Introduction
Variational integrators
Nonholonomic integrators
Lie group integrators

Short talk: High-order geometric methods for nonholonomic mechanical systems.

Rodrigo T. Sato Martín de Almagro

Supervisor:
David Martín de Diego

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Mechanical systems

- Described via Lagrangian or Hamiltonian formulation
- Built-in geometric properties (Manifold structure of configuration space, symplecticity)
- Built-in conservation laws due to symmetries (Noether theorem)

Question 1
Can we find numerical methods that respect / preserve these?
Mindful integration

As it turns out, mostly yes.

Structure preserving algorithms ([Hairer], [Sanz-Serna], [Munthe-Kaas], ...)

- We can try to respect the manifold structure of the configuration space.
- We can preserve at least first or second order invariants (energy, symplectic form).

For mechanical systems we take special interest in a set of constant step-size methods called *symplectic methods*. 
Symplectic integrators

Why do we like symplectic integrators?

- Good qualitative and quantitative behaviour.
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- Preserve state-space properties (symplecticity).
### Why do we like symplectic integrators?

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- Energy not exactly preserved... [Ge & Marsden]
**Why do we like symplectic integrators?**

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- ... but good long-term energy behaviour.

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**Figure 1.** Energy computed with variational Newmark method.

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**Figure 2.** Nonholonomic integrators.

**Figure 3.** Area preservation of numerical methods for the pendulum; same initial sets as in Fig. 2.2.

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**Example 3.2.** We consider the pendulum problem of Example 2.5 with the same initial conditions. If we take initial conditions $(\dot{\theta} = \omega, \theta = \gamma)$, we compute several steps with step size $h=\pi/2$ for the first order methods, and $h=\pi/4$ for the second order methods (right column): explicit Euler method (I.1.5), symplectic Euler method (I.1.9), the implicit midpoint rule (the right one), the Störmer–Verlet scheme (I.1.17), and the implicit midpoint rule for the derivative.

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**Introduction**

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**Symplectic integrators**
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- Energy not exactly preserved... [Ge & Marsden]
- ... but good long-term energy behaviour.

How come energy behaves so well?

Theorems ([Moser], [Benettin & Giogilli], [Tang], [Murua]...) warrant that symplectic integrators are integrating exactly some existing Hamiltonian system that is close to the original one.
### Why do we like symplectic integrators?
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### How come energy behaves so well?
Theorems ([Moser], [Benettin & Giogilli], [Tang], [Murua]...) warrant that symplectic integrators are integrating exactly some existing Hamiltonian system that is close to the original one.

### Question 2
How do we build them?
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Variational integrators are always symplectic.

Idea ([Veselov], [Suris], [Marsden & West]...)

- Substitute continuous state space with discrete one.
Variational integrators are always symplectic.

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Generating symplectic integrators easily

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- Build a discrete analogue of Hamilton’s principle.
Generating symplectic integrators easily

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- Substitute continuous state space with discrete one.
- Build a discrete analogue of Hamilton’s principle.
- Derive equations of motion and conserved quantities from the principle.
Generating symplectic integrators easily

Variational integrators are always symplectic.

**Idea ([Veselov], [Suris], [Marsden & West]...)**

- Substitute continuous state space with discrete one.
- Build a discrete analogue of Hamilton’s principle.
- Derive equations of motion and conservations from the principle.

Discrete equations of motion = Difference equations (a.k.a. **our integrator**).
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Building blocks

Exact discrete Lagrangian

\[ L_d^e(q_0, q_1) = \int_0^h L(q(\tau), \dot{q}(\tau))d\tau \]

where \( q(t) \) solution of the Euler-Lagrange eqs. with fixed boundary values \( q(0) = q_0, q(h) = q_1 \).

Approximation. Discrete Lagrangian

\( L_d \) approx. of order \( r \) if \( \exists C_1 > 0, h_1 > h > 0 \) s.t.

\[ \| L_d(q(0), q(h)) - L_d^e(q(0), q(h)) \| \leq C_1 h^{r+1} \]
Discrete principle and governing equations

Discrete Hamilton’s principle

Discrete curve \( q_d = \{ q_i \}_{i=0}^{N} \) solution of the discrete Lagrangian system ⇔ critical point of the functional:

\[
J_d(q_d) = \sum_{k=0}^{N-1} L_d(q_k, q_{k+1})
\]

Discrete Euler-Lagrange (DEL) equations

\[
D_2 L_d(q_{k-1}, q_k) + D_1 L_d(q_k, q_{k+1}) = 0, \forall k = 1, \ldots, N - 1
\]
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High-order variational integrators

Connection with Hamiltonian mechanics

Discrete fibre derivatives

\[ \mathbb{F}L_d^+ : \quad Q \times Q \rightarrow T^* Q \]
\[ (q_0, q_1) \mapsto (q_1, p_1 \equiv D_2 L_d(t_0, q_0, q_1)) \]

\[ \mathbb{F}L_d^- : \quad Q \times Q \rightarrow T^* Q \]
\[ (q_0, q_1) \mapsto (q_0, p_0 \equiv -D_1 L_d(t_0, q_0, q_1)) \]

These provide interpretation of DEL equations as matching of momenta:

\[ p_k^- = D_2 L_d(q_{k-1}, q_k) = -D_1 L_d(q_k, q_{k+1}) = p_k^+ \]
Theorem. Variational error [Marsden & West, Patrick & Cuell]

If $\tilde{F}_{L_d}$ Hamiltonian map of an order $r$ discrete Lagrangian $L_d$, then

$$\tilde{F}_{L_d} = \tilde{F}_{L_d}^e + O(h^{r+1}).$$
The starting point

**Hamilton-Pontryagin action**

\[(q, v, p) : [a, b] \subset \mathbb{R} \rightarrow TQ \oplus T^* Q, \ C^1([a, b]) \text{ curve with } C^2([a, b]) \text{ base component and fixed boundary values } q(a) = q_a, \ q(b) = q_b. \]

\[\mathcal{J}_{HP}(q, v, p) = \int_0^h \left[ L(q(t), v(t)) + \langle p(t), \dot{q}(t) - v(t) \rangle \right] dt\]

**Dynamical equations**

\[\frac{dp(t)}{dt} = D_1L(q(t), v(t)), \]
\[p(t) = D_2L(q(t), v(t)), \]
\[\frac{dq(t)}{dt} = v(t), \ \forall t \in [0, h].\]
Discretizing the action

Discrete Hamilton-Pontryagin action

\[
(\mathcal{J}_{\mathcal{HP}})_d = \sum_{k=0}^{N-1} \sum_{i=1}^{s} hb_i \left[ L \left( Q_k^i, V_k^i \right) + \left\langle p_k^i, \frac{Q_k^i - q_k}{h} - \sum_{j=1}^{s} a_{ij} V_k^j \right\rangle + \left\langle p_{k+1}, \frac{q_{k+1} - q_k}{h} - \sum_{j=1}^{s} b_j V_k^j \right\rangle \right]
\]

where \((a_{ij}, b_j)\) coefficients of a Runge-Kutta (RK) method.
Discrete dynamics in $T^*Q$

Discrete dynamical equations: Symplectic partitioned RK methods

\[
q_{k+1} = q_k + h \sum_{j=1}^{s} b_j V^j_k, \quad p_{k+1} = p_k + h \sum_{i=1}^{s} \hat{b}_j W^j_k,
\]

\[
Q^i_k = q_k + h \sum_{j=1}^{s} a_{ij} V^j_k, \quad P^i_k = p_k + h \sum_{j=1}^{s} \hat{a}_{ij} W^j_k,
\]

\[
W^i_k = D_1 L(Q^i_k, V^i_k), \quad P^i_k = D_2 L(Q^i_k, V^i_k),
\]

where $(\hat{a}_{ij}, \hat{b}_j)$ satisfy $b_i \hat{a}_{ij} + \hat{b}_j a_{ji} = b_i \hat{b}_j$ and $\hat{b}_i = b_i$. 
Discrete dynamics in $TQ$

Discrete dynamical equations: Symplectic partitioned RK methods

\[
q_{k+1} = q_k + h \sum_{j=1}^{s} b_j V_k^j, \quad p_{k+1} = p_k + h \sum_{i=1}^{s} \hat{b}_j W_k^j, \\
Q_k^i = q_k + h \sum_{j=1}^{s} a_{ij} V_k^j, \quad P_k^i = p_k + h \sum_{j=1}^{s} \hat{a}_{ij} W_k^j, \\
W_k^i = D_1 L(Q_k^i, V_k^i), \quad P_k^i = D_2 L(Q_k^i, V_k^i), \\
p_k = D_2 L(q_k, v_k), \quad p_{k+1} = D_2 L(q_{k+1}, v_{k+1}),
\]
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Nonholonomic mechanics

**Nonholonomic Lagrangian system**

\((L, Q, N)\) with \(N\), constrain manifold with \(i_N : N \leftrightarrow TQ\). Locally described by null-set of \(\Phi : TQ \rightarrow \mathbb{R}^m, \ m = \text{codim}_{TQ} N\).

**Dynamical equations**

\[
\begin{cases}
\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}^i} \right) - \frac{\partial L}{\partial q^i} = \left\langle \lambda, \frac{\partial \Phi}{\partial q^i} \right\rangle, \\
\Phi(q, \dot{q}) = 0
\end{cases}
\]

NON-VARIATIONAL (NOR SYMPLECTIC)!! Obtained via Chetaev’s principle. \(\lambda\) are Lagrange multipliers.

Should we throw away our variational integrators?
No, we can still build from the variational substrate. Previous attempts by [de León, Martín de Diego & Santamaría], [Cortés & Martínez], [Ferraro, Iglesias & Martín de Diego], [Jay]...

Idea

Somehow construct discrete nonholonomic fibre derivatives $\mathbb{F} \left( L^N_d \right)^\pm : Q \times Q \to M$, where $M = \mathbb{F} L^N (N)$ and $L^N = L \circ i_N$.

Augmented point of view

Easier to build $\Gamma^\pm_d : Q \times \Lambda \times Q \times \Lambda \to T^* Q \times \Lambda$, where $\Lambda \cong \mathbb{R}^m$, and find $\lambda_0, \lambda_1$ s.t. $\Gamma^\pm_d (q_0, \lambda_0, q_1, \lambda_1) \in T^* Q|_M \times \Lambda$. 
Discrete nonholonomic mechanics II

For a certain family of RK methods \((a_{ij}, b_j)\) (Lobatto-type):

**Nonholonomic integrator**

\[
q_{k+1} = q_k + h \sum_{i=1}^{s} b_i V^i_k, \quad p_{k+1} = p_k + h \sum_{i=1}^{s} \hat{b}_i W^i_k ,
\]

\[
Q^i_k = q_k + h \sum_{j=1}^{s} a_{ij} V^j_k, \quad P^i_k = p_k + h \sum_{j=1}^{s} \hat{a}_{ij} W^j_k ,
\]

\[
W^i_k = D_1 L(Q^i_k, V^i_k) + \left< \Lambda^i_k, D_2 \Phi(Q^i_k, V^i_k) \right>, \quad P^i_k = D_2 L(Q^i_k, V^i_k),
\]

\[
\Psi(q^i_k, p^i_k) = 0
\]

where \((\hat{a}_{ij}, \hat{b}_j)\) satisfy \(b_i \hat{a}_{ij} + \hat{b}_j a_{ji} = b_i \hat{b}_j\) and \(\hat{b}_i = b_i\) and \(\Psi = \Phi \circ FL^{-1}\).

This generates a well-defined nonholonomic Hamiltonian flow

\[
\tilde{F}_{L_d}^{\Lambda} : T^* Q|_M \times \Lambda \rightarrow T^* Q|_M \times \Lambda, (q_0, p_0, \lambda_0) \mapsto (q_1, p_1, \lambda_1).
\]
Nonholonomic integrator

\[ q_{k+1} = q_k + h \sum_{i=1}^{s} b_i V_k^i, \]

\[ p_{k+1} = p_k + h \sum_{i=1}^{s} \hat{b}_i W_k^i, \]

\[ Q_k^i = q_k + h \sum_{j=1}^{s} a_{ij} V_k^j, \]

\[ P_k^i = p_k + h \sum_{j=1}^{s} \hat{a}_{ij} W_k^j, \]

\[ W_k^i = D_1 L(Q_k^i, V_k^i) + \left\langle \Lambda_k^i, D_2 \Phi(Q_k^i, V_k^i) \right\rangle, \]

\[ P_k^i = D_2 L(Q_k^i, V_k^i), \]

\[ q_k^i = Q_k^i, \]

\[ p_k^i = p_k + h \sum_{j=1}^{s} a_{ij} W_k^j, \]

\[ p_k = D_2 L(q_k, v_k), \]

\[ p_k^i = D_2 L(q_k^i, v_k^i) \]

\[ \Phi(q_k^i, v_k^i) = 0 \]
Key players

\[ Q^i_k = q_k + h \sum_{j=1}^{s} a^j_{ij} V^j_k, \quad P^i_k = p_k + h \sum_{j=1}^{s} \hat{a}^j_{ij} W^j_k, \quad p^i_k = p_k + h \sum_{j=1}^{s} a^j_{ij} W^j_k \]
Key players

\[ Q^i_k = q_k + h \sum_{j=1}^{s} a_{ij} V^j_k, \quad P^i_k = p_k + h \sum_{j=1}^{s} \hat{a}_{ij} W^j_k, \quad p^i_k = p_k + h \sum_{j=1}^{s} a_{ij} W^j_k \]
Key players

\[ Q^i_k = q_k + h \sum_{j=1}^{s} a_{ij} V^j_k, \quad P^i_k = p_k + h \sum_{j=1}^{s} \hat{a}_{ij} W^j_k, \quad p^i_k = p_k + h \sum_{j=1}^{s} a_{ij} W^j_k. \]
Discrete nonholonomic mechanics IV

Key players

\[ Q_k^i = q_k + h \sum_{j=1}^{s} a_{ij} V_k^j, \quad P_k^i = p_k + h \sum_{j=1}^{s} \hat{a}_{ij} W_k^j, \quad p_k^i = p_k + h \sum_{j=1}^{s} a_{ij} W_k^j \]
Discrete nonholonomic mechanics V
Unfortunately, the variational error theorem does not apply. We need to prove order using numerical analysis techniques.

**Theorem. Global error**

If we use an $s$-stage member of the Lobatto-type family [...] the order of the nonholonomic Hamiltonian flow generated by the former integrator is $r = 2s - 2$ in $M$ thus achieving parity with the expected variational error.
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The starting point (again)

Hamilton-Pontryagin action on Lie groups

\[(g, \nu, p) : [a, b] \subset \mathbb{R} \rightarrow TG := TG \oplus T^* G.\]

\[\mathcal{J}_{HP}(g, \nu, p) = \int_0^h \left[ L(g(t), \nu(t)) + \langle p(t), \dot{g}(t) - \nu(t) \rangle \right] dt\]

Dynamical equations

\[\frac{dp(t)}{dt} = D_1 L(g(t), \nu(t)),\]
\[p(t) = D_2 L(g(t), \nu(t)),\]
\[\frac{dg(t)}{dt} = \nu(t), \quad \forall t \in [0, h].\]
Partially reduced case

Reduced Hamilton-Pontryagin action

\[(g, \eta, \mu) : [a, b] \subset \mathbb{R} \rightarrow G \times \mathfrak{g} \times \mathfrak{g}^*, \ell : G \times \mathfrak{g} \rightarrow \mathbb{R}.\]

\[\mathcal{J}_{\mathcal{H}P}(g, \eta, \mu) = \int_{0}^{h} \left[ \ell(g(t), \eta(t)) + \langle \mu(t), g^{-1}(t) \dot{g}(t) - \eta(t) \rangle \right] dt\]

Reduced Dynamical equations

\[\frac{d\mu(t)}{dt} = \text{ad}_{\eta(t)}^* \mu(t) + \left(L_{g(t)}\right)^* D_1 \ell(g(t), \eta(t)),\]

\[\mu(t) = D_2 L(g(t), \eta(t)),\]

\[\frac{dg(t)}{dt} = \left(L_{g(t)}\right)_* \eta(t), \quad \forall t \in [0, h].\]
Assume $L_{h^{-1}}g \in U_e$ and let $\tau : g \rightarrow U_e \subset G$ be a retraction.

\[
(\xi, \eta, \mu) = T_{L_{h^{-1}}g} \tau^{-1} T_g L_{h^{-1}}(g, v_g, p_g)
\]
\[
= (\tau^{-1}(L_{h^{-1}}g), d^L \tau^{-1}_{\tau^{-1}(L_{h^{-1}}g)} T_g L_{g^{-1}} v_g, (d^L \tau^{-1}_{\tau^{-1}(L_{h^{-1}}g)})^* (T_e L_g)^* p_g)
\]
\[
(g, v_g, p_g) = T_{\tau(\xi)} L_h T_{\xi} \tau(\xi, \eta, \mu)
\]
\[
= (L_h \tau(\xi), T_e L_h \tau(\xi) d^L \tau \eta, (T_{L_h \tau(\xi)} L(L_h \tau(\xi))^{-1})^* (d^L \tau^{-1}_\xi)^* \mu_{\xi})
\]

where $d^L \tau : g \times g \rightarrow g$ left-trivialized tangent of $\tau$. 
Variational Lie group integrators

Reduced discrete Hamilton-Pontryagin action

\[ \ell : G \times \mathfrak{g} \to \mathbb{R} \text{ partially reduced Lagrangian.} \]

\[
(\mathcal{J}_{\mathcal{HP}})_d = \sum_{k=0}^{N-1} \sum_{i=1}^{s} h \left[ b_i \ell \left( g_k \tau(\xi^i_k), d^L \tau \xi^i_k \eta^i_k \right) \right] 
+ \left\langle \tilde{M}_k, \frac{1}{h} \xi^i_k \right. 
- \sum_{j=1}^{s} a_{ij} \eta^j_k \left. \right\rangle 
+ \left\langle \tilde{\mu}_{k+1}, \frac{1}{h} \tau^{-1}((g_k)^{-1} g_{k+1}) \right. 
- \sum_{j=1}^{s} b_j \eta^j_k \left. \right\rangle \right] 
\]
Variational Lie group integrators

Discrete dynamical equations

\[ \xi_k^i = \tau^{-1} \left( g_k^{-1} G_k^i \right) = h \sum_{j=1}^{s} a_{ij} \eta_k^j, \]

\[ \xi_{k+1}^i = \tau^{-1} \left( g_{k+1}^{-1} g_k \right) = h \sum_{j=1}^{s} b_j \eta_k^j, \]

\[ M_k^i = \text{Ad}^*_{\tau(\xi_{k+1}^i)} \begin{bmatrix} \mu_k + h \sum_{j=1}^{s} b_j \left( d^L \tau^{-1} \xi_j^i - a_{ji} \frac{d^L \tau^{-1}}{b_i} \right) \end{bmatrix} \ast N_k^i, \]

\[ \mu_{k+1} = \text{Ad}^*_{\tau(\xi_k^i)} \begin{bmatrix} \mu_k + h \sum_{j=1}^{s} b_j \left( d^L \tau^{-1} \xi_j^i \right) \end{bmatrix} \ast N_k^i, \]

\[ N_k^i = \left( d^L \tau \xi_k^i \right) \ast L_{g_k \tau(\xi_k^i)}^* D_1 \ell \left( g_k \tau(\xi_k^i), d^L \tau \xi_k^i \eta_k^i \right), \]

\[ M_k^i = \left( d^L \tau^{-1}_k \xi_{k+1}^i \right) \ast \begin{bmatrix} \Pi_k^i + h \sum_{j=1}^{s} b_j \frac{a_{ji}}{b_i} \left( dd^L \tau \xi_j^i \right) \ast (\eta_k^j, \Pi_k^j) \end{bmatrix}, \]

\[ \Pi_k^i = \left( d^L \tau \xi_k^i \right) \ast D_2 \ell \left( g_k \tau(\xi_k^i), d^L \tau \xi_k^i \eta_k^i \right), \]

\[ \mu_k = \left( d^L \tau^{-1}_k \xi_{k-1} \right) \ast \tilde{\mu}_k. \]
Second trivialized differential of $\tau$

$\dd d^L \tau : \mathfrak{g} \times \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$ linear map on second and third arguments s.t.:

$$\partial_{\xi} \left( d^L \tau_{\xi} \eta \right) \delta \xi = d^L \tau_{\xi} \dd d^L \tau_{\xi} (\eta, \delta \xi).$$

Appears naturally when considering elements from $T^{(2)} G$ represented by elements $(\xi, \eta, \zeta) \in T^{(2)} \mathfrak{g}$:

$$\left( \tau(\xi), \tau(\xi) d^L \tau_{\xi} \eta, \tau(\xi) d^L \tau_{\xi} \left[ \zeta + \dd d^L \tau_{\xi} (\eta, \eta) \right] \right)$$
Nonholonomic Lie group integrators

Modified discrete dynamical equations

\[ N^i_k = \left( d^L \tau_{\xi_k^i} \right)^* \left[ L^*_{g_k \tau(\xi_k^i)} D_1 \ell \left( g_k \tau(\xi_k^i), d^L \tau_{\xi_k^i} \eta_k^i \right) \\
+ \left\langle \Lambda^i_k, D_2 \phi \left( g_k \tau(\xi_k^i), d^L \tau_{\xi_k^i} \eta_k^i \right) \right]\right] \]

\[ g_k^i = G_k^i \]

\[ \mu_k^i = \text{Ad}_{\tau(\xi_k^i)}^* \left[ \mu_k + h \sum_{j=1}^{s} a_{ij} \left( d^L \tau_{\xi_k^j}^{-1} \right)^* N^j_k \right] \]

\[ \psi \left( g_k^i, \mu_k^i \right) = 0 \]

where \( \phi : G \times g \rightarrow \mathbb{R} \) and \( \phi \circ F \ell^{-1} = \psi : G \times g^* \rightarrow \mathbb{R} \).

Convergence rates coincide with their vector space counterparts.
THANKS FOR YOUR ATTENTION!