Discretizations of Lagrangian Mechanics†

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†With Charles Cuell
Continuous Lagrangian system:

\[ Q, \quad L: TQ \to \mathbb{R}, \quad S = \int L(q'(t)) \, dt, \quad \delta S = 0, \]
\[ q(a) = q_1, \quad q(b) = q_2 \]
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Discrete means discrete time: \( q(t) \leftrightarrow q_i \).
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Moser-Veselov discretization:

\[ Q, \quad L_d: Q \times Q \rightarrow \mathbb{R}, \quad S_d = \sum L_d(q_{i+1}, q_i), \quad dS_d = 0 \]
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New framework:

- new discretizations \( \cong \) Moser-Veselov discretizations, but \( \cong \) not explicit
- Moser-Veselov discretizations \( \subseteq \) new discretizations
Equivalent framework to Moser-Veselov. But:
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- more geometrically appealing
Discretizations of Lagrangian Mechanics

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- helps in the construction of numerical integrators

The new framework makes it easier to create sophisticated new discretizations, all the way through nonlinear, nonholonomic systems. It clarifies discretizations of Lagrangian systems, and it should help wherever such discretizations are used.
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2 Basics
   - curve segments for as discrete tangent vectors
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   - Discretizations of Lagrangian systems
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6 Existence, uniqueness, and accuracy of the discrete flow
The discrete representation of a tangent vector is a curve segment. Replace $TQ$ with a set $\mathcal{V}$ of curve segments in $Q$.

There should be one curve segment for every $v_q$, so usually $\mathcal{V} = TQ$. 
Lifting the continuous variational principle from curves in the configuration space $Q$ to curves in the phase space $TQ$.

\[ v(t) = \frac{dq}{dt}, \quad S = \int L(v(t)) \, dt \]
First order constraint:

\[ \{ q'(t) \} = \left\{ v(t) : \frac{d}{dt}(\tau_Q \circ v(t)) = v(t) \right\} \]

So the variational principle

is equivalent to
First order constraint:

\[ \{ q'(t) \} = \left\{ v(t) : \frac{d}{dt} (\tau_Q \circ v(t)) = v(t) \right\} \]

So the variational principle

\[ L : TQ \to \mathbb{R}, \quad S = \int L(q'(t)) \, dt, \quad \delta S = 0, \]

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So the variational principle

\[ L : TQ \rightarrow \mathbb{R}, \quad S = \int L(q'(t)) \, dt, \quad \delta S = 0, \quad q(a) = q_1, \quad q(b) = q_2 \]

is equivalent to

\[ L : TQ \rightarrow \mathbb{R}, \quad S = \int L(v(t)) \, dt, \quad \delta S \cdot \delta v = 0, \quad T_{\tau_Q}(\delta v(a)) = 0, \quad T_{\tau_Q}(\delta v(b)) = 0, \quad \frac{d}{dt} \left( \tau_Q \circ v(t) \right) = v(t) \]
Given a discrete tangent bundle and a discrete Lagrangian

\[ \mathcal{V}, \quad \partial^+: \mathcal{V} \to \mathbb{R}, \quad \partial^-: \mathcal{V} \to \mathbb{R} \]

\[ L_d: \mathcal{V} \to \mathbb{R} \]

we use the action

\[ S = \sum L_d(v_i) \]

To find the discrete analogue of the Lagrangian system, only it is required discrete analogue of the first order constraint.
A discrete tangent bundle for \( \{ q \} = \mathbb{R}^n \) is \( \{ q, v \} = \mathbb{R}^n \times \mathbb{R}^n \) with

\[
\partial^-(q, v) = q, \quad \partial^+(q, v) = q + hv
\]
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The equations

\[
q_1 = \partial^-(q, v) = q, \quad q_2 = \partial^+(q, v) = q + h v
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have solution

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q = q_1, \quad v = \frac{q_2 - q_1}{h}
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have solution
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q = q_1, \quad v = \frac{q_2 - q_1}{h}
\]

The derivative of the sequence \( q_i \) is
\[
\nu_i = (\partial^\pm)^{-1}(q_{i+1}, q_i), \quad \partial^\pm \equiv (\partial^+, \partial^-)
\]
\[ v_i = (\partial^\pm)^{-1}(q_{i+1}, q_i), \quad \partial^\pm \equiv (\partial^+, \partial^-) \]
\( v_i = (\partial^{\pm})^{-1}(q_{i+1}, q_i), \quad \partial^{\pm} \equiv (\partial^+, \partial^-) \)

The derivative \( v_i \) of \( q_i \) satisfies \( \partial^+(v_{i-1}) = \partial^-(v_i) \)
\[ v_i = (\partial^\pm)^{-1}(q_{i+1}, q_i), \quad \partial^\pm \equiv (\partial^+, \partial^-) \]

The derivative \( v_i \) of \( q_i \) satisfies \( \partial^+(v_{i-1}) = \partial^-(v_i) \)

If \( v_i \) satisfies \( \partial^-(v_{i+1}) = \partial^+(v_i) \) then it is the derivative of \( q_i \) defined by \( q_i = \partial^+(v_{i-1}) = \partial^-(v_i) \)
\[ v_i = (\partial^\pm)^{-1}(q_{i+1}, q_i), \quad \partial^\pm \equiv (\partial^+, \partial^-) \]

The derivative \( v_i \) of \( q_i \) satisfies \( \partial^+(v_{i-1}) = \partial^-(v_i) \)

If \( v_i \) satisfies \( \partial^-(v_{i+1}) = \partial^+(v_i) \) then it is the derivative of \( q_i \) defined by \( q_i = \partial^+(v_{i-1}) = \partial^-(v_i) \)

The discrete first order condition is

\[ \partial^+(v_i) = \partial^-(v_{i+1}) \]

Same as: the curve segments connect
$$S = \sum_{i=1}^{L} d_i(v_i),$$

$$dS \cdot \delta v_i = 0,$$

$$\partial^+ (v_i) = \partial^- (v_{i+1}),$$

$$T \partial^+ (\delta v_i) = T \partial^- (\delta v_{i+1}),$$

$$T \partial^- (\delta v_0) = 0,$$

$$T \partial^+ (\delta v_N) = 0.$$
\[ S_d = \sum_{i=1}^{N} L_d(v_i), \quad dS_d \cdot \delta v_i = 0 \]
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S_d = \sum_{i=1}^{N} L_d(v_i), \quad dS_d \cdot \delta v_i = 0
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\[ S_d = \sum_{i=1}^{N} L_d(v_i), \quad dS_d \cdot \delta v_i = 0 \]

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\[ T \partial^-(\delta v_0) = 0, \quad T \partial^+(\delta v_N) = 0 \]
A discretization of $T^* \mathcal{M}$ is a tuple $(\psi, \alpha^+, \alpha^-)$, where

1. $\psi: U \subseteq \mathbb{R}^2 \times \mathcal{M} \to \mathcal{M}$, $\alpha^+: [0, a) \to \mathbb{R} \geq 0$, $\alpha^-: [0, a) \to \mathbb{R} \leq 0$,

are such that

2. $U$ is open and $\{0\} \times \{0\} \times \mathcal{M} \subseteq U$;

3. $\alpha^+, \alpha^-$ are $C^1$, $\alpha^+(0) = \alpha^-(0) = 0$, and $\dot{\alpha}^+ \equiv d \alpha^+ dh(0)$, $\dot{\alpha}^- \equiv d \alpha^- dh(0)$, satisfy $\dot{\alpha}^+ - \dot{\alpha}^- = 1$;

4. the boundary maps defined by $\partial^- h(v_m) \equiv \psi(h, \alpha^-(h), v_m)$, $\partial^+ h(v_m) \equiv \psi(h, \alpha^+(h), v_m)$, are $C^1$ and $d dh \big|_{h=0} \partial^+ h(v_m) = \dot{\alpha}^+ v_m$, $d dh \big|_{h=0} \partial^- h(v_m) = \dot{\alpha}^- v_m$. 


A discretization of $T\mathcal{M}$ is a tuple $(\psi, \alpha^+, \alpha^-)$, where

$$\psi: U \subseteq \mathbb{R}^2 \times \mathcal{M} \rightarrow \mathcal{M}, \quad \alpha^+: [0, a) \rightarrow \mathbb{R}_{\geq 0}, \quad \alpha^-: [0, a) \rightarrow \mathbb{R}_{\leq 0},$$

are such that

1. $U$ is open and $\{0\} \times \{0\} \times \mathcal{M} \subseteq U$;
2. $\alpha^+, \alpha^-$ are $C^1$, $\alpha^+(0) = \alpha^-(0) = 0$, and
   $$\dot{\alpha}^+ \equiv \frac{d\alpha^+}{dh}(0), \quad \dot{\alpha}^- \equiv \frac{d\alpha^+}{dh}(0),$$
   satisfy $\dot{\alpha}^+ - \dot{\alpha}^- = 1$;
3. $\psi(h, 0, \nu_m) = m$, and $\frac{\partial \psi}{\partial t}(h, 0, \nu_m) = \nu_m$;
4. the boundary maps defined by
   $$\partial^-_h(\nu_m) \equiv \psi(h, \alpha^-(h), \nu_m), \quad \partial^+_h(\nu_m) \equiv \psi(h, \alpha^+(h), \nu_m),$$
   are $C^1$ and
   $$\frac{d}{dh}\bigg|_{h=0} \partial^+_h(\nu_m) = \dot{\alpha}^+ \nu_m, \quad \frac{d}{dh}\bigg|_{h=0} \partial^-_h(\nu_m) = \dot{\alpha}^- \nu_m.$$
Let $\mathcal{M}$ be a manifold. A \textit{discrete tangent bundle of} $\mathcal{M}$ is a tuple $(\mathcal{V}, \partial^+, \partial^-)$, where $\mathcal{V}$ is a manifold, $\dim \mathcal{V} = 2 \dim \mathcal{M}$ and $\partial^+: \mathcal{V} \to \mathcal{M}$ and $\partial^-: \mathcal{V} \to \mathcal{M}$ satisfy

1. $\partial^+$ and $\partial^-$ are submersions such that $\ker T\partial^+ \cap \ker T\partial^- = 0$; and

2. for all $m \in \mathcal{M}$, the \textit{backward fiber} $\mathcal{V}_m^+ \equiv (\partial^+)^{-1}(m)$ and the \textit{forward fiber} $\mathcal{V}_m^- \equiv (\partial^-)^{-1}(m)$ meet in exactly one point, denoted $0_m$.

The \textit{discrete zero section} is $0_\mathcal{V} \equiv (\partial^\pm)^{-1}\Delta(\mathcal{M} \times \mathcal{M})$, where $\Delta(\mathcal{M} \times \mathcal{M})$ is the diagonal of $\mathcal{M} \times \mathcal{M}$. 
Discretizations of tangent bundles
\( \mathcal{M} = \mathbb{R}^k \), \( \psi(h, t, (m, v)) \equiv m + tv + O(h^2) \)
\[ M = \mathbb{R}^k, \quad \psi(h, t, (m, v)) \equiv m + tv + O(h^2) \]

\[ m^- = m + \alpha^-(h)v + O(h^2), \quad m^+ = m + \alpha^+(h)v + O(h^2) \]
\[ \mathcal{M} = \mathbb{R}^k, \quad \psi(h, t, (m, v)) \equiv m + tv + O(h^2) \]

\[ m^- = m + \alpha^-(h)v + O(h^2), \quad m^+ = m + \alpha^+(h)v + O(h^2) \]

\[ h = 0 : \quad m^- = m, \quad m^+ = m \]
\[ \mathcal{M} = \mathbb{R}^k, \quad \psi(h, t, (m, v)) \equiv m + tv + O(h^2) \]

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\[ h = 0 : \quad m^- = m, \quad m^+ = m \]

\[ \bar{m} = \frac{m^+ + m^-}{2}, \quad z = \frac{m^+ - m^-}{h} \]
\( \mathcal{M} = \mathbb{R}^k, \quad \psi(h, t, (m, v)) \equiv m + tv + O(h^2) \)

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\[ \bar{m} = \frac{m^+ + m^-}{2}, \quad z = \frac{m^+ - m^-}{h} \]

\[ \bar{m} = m + \frac{\alpha^+(h) + \alpha^-(h)}{2}v + O(h^2), \quad z = v + O(h) \]
\[ \mathcal{M} = \mathbb{R}^k, \quad \psi(h, t, (m, v)) \equiv m + tv + O(h^2) \]

\[ m^- = m + \alpha^-(h)v + O(h^2), \quad m^+ = m + \alpha^+(h)v + O(h^2) \]

\[ h = 0 : \quad m^- = m, \quad m^+ = m \]

\[ \tilde{m} = \frac{m^+ + m^-}{2}, \quad z = \frac{m^+ - m^-}{h} \]

\[ \tilde{m} = m + \frac{\alpha^+(h) + \alpha^-(h)}{2}v + O(h^2), \quad z = v + O(h) \]

\[ h = 0 : \quad \tilde{m} = m, \quad z = v \]
Discretizations of tangent bundles


A discretization of a Lagrangian system $L: TQ \to \mathbb{R}$ is a tuple $(L_h, \psi, \alpha^+, \alpha^-)$ where $(\psi, \alpha^+, \alpha^-)$ is a discretization of $TQ$ and $L_h: TQ \to \mathbb{R}$ is a function such that

$$L_h(v_q) = \int_{\alpha^-(h)}^{\alpha^+(h)} L \circ \frac{\partial \psi}{\partial t}(h, t, v_q) \, dt + O(h^2).$$

A discrete Lagrangian system is a tuple $(L_d, \partial^+, \partial^-, \mathcal{V}, Q)$ where $L_d: \mathcal{V} \to \mathbb{R}$ and $(\mathcal{V}, \partial^+, \partial^-)$ is a discrete tangent bundle on $Q.$
The variational technology in

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- identifies the symplectic form
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- identifies the symplectic form
- proves symplecticity of the discrete flow
The variational technology in

J. E. Marsden, G. W. Patrick, and S. Shkoller [1998].

- identifies the symplectic form
- proves symplecticity of the discrete flow
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\[ \theta_L^-(\nu) = -dL(\nu) T \pi^-, \quad \theta_L^+(\nu) = dL(\nu) T \pi^+, \]

\[ d\theta_L^+ = -d\theta_L^- = -\omega_L \]

\[ J^\xi = \iota_\xi \nu \theta_L^+ \]
Given \( w_1 = (q_1, v_1) \in TQ \) solve, for \( w_2 = (q_2, v_2) \in T\hat{Q} \), the equations

\[
DL_h(w_1) = \lambda^- D\hat{\theta}_h^- (w_1) + \mu D\hat{\theta}_h^+ (w_1) + \nu_1^- [Dg(q_1), 0] + \nu_2^- [D^2g(q_1)v_1, Dg(q_1)]
\]

\[
DL_h(w_2) = \lambda^+ D\hat{\theta}_h^+ (w_2) - \mu D\hat{\theta}_h^- (w_2) + \nu_1^+ [Dg(q_2), 0] + \nu_2^+ [D^2g(q_2)v_2, Dg(q_2)]
\]

\[
\bar{q} = \hat{\theta}_h^+(w_1) + Dg(\bar{q})^T \bar{\theta}_1, \quad \bar{q} = \hat{\theta}_h^-(w_2) + Dg(\bar{q})^T \bar{\theta}_2
\]

\[
g(\bar{q}) = 0
\]

\[
\lambda^- Dg(q_1^-)^T = 0, \quad \lambda^+ Dg(q_2^+)^T = 0 \quad \mu Dg(\bar{q})^T = 0
\]

\[
g(q_2) = 0, \quad Dg(q_2)v_2 = 0
\]

\[
g(q_1^-) = 0, \quad g(q_2^+) = 0
\]

\[
q_1^- = \hat{\theta}_h^- (w_1) + Dg(q_1^-)^T \theta^-, \quad q_2^+ = \hat{\theta}_h^+(w_2) + Dg(q_2^+)^T \theta^+
\]

Lagrange multipliers \( \lambda^-, \lambda^+, \mu \)

Lagrange multipliers \( \nu_1^+, \nu_2^+, \nu_1^-, \nu_2^- \)

Time advanced state \( (q_2, v_2) \in TQ \)

Midpoint \( \bar{q} \)

Variables \( \bar{\theta}_1, \bar{\theta}_2, \theta^-, \theta^+ \)

Variables \( q_1^-, q_2^+ \)

\[8N + 8r\]
$L : TQ \rightarrow \mathbb{R}, \ \psi(h, t, v_q), \ L_d = \int_{\alpha^-(h)}^{\alpha^+(h)} L \left( \frac{\partial \psi}{\partial t}(h, t, v_q) \right) dt + O(h^2)$
\[ L: TQ \rightarrow \mathbb{R}, \ \psi(h, t, v_q), \ L_d = \int_{\alpha^-(h)}^{\alpha^+(h)} L \left( \frac{\partial \psi}{\partial t}(h, t, v_q) \right) \ dt + O(h^2) \]

Want: for small enough \( h \), for all \( v \) there is a unique \( \tilde{v} \) such that

\[ dL_d(v)\delta v + dL_d(\tilde{v})\delta v = 0, \]
\[ \partial^+(v) = \partial^-(\tilde{v}), \]
\[ T \partial^- \delta v = 0, \quad T \partial^+ \delta \tilde{v} = 0, \quad T \partial^+ \delta v = T \partial^- \delta \tilde{v} \]
L: $TQ \to \mathbb{R}$, $\psi(h, t, v_q)$, $L_d = \int_{\alpha^-(h)}^{\alpha^+(h)} L \left( \frac{\partial \psi}{\partial t}(h, t, v_q) \right) dt + O(h^2)$

Want: for small enough $h$, for all $v$ there is a unique $\tilde{v}$ such that

$$dL_d(v)\delta v + dL_d(\tilde{v})\delta v = 0,$$

$$\partial^+(v) = \partial^-(\tilde{v}),$$

$$T\partial^- \delta v = 0, \quad T\partial^+ \delta \tilde{v} = 0, \quad T\partial^+ \delta v = T\partial^- \delta \tilde{v}$$

Must be a perturbative proof at $h = 0$. 
\[ L: \mathcal{T}Q \rightarrow \mathbb{R}, \quad \psi(h, t, \nu_q), \quad L_d = \int_{\alpha^-(h)}^{\alpha^+(h)} L \left( \frac{\partial \psi}{\partial t} (h, t, \nu_q) \right) dt + O(h^2) \]

Want: for small enough \( h \), for all \( \nu \) there is a unique \( \tilde{\nu} \) such that

\[
dL_d(\nu) \delta \nu + dL_d(\tilde{\nu}) \delta \nu = 0, \\
\partial^+ (\nu) = \partial^- (\tilde{\nu}), \\
T \partial^- \delta \nu = 0, \quad T \partial^+ \delta \tilde{\nu} = 0, \quad T \partial^+ \delta \nu = T \partial^- \delta \tilde{\nu}
\]

Must be a perturbative proof at \( h = 0 \).

But \( h = 0 \) this problem is badly degenerate:

\[
h = 0 : \quad \partial^- (\nu_q) = \partial^+ (\nu_q) = q, \quad L_d = 0
\]

Discrete existence and uniqueness
Blow up the variational principle at $h = 0$.

$$S_d(v, \tilde{v}) = L(v) + L(\tilde{v}), \quad v, \tilde{v} \in T_q Q,$$

$$\frac{v + \tilde{v}}{2} = z_q$$

Nondegenerate if $L$ is hyperregular and the solution is $v_q = \tilde{v}_q = z_q$. 
Blow up the variational principle at $h = 0$.

\[ S_d(v, \tilde{v}) = L(v) + L(\tilde{v}), \quad v, \tilde{v} \in T_q Q, \]
\[ \frac{v + \tilde{v}}{2} = z_q \]

Nondegenerate if $L$ is hyperregular and the solution is $v_q = \tilde{v}_q = z_q$.

Semiglobal inverse function theorem; tubular neighbourhood.
Want: if $\psi, \tilde{\psi}$ and $L_d, \tilde{L}_d$ match to order $r$, then $F, \tilde{F}$ match to order $\psi$. 
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Easy: $\tilde{F} = F + \mathcal{O}(h^{r-1})$. Its $r - 1$ because of a division by $h$ in the blow-up.
Want: if $\psi, \tilde{\psi}$ and $L_d, \tilde{L}_d$ match to order $r$, then $F, \tilde{F}$ match to order $\psi$.

**Easy:** $\tilde{F} = F + O(h^{r-1})$. Its $r - 1$ because of a division by $h$ in the blow-up.

**Difficult:** $\tilde{F} = F + O(h^r)$.
Want: if $\psi, \tilde{\psi}$ and $L_d, \tilde{L}_d$ match to order $r$, then $F, \tilde{F}$ match to order $\psi$.

Easy: $\tilde{F} = F + O(h^{r-1})$. Its $r - 1$ because of a division by $h$ in the blow-up.

Difficult: $\tilde{F} = F + O(h^r)$.

- $F, \tilde{F}$ are obtained from graphs $\Gamma, \tilde{\Gamma}$. 

$\tilde{\Gamma} = \Gamma + O(h^{r-1})$

$rsd(r)(v, \tilde{v})$ is symmetric. It affects the graphs symmetrically.

That does not affect the maps.
Want: if $\psi, \tilde{\psi}$ and $L_d, \tilde{L}_d$ match to order $r$, then $F, \tilde{F}$ match to order $\psi$.

Easy: $\tilde{F} = F + O(h^{r-1})$. Its $r - 1$ because of a division by $h$ in the blow-up.

Difficult: $\tilde{F} = F + O(h^r)$.

- $F, \tilde{F}$ are obtained from graphs $\Gamma, \tilde{\Gamma}$.
- $\Gamma = \tilde{\Gamma} + O(h^{r-1})$
Want: if $\psi, \tilde{\psi}$ and $L_d, \tilde{L}_d$ match to order $r$, then $F, \tilde{F}$ match to order $\psi$.

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Easy: $\tilde{F} = F + O(h^{r-1})$. Its $r - 1$ because of a division by $h$ in the blow-up.

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- $F, \tilde{F}$ are obtained from graphs $\Gamma, \tilde{\Gamma}$.
- $\Gamma = \tilde{\Gamma} + O(h^{r-1})$
- $\Gamma = \tilde{\Gamma} + \text{rsd}^r(v, \tilde{v})$
- $\text{rsd}^r(v, \tilde{v})$ is symmetric. It affects the graphs symmetrically. That does not affect the maps.