Developing Geometric Integrators for Hamiltonizable Nonholonomic Systems

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Career Options for Underrepresented Groups in the Mathematical Sciences

Overview

1. Geometric Mechanics

2. Nonholonomic Mechanics
   - Equations of Motion

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3. Hamiltonization
   - Associated Second Order Systems
4. Variational Integrators

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6. Acknowledgements

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- Geometric Mechanics is, roughly, mechanics on a manifold Q called the *configuration space*.
- The *Lagrangian* $L : TQ \to \mathbb{R}$, $L = L(q, \dot{q})$ or equivalently the *Hamiltonian* $H : T^*Q \to \mathbb{R}$, $H = H(q, p)$ completely determine the dynamics via *Hamilton's equations*:

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Hamilton's Equations

Let (M, ω) be a symplectic manifold and $H : M \to \mathbb{R}$ a Hamiltonian on M. The vector field X_H determined by the condition:

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- Locally, Hamilton's equations are:

$$\dot{q}^i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial \dot{q}^i},$$

and are equivalent to the *Euler-Lagrange equations*:

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

- All of the fundamental modern physical theories can be described in this way:
  1. $L = \frac{1}{2}g_{ij}\dot{q}^i\dot{q}^j - V(q)$ (system with N degrees of freedom)
  2. $L = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} + \frac{1}{c}j_\mu A_\mu$ (Electromagnetism)
  3. $L = \frac{1}{2\kappa}R$ (General Relativity)
  4. $L = i\hbar\overline{\Psi}\Psi - \frac{\hbar^2}{2m}\nabla\overline{\Psi}\cdot\Psi - V(r)\overline{\Psi}\Psi$ (Quantum Mechanics)

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- The EL equations also result from *Hamilton's principle*, which states that the trajectories of a mechanical system between any two times t_a and t_b extremizes the action S, where:

$$S = \int_a^b L(q, \dot{q}) \, dt.$$

- Mechanical systems whose dynamics are *Lagrangian* (follow from the Euler-Lagrange equations for some L) are also called *variational*.

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Nonholonomic Mechanics

Definition

A *nonholonomic system with symmetry* on a configuration manifold Q (*dim* $Q = n$) is a triple $(L, G, \mathcal{D})$, where:

- $L : TQ \to \mathbb{R}$ is a regular *Lagrangian* of mechanical type $L = T - V$, where $T : TQ \to \mathbb{R}$ is the kinetic energy corresponding to a Riemannian metric g on Q, and $V : Q \to \mathbb{R}$ is the potential energy.

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Equations of Motion

The simplest nonholonomic system on $Q = \mathbb{R}^n$, coordinatized by $q = (r, s)$, has Lagrangian $L(r, \dot{r}, \dot{s})$ and equations of motion:

$$\frac{d}{dt}\frac{\partial L_c}{\partial \dot{r}^\alpha} - \frac{\partial L_c}{\partial r^\alpha} = -\frac{\partial L}{\partial \dot{s}^a} B^a_{\alpha\beta}\dot{r}^\beta,$$

along with the constraint equations $\dot{s}^a = -A^a_\alpha(r)\dot{r}^\alpha$.

- Here the $B^a_{\alpha\beta}$ are the local components of the curvature of A:

$$B^a_{\alpha\beta} = \frac{\partial A^a_\alpha}{\partial r^\beta} - \frac{\partial A^a_\beta}{\partial r^\alpha},$$

  and $L_c = L(r, \dot{r}, \dot{s} = -A \cdot \dot{r})$ is the constrained Lagrangian.
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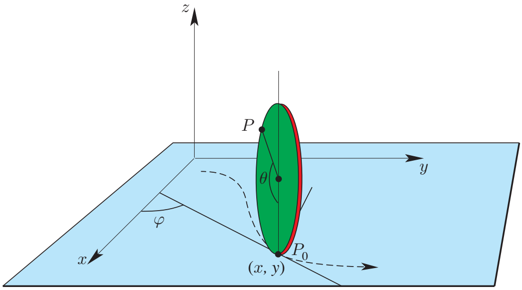
- Example: The vertically rolling disk [1]:



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L &= \frac{1}{2}(\dot{x}^2 + \dot{y}^2) + \frac{1}{2}\dot{\theta}^2 + \frac{1}{2}\dot{\varphi}^2, \\
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Second-Order Associated Systems

A system of second-order ordinary differential equations will be called a *second-order system associated to a nonholonomic system* if its solution set contains the nonholonomic system's solution set.

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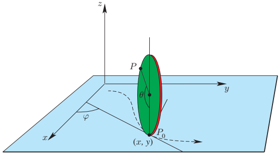

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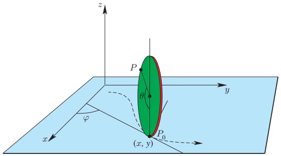

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- The associated second-order system of type I:

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- Now, consider the class of nonholonomic systems where the Lagrangian and constraints are given by:

$$L = \frac{1}{2}\left(I_1\dot{r}_1^2 + I_2\dot{r}_2^2 + \sum_\alpha I_\alpha \dot{s}_\alpha^2\right),$$
$$\dot{s}_\alpha = -A_\alpha(r_1)\dot{r}_2.$$

- The nonholonomic equations of motion are:

$$\ddot{r}_1 = 0, \quad \ddot{r}_2 = -N^2\Big(\sum_\beta I_\beta A_\beta A_\beta'\Big)\dot{r}_1\dot{r}_2, \quad \dot{s}_\alpha = -A_\alpha\dot{r}_2,$$

where $N(r_1)$ is the (in general non-constant) invariant measure density of the nonholonomic system:

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Theorem [1]

The function

$$L = \rho(\dot{r}_1) + \frac{1}{2N}\left(C_2\frac{\dot{r}_2^2}{\dot{r}_1} + \sum_\beta C_\beta \frac{\dot{s}_\beta^2}{A_\beta \dot{r}_1}\right),$$

with $d^2\rho/d\dot{r}_1^2 \neq 0$ and all $C_\alpha \neq 0$ is a regular Lagrangian for the associated systems of type II. If the invariant measure density N is a constant, then also

$$L = \rho(\dot{r}_1) + \sigma(\dot{r}_2) + \frac{1}{2N}\sum_\beta a_\beta \frac{\dot{s}_\beta^2}{A_\beta \dot{r}_1},$$

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[1] Bloch, A.M., Fernandez, O.E. and Mestdag, T. "Hamiltonization and the Inverse Problem of the Calculus of Variations," *Rep. Math. Phy.* 63 (2009), 225-249.

Variational Integrators

- *Mechanical (geometric) integrators* preserve some of the invariants of a mechanical system, such as energy, momentum, or the symplectic form.
- *Variational integrators* are *symplectic-momentum* mechanical integrators resulting from the discretization of Hamilton's principle.

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- Similarly, discretizing the Lagrange-d'Alembert principle yields [1] the *discrete Lagrange-d'Alembert* (DLA) equations, which give a *nonholonomic integrator* for a system subjected to the nonholonomic constraints $\omega_i^a \dot{q}^i = 0$.

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- For Q the n-dimensional configuration manifold and $L_d : Q \times Q \to \mathbb{R}$ the discrete Lagrangian, the DEL equations are:

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

where $q_k \in Q$ for $k \in \{0, 1, \ldots, N\}$ (k is the discrete time).

- For a system subjected to the the nonholonomic constraints $\omega_i^a \dot{q}^i = 0$, the DLA equations are:

$$\begin{aligned} [D_1 L_d(q_k, q_{k+1}) + D_2 L_d(q_{k-1}, q_k)]_i &= (\lambda_k)_a \omega_i^a(q_k), \\ \omega_d^a(q_k, q_{k+1}) &= 0, \end{aligned}$$

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- For a given k and α, we typically take the discretizations to be:

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\begin{aligned}
L_d(q_1, q_2) &= L\left(q = (1-\alpha)q_1 + \alpha q_2, \dot{q} = \frac{q_2 - q_1}{k}\right), \\
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- Example: The Vertical Disk. Here $(r_1, r_2, s_\alpha) = (\phi, \theta, x, y)$, and the nonholonomic solutions are (circles) given by:

$$\theta(t) = u_\theta t + \theta_0, \quad \phi(t) = u_\phi t + \phi_0,$$
$$x(t) = \left(\frac{u_\theta}{u_\phi}\right) R \sin(\phi(t)) + x_0, \quad y(t) = -\left(\frac{u_\theta}{u_\phi}\right) R \cos(\phi(t)) + y_0.$$

- The system is Hamiltonizable, and from the previous Theorem we can choose a simple Lagrangian (for convenience, let $m = R = 1$), such as:

$$\tilde{L} = \frac{1}{2}\left(\dot{\phi}^2 + \dot{\theta}^2 + \frac{\dot{x}^2}{\cos\phi\dot{\phi}} + \frac{\dot{y}^2}{\sin\phi\dot{\phi}}\right).$$

- Example: The Vertical Disk. Here $(r_1, r_2, s_\alpha) = (\phi, \theta, x, y)$, and the nonholonomic solutions are (circles) given by:

$$\theta(t) = u_\theta t + \theta_0, \quad \phi(t) = u_\phi t + \phi_0,$$
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- In order to reproduce the nonholonomic mechanics, we must choose the initial conditions $(x_0, y_0, \theta_0, \phi_0, x_1, y_2, \theta_1, \phi_1)$ such that they satisfy the constraints:

$$x_1 = x_0 + \cos\phi_0\left(\theta_1 - \theta_0\right), \quad y_1 = y_0 + \sin\phi_0\left(\theta_1 - \theta_0\right).$$

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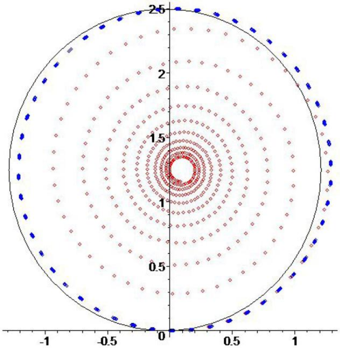

Figure: Comparison: Black = actual solution, Blue = variational, Red = nonholonomic

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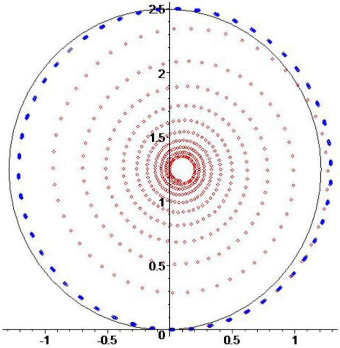

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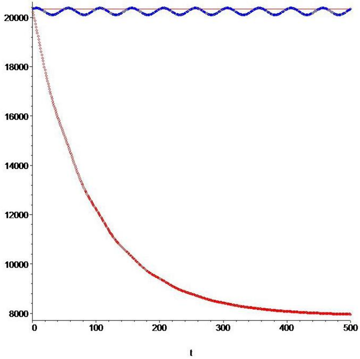
- Moreover, the *energy* is also better preserved by the variational integrator:



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- However, although the *constraints* are in theory preserved (the variational integrator is a symplectic-momentum integrator, and our constraints here are momentum conservation laws), they are not exactly preserved in practice by the variational integrator:

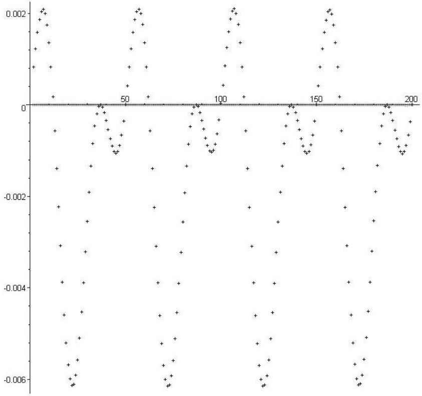

Figure: Plot of $\dot{x} - R\cos\phi\dot{\theta} = 0$, Plus = full variational, Box = constrained variational

- We can fix this by only simulating the constrained dynamics (θ and ψ) and simply enforcing the discrete constraints $\omega_d^a(q_k, q_{k+1}) = 0$ throughout the motion.

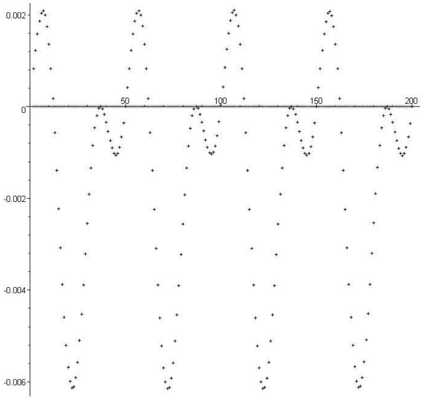

Figure: Plot of $\dot{x} - R\cos\phi\dot{\theta} = 0$, Plus = full variational, Box = constrained variational

- This modified variational integrator *retains the accuracy we saw before*, but of course now numerically preserves the constraints exactly.

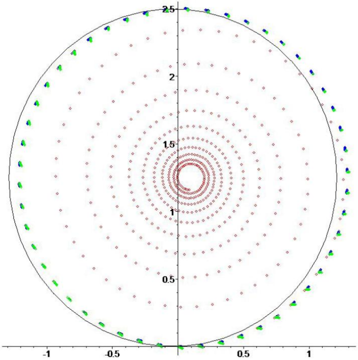

Figure: Comparison: Black = actual solution, Blue = variational, Red = nonholonomic, Green = modified variational

- Lastly, changing α shows that *the variational integrator is stable*, whereas the nonholonomic integrator is not.

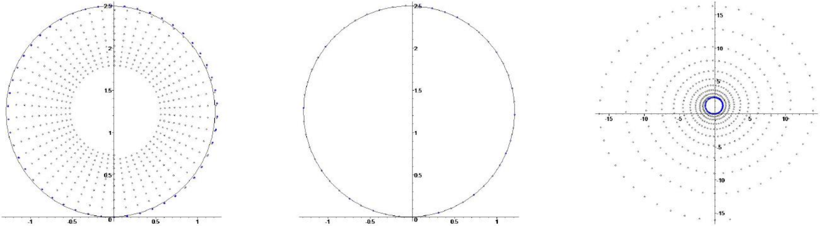

Figure: Comparison: Black = actual solution, Blue = variational, Circles = nonholonomic, for $\alpha = 1/3, 1/2, 1$

- Thus, these variational integrators applied to the Hamiltonized system:
  1. Preserve the energy better (a plus since they are only symplectic-momentum integrators)
  2. Preserve the constraints exactly (just as the nonholonomic integrator does)

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Applications and Future Work

- We have studied and generalized several methods used for Hamiltonization, and the class of Hamiltonizable nonholonomic systems is large.
- One such Hamiltonization technique involves time reparameterization, and the development of a variational integrator similar to the results presented here would provide alternative simulation methods for common *isokinetic and isothermal problems in molecular dynamics* (some of which make use of time reparameterizations as well).

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Acknowledgements

Thank you!

- References:

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