to the Euler-Lagrange IVP with intial conditions (q_0, v_0), where v_0 satisfies $\pi_Q \circ \Phi_h(q_0, v_0) = q_1$.

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- Denote the solution of the Euler-Lagrange IVP with intial conditions $(q_0, \tilde{v}_0)$ by $(\tilde{q}(t), \tilde{v}(t))$.

Proof

- Denote the solution to the Euler-Lagrange BVP with boundary conditions (q_0, q_1) by $(q(t), v(t))$ for $t \in [0, h]$.
- Then $(q(t), v(t))$ is also a solution to the Euler-Lagrange IVP with intial conditions (q_0, v_0), where v_0 satisfies $\pi_Q \circ \Phi_h(q_0, v_0) = q_1$.
- Denote the solution of the Euler-Lagrange IVP with intial conditions $(q_0, \tilde{v}_0)$ by $(\tilde{q}(t), \tilde{v}(t))$.
- Let $(q_d(t), v_d(t))$ denote the values generated by the order r Taylor's method with initial conditions $(q_0, \tilde{v}_0)$.

Proof

Let M be the Lipschitz constant with respect to initial velocity of the well-posed Euler-Lagrange IVP. Then,

$$\|(q(t), v(t)) - (\tilde{q}(t), \tilde{v}(t))\| \leq M\|v_0 - \tilde{v}_0\| \leq \mathcal{O}(h^{r+1}).$$

Combining this inequality with our r-order method yields,

$$\begin{aligned}
&\|(q(t), v(t)) - (q_d(t), v_d(t))\| \\
&= \|(q(t), v(t)) - (\tilde{q}(t), \tilde{v}(t)) + (\tilde{q}(t), \tilde{v}(t)) - (q_d(t), v_d(t))\| \\
&\leq \|(q(t), v(t)) - (\tilde{q}(t), \tilde{v}(t))\| + \|(\tilde{q}(t), \tilde{v}(t)) - (q_d(t), v_d(t))\| \\
&\leq \mathcal{O}(h^{r+1}).
\end{aligned}$$

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- What if we used our r-order Taylor's method to solve for $\tilde{v}_0$

$$\pi_Q \circ \Psi_h(q_0, \tilde{v}_0) = q_1$$

2nd order Taylor's method

$$q_1 = q_0 + hv_0 + \frac{h^2}{2} f(q_0) + \mathcal{O}(h^3)$$

$$v_0 = \frac{q_1 - q_0}{h} - \frac{h}{2} f(q_0) + \mathcal{O}(h^2)$$

2nd order Taylor's method

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$$v_0 = \frac{q_1 - q_0}{h} - \frac{h}{2} f(q_0) + \mathcal{O}(h^2)$$

- Setting $\tilde{v}_0 = \frac{q_1 - q_0}{h} - \frac{h}{2} f(q_0)$ only provides a 1st order approximation to the intitial velocity!

- Recall the Taylor's method is approximating elements in TQ, thus the full 2nd order Taylor's method is,

$$\begin{bmatrix} q_d(h) \\ v_d(h) \end{bmatrix} = \begin{bmatrix} q_0 \\ v_0 \end{bmatrix} + \begin{bmatrix} v_0 \\ f(q_0) \end{bmatrix} h + \begin{bmatrix} f(q_0) \\ \nabla f(q_0) v_0 \end{bmatrix} \frac{h^2}{2}.$$

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- Since we already must calculate $\nabla f(q_0)$ for the 2nd order Taylor's method, we can use it on our inverse problem to make $\tilde{v}_0$ a 2nd order approximation to v_0, at no additional computational cost.

Theorem

$\tilde{v}_0$ as defined by, $\pi_Q \circ \hat{\Psi}_h(q_0, \tilde{v}_0) = q_1$, where $\hat{\Psi}_h$ is a $r+1$-order Taylor's method, approximates v_0 with order of accuracy r.

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Taylor discrete Lagrangian

Given a r-order Taylor method and a s-order accurate numerical quadrature formula with quadrature weights b_i and quadrature nodes c_i, we construct the **Taylor discrete Lagrangian**,

$$L_d(q_0, q_1; h) = h \sum_{i=0}^{n} b_i L(\Psi_{c_i h}(q_0, \tilde{v}_0)),$$

where $\pi_Q \circ \hat{\Psi}_h(q_0, \tilde{v}_0) = q_1$.

Theorem

Given a r-order Taylor's method Ψ_h, a s-order accurate quadrature formula, and a Lagrangian L that is Lipschitz continuous in both variables, the associated Taylor discrete Lagrangian approximates the exact discrete Lagrangian with order of accuracy $\min(r+1, s)$.

Proof

$$q_{01}(c_i h) = q_d(c_i h) + \mathcal{O}(h^{r+1}),$$
$$v_{01}(c_i h) = v_d(c_i h) + \mathcal{O}(h^{r+1}).$$

$$L_d^E(q_0, q_1; h) = \int_0^h L(q_{01}(t), v_{01}(t))dt$$

$$= \left[h \sum_{i=1}^m b_i L(q_{01}(c_i h), v_{01}(c_i h))\right] + \mathcal{O}(h^{s+1})$$

$$= \left[h \sum_{i=1}^m b_i L(q_d(c_i h) + \mathcal{O}(h^{r+1}), v_d(c_i h) + \mathcal{O}(h^{r+1}))\right] + \mathcal{O}(h^{s+1})$$

Proof cont'd

$$= \left[h \sum_{i=1}^{m} b_i L(q_d(c_i h), v_d(c_i h)) \right] + \mathcal{O}(h^{r+2}) + \mathcal{O}(h^{s+1})$$

$$= L_d(q_0, q_1; h) + \mathcal{O}(h^{r+2}) + \mathcal{O}(h^{s+1})$$

$$= L_d(q_0, q_1; h) + \mathcal{O}(h^{\min(r+1,s)+1})$$

2nd order Taylor Variational Integrator

- Assume the Lagrangian has the form,

$$L(q(t), \dot{q}(t)) = \frac{1}{2}\dot{q}^T(t)M\dot{q}(t) - V(q(t)),$$

where M is symmetric positive definite and V is sufficiently smooth.

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- The corresponding Euler-Lagrange equation is,

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- We construct the 2nd order Taylor variational integrator using a 1st order Taylor's method combined with the trapezoid rule.

2nd order Taylor Variational Integrator

- The 1st order Taylor's method yields,

$$q_1 = q_0 + \tilde{v}_0 h$$

$$v_1 = \tilde{v}_0 - M^{-1} \triangledown V(q_0) h$$

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$$q_1 = q_0 + \tilde{v}_0 h - M^{-1} \triangledown V(q_0) \frac{h^2}{2}$$

- $$\tilde{v}_0 = \frac{q_1 - q_0}{h} + M^{-1} \triangledown V(q_0) \frac{h}{2}$$

- Using the trapezoidal quadrature rule our discrete Lagrangian becomes,

$$L_d(q_0, q_1) = \frac{h}{2}(\tilde{v}_0^T M \tilde{v}_0 - V(q_0) + v_1^T M v_1 - V(q_1)).$$

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- Given q_0 and p_0 our one-step method is defined implicitly by,

$$p_0 = -D_1 L_d(q_0, q_1)$$

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$$p_0 = -D_1 L_d(q_0, q_1)$$

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- Working out these equations gives the following explicit one-step method,

$$q_1 = q_0 + hM^{-1}p_0 - \frac{h^2}{2}M^{-1}\nabla V(q_0) + \frac{h^4}{4}M^{-1}\nabla\nabla V(q_0)M^{-1}\nabla V(q_0)$$

$$p_1 = p_0 - \frac{h}{2}(\nabla V(q_0) + \nabla V(q_1)) + \frac{h^3}{4}\nabla\nabla V(q_0)M^{-1}\nabla V(q_0)$$

Higher-Order Taylor Variational Integrators

The 2nd and 3rd order TVI have can have explicit forms depending on the Euler-Lagrange equations, but all higher-order methods will be implicit and require non-linear solvers.

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Higher-Order Taylor Variational Integrators

The 2nd and 3rd order TVI have can have explicit forms depending on the Euler-Lagrange equations, but all higher-order methods will be implicit and require non-linear solvers.

- A good initial guess to $\tilde{v}_0$ can be found by taking the Legendre Transform of the initial momentum.
- A good initial guess for q_1 and other values can be found by utilizing Taylor's method.

Numerical Considerations

- Taylor's method is well-suited to provide additional quadrature nodes without the need for additional function evaluations.

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- The derivatives required for Taylor's method are computed accurately and at the cost of a function evaluation by using Automatic Differentiation.
- Any one-step method could be used in place of Taylor's method, but it would require both a r order and r+1 order to develop the variational integrator.

Outline

1. Classical Mechanics
2. Numerical Example
3. Discrete Mechanics
4. Taylor Variational Integrator
5. Discrete Hamiltonian Variational Integrators

Exact Discrete Hamiltonian

$$H_d^{+,E}(q_0, p_1; h) = p(h)q(h) - \int_0^h [p(t)v(t) - H(q(t), p(t))]_{v=\frac{\partial H}{\partial p}} dt,$$

where $(q(t), p(t))$ is a solution of Hamilton's equations satisfying the boundary conditions $q(0) = q_0$ and $p(h) = p_1$.

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Discrete Right Hamilton's Equations

$$q_1 = D_2 H_d^+(q_0, p_1)$$

$$p_0 = D_1 H_d^+(q_0, p_1)$$

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- If the Lagrangian is degenerate, then the Legendre transform is not invertible, and it may make more sense to approach the problem from the Hamiltonian side.
- Letting $h \to 0$ causes a breakdown in the well-posedness of a BVP, with Dirichlet boundary conditions $q(0) = q_0$ and $q(h) = q_1$, as the initial velocity becomes unbounded.
- Letting $h \to 0$ does not cause this singularity when the boundary conditions are $q(0) = q_0$ and $p(h) = p_1$.

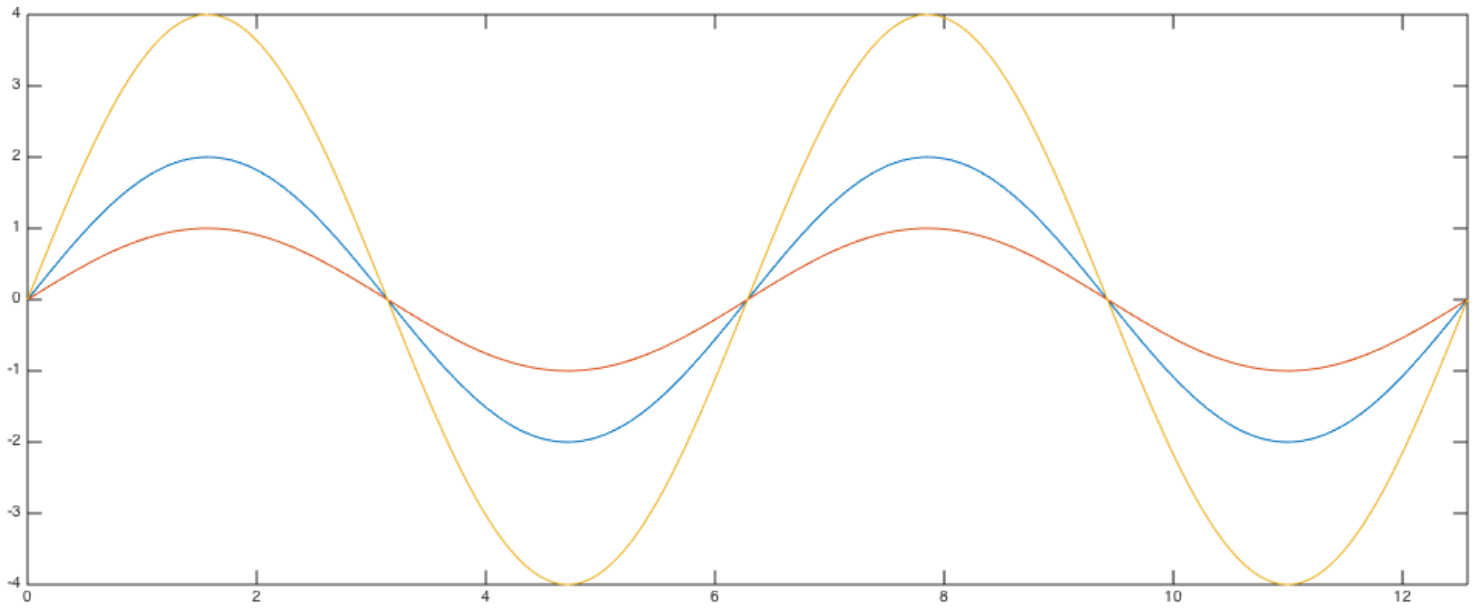
Harmonic Oscillator

Consider the harmonic oscillator given by the Euler-Lagrange BVP,

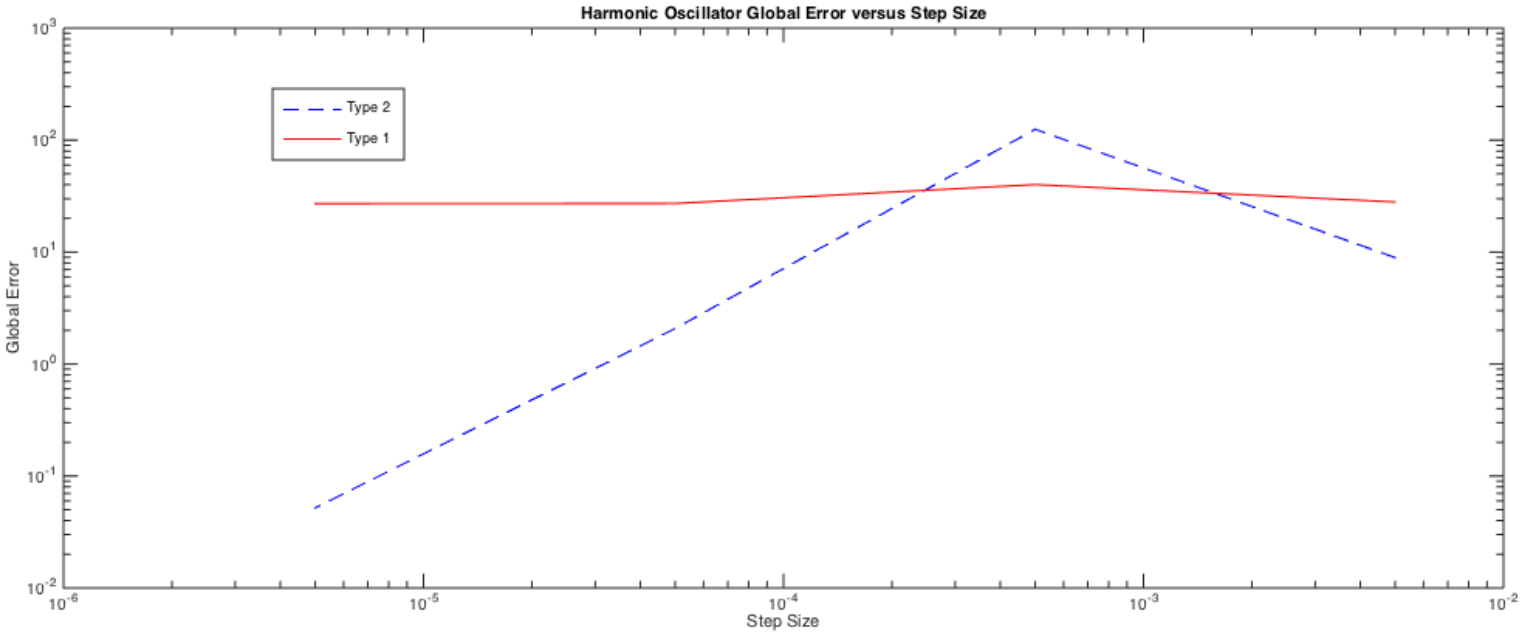
$$\ddot{q}(t) = -kx,$$

where $q(0) = 0$ and $q(\frac{\pi}{\sqrt{k}}) = 0$. This BVP does not have a unique solution!

Harmonic Oscillator



Harmonic Oscillator Period=0.025



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- The exact discrete Hamiltonian is a type 2 generating function of the exact flow of Hamilton's equations.(Leok, Zhang 2011)
- The map defined by constructing a discrete right Hamitonian and applying the discrete right Hamilton's equations is symplectic and preserves momentum maps. (Leok, Zhang 2011)

Definition

Given the discrete right Hamilton's equation, $q_1 = D_2 H_d^+(q_0, p_1)$ and $p_0 = D_1 H_d^+(q_0, p_1)$ we define the following maps:

$$\tilde{F}_{H_d^+} : (q_k, p_k) \mapsto (q_{k+1}, p_{k+1})$$

$$F_{H_d^+} : (q_k, p_{k+1}) \mapsto (q_{k+1}, p_{k+2})$$

Definition

Define the **discrete left and right Legendre Transforms** by,

$$\mathbb{F}^+ H_d^+(q_0, p_1) \cdot \delta p_1 = D_2 H_d^+(q_0, p_1) \cdot \delta p_1$$

$$\mathbb{F}^- H_d^+(q_0, p_1) \cdot \delta q_0 = D_1 H_d^+(q_0, p_1) \cdot \delta q_0.$$

Thus we have the maps,

$$\mathbb{F}^+ H_d^+ : (q_k, p_{k+1}) \mapsto (q_{k+1}, p_{k+1}) = (D_2 H_d^+(q_0, p_1), p_{k+1})$$

$$\mathbb{F}^- H_d^+ : (q_k, p_{k+1}) \mapsto (q_k, p_k) = (q_0, D_1 H_d^+(q_0, p_1))$$

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$$\mathbb{F}^+ H_d^+ : (q_k, p_{k+1}) \mapsto (q_{k+1}, p_{k+1}) = (D_2 H_d^+(q_0, p_1), p_{k+1})$$

$$\mathbb{F}^- H_d^+ : (q_k, p_{k+1}) \mapsto (q_k, p_k) = (q_0, D_1 H_d^+(q_0, p_1))$$

- Note that this implies, $\mathbb{F}^+ H_d^+ = \mathbb{F}^- H_d^+ \circ F_{H_d^+}$ and $\mathbb{F}^- H_d^+(q_1, p_2) = \mathbb{F}^+ H_d^+(q_0, p_1)$.

$$
\begin{tikzcd}
 & (q_k, p_k) \arrow[rr, "\tilde{F}_{H_d^+}"] & & (q_{k+1}, p_{k+1}) & \\
(q_{k-1}, p_k) \arrow[ur, "\mathbb{F}^+ H_d^+"] \arrow[rr, "F_{H_d^+}"'] & & (q_k, p_{k+1}) \arrow[ul, "\mathbb{F}^- H_d^+ \, \mathbb{F}^+ H_d^+"'] \arrow[ur] \arrow[rr, "F_{H_d^+}"'] & & (q_{k+1}, p_{k+2}) \arrow[ul, "\mathbb{F}^- H_d^+"']
\end{tikzcd}
$$

- The previous commutative diagram implies the discrete Hamiltonian map is given by,

$$\tilde{F}_{H_d^{+,E}}(q(0), p(h), h) = \mathbb{F}^+ H_d^+ \circ (\mathbb{F}^- H_d^+)^{-1}.$$

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- We say the discrete right Hamiltonian is of order r if,

$$\|H_d^+(q(0), p(h), h) - H_d^{+,E}(q(0), p(h), h)\| \leq Ch^{r+1}.$$

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- Equivalently, this may be expressed as,

$$H_d^+(q(0), p(h), h) = H_d^{+,E}(q(0), p(h), h) + h^{r+1} e(q(0), p(h), h),$$

where $e(q(0), p(h), h)$ is bounded on compact sets.

Theorem

If a discrete right Hamiltonian, $H_d^+ : T^*Q \to \mathbb{R}$, approximates the exact discrete Hamiltonian, $H_d^{+,E} : T^*Q \to \mathbb{R}$ to order r, i.e.,

$$H_d^+(q_0, p_1; h) = H_d^{+,E}(q_0, p_1; h) + \mathcal{O}(h^{r+1}),$$

then the discrete map, $\tilde{F}_{H_d^+} : (q_k, p_k) \mapsto (q_{k+1}, p_{k+1})$, viewed as a one-step method, is order r accurate.

proof

- By assumption we have,

$$H_d^+(q(0), p(h), h) = H_d^{+,E}(q(0), p(h), h) + h^{r+1} e(q(0), p(h), h).$$

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$$H_d^+(q(0), p(h), h) = H_d^{+,E}(q(0), p(h), h) + h^{r+1} e(q(0), p(h), h).$$

- Differentiating then yields,

$$D_1 H_d^+(q(0), p(h), h) = D_1 H_d^{+,E}(q(0), p(h), h) + h^{r+1} D_1 e(q(0), p(h), h$$

where $\|D_1 e(q(0), p(h), h)\| \leq \hat{C}$.

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- $\|\mathbb{F}^- H_d^+(q(0), p(h), h) - \mathbb{F}^- H_d^{+,E}(q(0), p(h), h)\|$
- The same can be shown for $\mathbb{F}^+$.

proof

- Given smooth functions related by,

$$f_1(x,h) = g_1(x,h) + h^{r+1}e_1(x,h)$$

$$f_2(x,h) = g_2(x,h) + h^{r+1}e_2(x,h),$$

the following can be shown.

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the following can be shown.

- $$f_2(f_1(x,h),h) = g_2(g_1(x,h),h) + h^{r+1}e_{12}(x,h)$$
$$f_1^{-1}(y,h) = g_1^{-1}(y,h) + h^{r+1}\bar{e}_1(y,h)$$

proof

- Combining this with the fact that $\tilde{F}_{H_d^+} = \mathbb{F}^+ H_d^+ \circ (\mathbb{F}^- H_d^+)^{-1}$ yields,

$$\tilde{F}_{H_d^+}(q(0), p(h), h) = \tilde{F}_{H_d^{+,E}}(q(0), p(h), h) + h^{r+1} e_3(q(0), p(h), h).$$

TVI on the Hamiltonian side

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- Using an order r Taylor's method results in an order r TVI.
- $$H_d^+(q_0, p_1; h) = p_1 q_1 - \frac{h}{2}(p_0^T \dot{q}_0 - H(q_0, p_0) + p_1^T \dot{q}_1 - H(q_1, p_1))$$

TVI on the Hamiltonian side

- The inverse problem for $\tilde{p}_0$ is,

$$p_1 = \pi_{T^*Q} \circ \Psi_h(q_0, p_1) = \tilde{p}_0 - \nabla V(q_0) + \dots.$$

TVI on the Hamiltonian side

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$$p_1 = \pi_{T^*Q} \circ \Psi_h(q_0, p_1) = \tilde{p}_0 - \nabla V(q_0) + \dots.$$

- Upshot: No need to construct a higher order-method for the inverse problem. Thus, this generalizes easily to any one-step method.

Future Work

- Analyze further the stability and other qualitative properties of the discrete Hamiltonian versus discrete Lagrangian variational integrator.

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- Analyze further the stability and other qualitative properties of the discrete Hamiltonian versus discrete Lagrangian variational integrator.
- Examine the stability of the discrete Hamiltonian variational integrator for high oscillatory mechanical systems.
- Further develop a symplectic method for dealing with mechanical systems involving a low and high frequency component via time averaging.
- Investigate the discretization of the boundary Lagrangian and possibly a boundary Hamiltonian for multi-symplectic field theories.