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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3. Discrete Mechanics
4. Taylor Variational Integrator
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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**.
Lagrangian Dynamical System

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Dynamics of the Lagrangian system

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

$$ S(q) = \int_0^T L(q(t), \dot{q}(t)) dt $$
A motion, \( q \), satisfies the **Euler – Lagrange** equations,

\[
\frac{d}{dt} \frac{\partial L}{\partial \dot{q}} - \frac{\partial L}{\partial q} = 0.
\]
Theorem

A motion, $q$, satisfies the **Euler – Lagrange** equations,

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

Proof

$$
0 = \delta S
= \delta \int_0^T L(q, \dot{q}) dt
= \int_0^T \delta L(q, \dot{q}) dt
= \int_0^T \frac{\partial L}{\partial q} \delta q + \frac{\partial L}{\partial \dot{q}} \delta \dot{q} dt
$$
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 fundamental 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 $\mathbb{F}L : TQ \rightarrow T^*Q$ by,

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

where $v, w \in T_qQ$. 
Legendre Transform

Definition

Given a Lagrangian system, define the fiber derivative \( F_L : TQ \to T^*Q \) by,

\[
F_L(v) \cdot w = \frac{d}{ds} \bigg|_{s=0} L(v + sw),
\]

where \( v, w \in T_qQ \).

Legendre Transform

\( F_L \) is called the **Legendre Transform**. For a finite dimensional configuration manifold,

\[
F_L : (q, \dot{q}) \to (q, \frac{\partial L}{\partial \dot{q}}) = (q, p).
\]
Definition

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

$$p = \frac{\partial L}{\partial \dot{q}}$$
Definition

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\[
p = \frac{\partial L}{\partial \dot{q}}
\]

Hamiltonian

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

\[
H(q, p) = p\dot{q} - L(q, \dot{q})\bigg|_{p=\frac{\partial L}{\partial \dot{q}}}.
\]
Hamilton’s Equations

Definition

The system of first-order differential equations,

\[ \dot{q} = \frac{\partial H}{\partial p} \]
\[ \dot{p} = -\frac{\partial H}{\partial q} \]

is called Hamilton’s Equations.
Hamilton’s Equations

**Definition**

The system of first-order differential equations,

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

is called **Hamilton’s Equations**.

**Theorem**

Hamilton’s equations are equivalent to the Euler-Lagrange equations.
Sketch of the Proof

\[ 0 = \dot{p} + \frac{\partial H}{\partial q} \]

\[ = \frac{d}{dt} p + \frac{\partial H}{\partial q} \]

Noting \( p = \frac{\partial L}{\partial \dot{q}} \) by definition, 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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Given a Lagrangian, \( L(q, \dot{q}) \), that is not explicitly a function of time, then the Hamiltonian is an invariant of the flow.

Proof

\[
\frac{dH}{dt} = \frac{\partial H}{\partial q} \frac{dq}{dt} + \frac{\partial H}{\partial p} \frac{dp}{dt} \\
= -\dot{p}\dot{q} + \dot{q}\dot{p} \\
= 0
\]
Can we build a numerical method that takes into account the underlying (geometric) structure of the dynamical system?
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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 $\theta$ the angle between the rod and the negative $y$-axis.

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

The corresponding Hamiltonian will then be the total energy of the system, which will remain constant.
The corresponding Euler-Lagrange equation is,

\[ \ddot{\theta} = -9.8 \sin(\theta) \]
Simple Pendulum

Taylor’s Method 2nd Order $h=0.1$
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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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,

\[
C_d(Q) = \{ q_d : \{ t_k \}_{k=0}^N \rightarrow Q \}
\]
Definition

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

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C_d(Q) = \{ q_d : \{ t_k \}_{k=0}^N \rightarrow Q \}
\]

Definition

The **discrete Action Sum**, \( S_d : C_d(Q) \rightarrow \mathbb{R} \) is defined as,

\[
S_d(q_0, q_1, \ldots, q_N) = \sum_{i=0}^{N-1} L_d(q_i, q_{i+1}).
\]
discrete Hamilton’s Principle

$q \in C_d(Q)$ is called a **Discrete Motion** if it satisfies,

$$\delta S_d = 0$$
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$$\delta S_d = 0$$

**Theorem**

Discrete motion’s satisfy the **discrete Euler – Lagrange** equations,

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

\[
\tilde{F}_{L_d} : (q_k, p_k) \mapsto (q_{k+1}, p_{k+1})
\]
Define the **discrete Legendre transforms**, \( \mathbb{F}^\pm L_d : Q \times Q \to T^* Q \), as,

\[
\begin{align*}
\mathbb{F}^+ L_d & : (q_0, q_1) \mapsto (q_1, p_1) = (q_1, D_2 L_d(q_0, q_1)), \\
\mathbb{F}^- L_d & : (q_0, q_1) \mapsto (q_0, p_0) = (q_0, -D_1 L_d(q_0, q_1)).
\end{align*}
\]

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.
\[
\begin{align*}
(q_k, p_k) & \xrightarrow{\tilde{F}_{Ld}} (q_{k+1}, p_{k+1}) \\
(q_{k-1}, q_k) & \xrightarrow{F_{Ld}} (q_k, q_{k+1}) \quad (q_{k+1}, q_{k+2})
\end{align*}
\]
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 \((0, h)\).
Theorem (Marsden and West, 2001)

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

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

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

\[
L^E_d(q_0, q_1; h) = \text{ext}_{q \in C^2([0,h],Q), q(0)=q_0, q(h)=q_1} \int_0^h L(q(t), \dot{q}(t)) \, dt,
\]

which leads naturally to Galerkin methods. Pick a finite dimensional subspace and a numerical quadrature method to build the discrete Lagrangian.(Leok, Shingel)
How do we construct the discrete Lagrangian?

- The variational form of the exact discrete Lagrangian is
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- The type-I generating function form of the exact discrete Lagrangian is
  \[ L_{d}^{E}(q_{0}, q_{1}; h) = \int_{0}^{h} L(q_{01}(t), \dot{q}_{01}(t)) dt, \]
  where \( q_{01}(0) = q_{0}, q_{01}(h) = q_{1}, \) and \( q_{01} \) satisfies the Euler-Lagrange 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.\textmd{\textcopyright{} 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)

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.
Goal: Construct a one-step method to solve an IVP for $t \in [0, T]$. 
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Step 1: Given the Euler-Lagrange BVP, use a $r$th order Taylor’s method on $TQ$ to solve for an approximation to $v_0$ implicitly defined by $q_1 = \pi_Q \circ \Phi_h(q_0, v_0)$. 

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.

$$p_k = -D_1 L_d(q_k, q_{k+1}), \quad p_{k+1} = D_2 L_d(q_k, q_{k+1}).$$
Goal: Construct a one-step method to solve an IVP for 
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The discrete Hamiltonian map, $\tilde{F}_{Ld} : (q_k, p_k) \mapsto (q_{k+1}, p_{k+1})$, viewed as a one-step method, will be initialized with some $(q_0, p_0) \in T^* Q$. 
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 \((q_0, p_0) \in T^*Q\).

\((q_0, q_1) = (\mathcal{F} - L_d)^{-1}(q_0, p_0)\) 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, $\Phi_t : TQ \rightarrow TQ$ combined with the canonical projection onto the configuration manifold, $\pi_Q : TQ \rightarrow Q$, gives an explicit connection to the Euler-Lagrange BVP.

$$(q_0, q_1) = (q_0, \pi_Q \circ \Phi_h(q_0, v_0)).$$
(q_0, v_0) \xrightarrow{\Phi_h} (q_1, v_1)

F_L \downarrow \Phi_h \downarrow F_L

(q_0, p_0) \xrightarrow{\tilde{F}_{LE}} (q_1, p_1)

F_{-LE_d} \downarrow \tilde{F}_{LE_d} \downarrow F_{+LE_d}

(q_0, q_1)
Euler-Lagrange Boundary 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 \((q(t), v(t))\).
Euler-Lagrange Boundary Value Problem

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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 initial 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 \(t \in [0, h]\).
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 initial conditions \((q_0, v_0)\), where \(v_0\) satisfies 
  \[\pi Q \circ \Phi_h(q_0, v_0) = q_1.\]
Proof

- Denote the solution to the Euler-Lagrange BVP with boundary conditions \((q_0, q_1)\) by \((q(t), \nu(t))\) for \(t \in [0, h]\).
- Then \((q(t), \nu(t))\) is also a solution to the Euler-Lagrange IVP with initial conditions \((q_0, \nu_0)\), where \(\nu_0\) satisfies \(\pi_Q \circ \Phi_h(q_0, \nu_0) = q_1\).
- Denote the solution of the Euler-Lagrange IVP with initial conditions \((q_0, \tilde{\nu}_0)\) by \((\tilde{q}(t), \tilde{\nu}(t))\).
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 initial 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 initial 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,

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

Combining this inequality with our $r$-order method yields,

$$\|(q(t), v(t)) - (q_d(t), v_d(t))\|$$

$$= \|(q(t), v(t)) - (\tilde{q}(t), \tilde{v}(t)) + (\tilde{q}(t), \tilde{v}(t)) - (q_d(t), v_d(t))\|$$

$$\leq \|(q(t), v(t)) - (\tilde{q}(t), \tilde{v}(t))\| + \|(\tilde{q}(t), \tilde{v}(t)) - (q_d(t), v_d(t))\|$$

$$\leq O(h^{r+1}).$$
We need an order r approximation to $v_0$. 
We need an order $r$ approximation to $v_0$.

Given $(q_0, q_1)$ we must approximately solve the inverse problem,

$$\pi Q \circ \Phi_h(q_0, v_0) = q_1.$$
We need an order $r$ approximation to $v_0$.

Given $(q_0, q_1)$ we must approximately solve the inverse problem,

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

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

$$\pi_Q \circ \Psi_h(q_0, \tilde{v}_0) = q_1.$$
Second order Taylor’s method

\[ q_1 = q_0 + h v_0 + \frac{h^2}{2} f(q_0) + \mathcal{O}(h^3) \]

\[ v_0 = \frac{q_1 - q_0}{h} - \frac{h}{2} f(q_0) + \mathcal{O}(h^2) \]
$2^{nd}$ order Taylor’s method

$q_1 = q_0 + h v_0 + \frac{h^2}{2} f(q_0) + \mathcal{O}(h^3)$

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

- Setting $\tilde{v}_0 = \frac{q_1 - q_0}{h} - \frac{h}{2} f(q_0)$ only provides a $1^{st}$ order approximation to the initial velocity!
Recall the Taylor’s method is approximating elements in $TQ$, thus the full $2^{nd}$ order Taylor’s method is,

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

Since we already must calculate $\nabla f(q_0)$ for the $2^{nd}$ order Taylor’s method, we can use it on our inverse problem to make $\tilde{v}_0$ a $2^{nd}$ order approximation to $v_0$, at no additional computational cost.
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\nu_d(h)
\end{bmatrix}
= 
\begin{bmatrix}
q_0 \\
\nu_0
\end{bmatrix}
+ 
\begin{bmatrix}
\nu_0 \\

f(q_0)
\end{bmatrix} h
+ 
\begin{bmatrix}
f(q_0) \\
\nabla f(q_0) \nu_0
\end{bmatrix}
\frac{h^2}{2}.
$$

Since we already must calculate $\nabla f(q_0)$ for the $2^{nd}$ order Taylor’s method, we can use it on our inverse problem to make $\tilde{\nu}_0$ a $2^{nd}$ order approximation to $\nu_0$, 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 \( r \).
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 \( r \).

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 $\Psi_h$, 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

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

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

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

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

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

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

\[ = L_d(q_0, q_1; h) + O(h^{\min(r+1,s)+1}) \]
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 2\textsuperscript{nd} order Taylor variational integrator using a 1\textsuperscript{st} order Taylor’s method combined with the trapezoid rule.
The 1<sup>st</sup> order Taylor’s method yields,

\[ q_1 = q_0 + \tilde{v}_0 h \]

\[ v_1 = \tilde{v}_0 - M^{-1} \nabla V(q_0) h \]
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To find \( \tilde{v}_0 \) we solve,

\[ q_1 = q_0 + \tilde{v}_0 h - M^{-1} \nabla V(q_0) \frac{h^2}{2} \]
2nd order Taylor Variational Integrator

- The 1st order Taylor’s method yields,

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- To find \( \tilde{v}_0 \) we solve,

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

\[ \tilde{v}_0 = \frac{q_1 - q_0}{h} + M^{-1} \nabla V(q_0) \frac{h}{2} \]
Using the trapezoidal quadrature rule our discrete Lagrangian becomes,

\[ L_d(q_0, q_1) = \frac{h}{2} (\tilde{v}_0^T M \tilde{v}_0 - V(q_0) + \nu_1^T M \nu_1 - V(q_1)). \]
Using the trapezoidal quadrature rule our discrete Lagrangian becomes,

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

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

\[ p_0 = -D_1 L_d(q_0, q_1) \]
\[ p_1 = D_2 L_d(q_0, q_1) \]
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Given \( q_0 \) and \( p_0 \) our one-step method is defined implicitly by,

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\begin{align*}
p_0 &= -D_1 L_d(q_0, q_1) \\
p_1 &= D_2 L_d(q_0, q_1)
\end{align*}
\]

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

\[
\begin{align*}
q_1 &= q_0 + hM^{-1}p_0 - \frac{h^2}{2} M^{-1} \nabla V(q_0) + \frac{h^4}{4} M^{-1} \nabla \nabla V(q_0) M^{-1} \nabla V(q_0) \\
p_1 &= p_0 - \frac{h}{2} (\nabla V(q_0) + \nabla V(q_1)) + \frac{h^3}{4} \nabla \nabla V(q_0) M^{-1} \nabla V(q_0)
\end{align*}
\]
Higher-Order Taylor Variational Integrators

The $2^{nd}$ and $3^{rd}$ 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.
Higher-Order Taylor Variational Integrators

The 2\textsuperscript{nd} and 3\textsuperscript{rd} 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.
Higher-Order Taylor Variational Integrators

The $2^{nd}$ and $3^{rd}$ 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.
Taylor’s method is well-suited to provide additional quadrature nodes without the need for additional function evaluations.
Numerical Considerations

- Taylor’s method is well-suited to provide additional quadrature nodes without the need for additional function evaluations.
- The derivatives required for Taylor’s method are computed accurately and at the cost of a function evaluation by using Automatic Differentiation.
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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

\[ H^{+,E}_d(q_0, p_1; h) = p(h)q(h) - \int_0^h \left[ p(t)v(t) - H(q(t), p(t)) \right] dt, \]

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

Discrete Right Hamilton’s Equations

\[ q_1 = D_2 H_d^+(q_0, p_1) \]
\[ p_0 = D_1 H_d^+(q_0, p_1) \]
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.
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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.
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 $p(h) = p_1$. 
Consider the harmonic oscillator given by the Euler-Lagrange BVP,

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

where \( q(0) = 0 \) and \( q\left( \frac{\pi}{\sqrt{k}} \right) = 0 \). This BVP does not have a unique solution!
Harmonic Oscillator
Harmonic Oscillator Period = 0.025

Harmonic Oscillator Global Error versus Step Size

- Type 2
- Type 1
Discrete variational Hamiltonian mechanics has been developed in papers by (Lall, West 2006) and (Leok, Zhang 2011).
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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 Hamiltonian 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,

\[ F^+ H^+_d(q_0, p_1) \cdot \delta p_1 = D_2 H^+_d(q_0, p_1) \cdot \delta p_1 \]

\[ F^- H^+_d(q_0, p_1) \cdot \delta q_0 = D_1 H^+_d(q_0, p_1) \cdot \delta q_0. \]

Thus we have the maps,

\[ F^+ H^+_d : (q_k, p_{k+1}) \mapsto (q_{k+1}, p_{k+1}) = (D_2 H^+_d(q_0, p_1), p_{k+1}) \]

\[ F^- H^+_d : (q_k, p_{k+1}) \mapsto (q_k, p_k) = (q_0, D_1 H^+_d(q_0, p_1)) \]
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,

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

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

Note that this implies, $\mathbb{F}^+ H_d^+ = \mathbb{F}^- H_d^+ \circ F_{H_d^+}$ and

$$
\mathbb{F}^- H_d^+(q_1, p_2) = \mathbb{F}^+ H_d^+(q_0, p_1).
$$
\[(q_k, p_k) \xrightarrow{F_{H_d}^+} (q_{k+1}, p_{k+1})\]

\[(q_{k-1}, p_k) \xrightarrow{F_{H_d}^+} (q_k, p_{k+1}) \xrightarrow{F_{H_d}^+} (q_{k+1}, p_{k+2})\]
The previous commutative diagram implies the discrete Hamiltonian map is given by,

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

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

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

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

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.,

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

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,

\[ H_d^+(q(0), p(h), h) = H_d^+,E(q(0), p(h), h) + h^{r+1} e(q(0), p(h), h). \]
proof

- By assumption we have,
  \[ H_d^+(q(0), p(h), h) = H_d^{+,E}(q(0), p(h), h) + h^{r+1}e(q(0), p(h), h). \]

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

By assumption we have,

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

\[ \| F^- H_d^+(q(0), p(h), h) - F^- H_d^{+,E}(q(0), p(h), h) \| \]
By assumption we have,

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

Differentiating then yields,

\[ D_1H_d^+(q(0), p(h), h) = D_1H_d^+,E(q(0), p(h), h) + h^{r+1}D_1e(q(0), p(h), h), \]

where \( \|D_1e(q(0), p(h), h)\| \leq \hat{C}. \)

\[ \|F^-H_d^+(q(0), p(h), h) - F^-H_d^+,E(q(0), p(h), h)\| \]

The same can be shown for \( F^+. \)
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.
Given smooth functions related by,

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the following can be shown.

\[ f_2(f_1(x, h), h) = g_2(g_1(x, h), h) + h^{r+1} e_{12}(x, h) \]
\[ f_1^{-1}(y, h) = g_1^{-1}(y, h) + h^{r+1} \tilde{e}_1(y, h) \]
proof

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

\[
\tilde{F}_{H_d^+}(q(0), p(h), h) = \tilde{F}_{H_d^+;E}(q(0), p(h), h) + hr^{1}e_3(q(0), p(h), h).
\]
All Taylor Variational Integrators on the Hamiltonian side are implicit.
TVI on the Hamiltonian side

- All Taylor Variational Integrators on the Hamiltonian side are implicit.
- Using an order $r$ Taylor’s method results in an order $r$ TVI.
TVI on the Hamiltonian side

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- Using an order $r$ Taylor’s method results in an order $r$ TVI.

$$H_d^+(q_0, p_1; h) = p_1 q_1 - \frac{h}{2} (p_0^T \dot{q}_0 - H(q_0, p_0) + p_1^T \dot{q}_1 - H(q_1, p_1))$$
The inverse problem for $\tilde{p}_0$ is,

$$p_1 = \pi_{T^*Q} \circ \Psi_h(q_0, p_1) = \tilde{p}_0 - \nabla V(q_0) + \ldots.$$
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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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- Examine the stability of the discrete Hamiltonian variational integrator for high oscillatory mechanical systems.
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- Further develop a symplectic method for dealing with mechanical systems involving a low and high frequency component via time averaging.
Future Work

- 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.