Hamiltonization and geometric integration of nonholonomic mechanical systems

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Lagrangian systems

Consider a mechanical system, with \( n \) generalized coordinates \((q^i)\), subject to forces that can be derived from a potential \( V(q) \). Let \( T(q, \dot{q}) \) be the kinetic energy.

\(~\) The function \( L(q, \dot{q}) = T(q, \dot{q}) - V(q) \) is the Lagrangian.

Then, the principle of Hamilton postulates:

"the trajectory \( q(t) \) between times \( t_1 \) and \( t_2 \) is such that \( \delta \int_{t_1}^{t_2} L(q(t), \dot{q}(t)) dt = 0 \), for all variations with fixed endpoints."

\(~\) The trajectory \( q(t) \) will satisfy the Euler-Lagrange equations

\[
\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}^i} \right) - \frac{\partial L}{\partial q^i} = 0.
\]
Example: A particle with mass $M$

A particle has coordinates $(q^i) \in \mathbb{R}^3$.

**Newton’s equations** of motion if the particle is subject to a force $F_i = -\frac{\partial V}{\partial q^i}$:

$$Ma = F \quad \Leftrightarrow \quad m\ddot{q}^i = -\frac{\partial V}{\partial q^i}.$$

The Lagrangian is $L(q, \dot{q}) = T(q, \dot{q}) - V(q) = \frac{1}{2}M\dot{q}^i \dot{q}^i - V(q)$.

We get:

$$\frac{\partial L}{\partial q^i} = -\frac{\partial V}{\partial q^i}, \quad \frac{\partial L}{\partial \dot{q}^i} = M\dot{q}^i,$$

and therefore

$$\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}^i} \right) - \frac{\partial L}{\partial q^i} = 0 \quad \Leftrightarrow \quad M\dddot{q}^i + \frac{\partial V}{\partial q^i} = 0.$$
Nonholonomic systems

Suppose that the system is subject to \( m \) non-holonomic (nonintegrable) constraints

\[ a_j^\alpha(q) \dot{q}^j = 0, \quad \alpha = 1, \ldots, m < n. \]

Then, the (extended) principle of Hamilton postulates that:

"the trajectory \( q(t) \) between times \( t_1 \) and \( t_2 \) is such that the constraints are satisfied and \( \delta \int_{t_1}^{t_2} L(q(t), \dot{q}(t)) dt = 0 \), for all variations satisfying \( a_j^\alpha \delta q^j = 0. \)"

\[
\begin{align*}
\Rightarrow \quad \int_{t_1}^{t_2} \left( \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}^j} \right) - \frac{\partial L}{\partial q^j} \right) \delta q^j dt &= 0 \\
\Rightarrow \quad \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}^j} \right) - \frac{\partial L}{\partial q^j} &= \sum_{\beta=1}^{m} \lambda_\beta a_j^\beta
\end{align*}
\]

This system of \( n + m \) equations can be solved for the \( n + m \) unknown functions \( q_j(t) \) and \( \lambda_\alpha(t) \).

The terms \( \sum_{\beta=1}^{m} \lambda_\beta a_j^\beta \) in the right hand side are related to the reaction forces!
An example: The vertically rolling disk

Coordinates:

- \((x, y)\): centre of mass \(C\),
- \(\varphi\): angle of the disk with the \((x, z)\)-plane,
- \(\theta\): angle of a fixed line on the disk and a vertical line.

Constraints: \(z = R\) (holonomic), rolling without slipping (non-holonomic):

\[
\mathbf{v}_A = 0 \iff \mathbf{v}_C = \omega \times \mathbf{AC} \iff \begin{cases} 
\dot{x} &= R \cos(\varphi) \dot{\theta} \\
\dot{y} &= R \sin(\varphi) \dot{\theta}
\end{cases}
\]

The Lagrangian is

\[
L = T = \frac{1}{2}M\mathbf{v}_C^2 + \frac{1}{2}I_C(\omega, \omega) = \frac{1}{2}M(\dot{x}^2 + \dot{y}^2) + \frac{1}{2}I\dot{\theta}^2 + \frac{1}{2}J\dot{\varphi}^2, \quad (I = \frac{1}{2}MR^2, J = \frac{1}{4}MR^2).
\]
Next to the constraints, the equations of motion are

\[
\begin{align*}
\frac{d}{dt}\left(\frac{\partial T}{\partial \dot{x}}\right) - \frac{\partial T}{\partial x} &= \lambda_1, \\
\frac{d}{dt}\left(\frac{\partial T}{\partial \dot{y}}\right) - \frac{\partial T}{\partial y} &= \lambda_2, \\
\frac{d}{dt}\left(\frac{\partial T}{\partial \dot{\theta}}\right) - \frac{\partial T}{\partial \theta} &= -\lambda_1 R \cos(\varphi) - \lambda_2 R \sin(\varphi), \\
\frac{d}{dt}\left(\frac{\partial T}{\partial \dot{\phi}}\right) - \frac{\partial T}{\partial \phi} &= 0,
\end{align*}
\]

\[\Leftrightarrow\]

\[
\begin{align*}
M \ddot{x} &= \lambda_1, \\
M \ddot{y} &= \lambda_2, \\
I \ddot{\theta} &= -\lambda_1 R \cos(\varphi) - \lambda_2 R \sin(\varphi), \\
J \ddot{\phi} &= 0,
\end{align*}
\]

\[\Rightarrow\] Use the constraints \(\dot{x} = R \cos(\varphi) \dot{\theta}, \dot{y} = R \sin(\varphi) \dot{\theta}\) to eliminate \(\lambda_1\) and \(\lambda_2\):

\[
\begin{align*}
\ddot{\theta} &= 0, \\
\ddot{\phi} &= 0, \\
\dot{x} &= R \cos(\varphi) \dot{\theta}, \\
\dot{y} &= R \sin(\varphi) \dot{\theta}.
\end{align*}
\]

\[\Rightarrow\] The solutions are \(\theta(t) = u_\theta t + \theta_0, \ \varphi(t) = u_\varphi t + \varphi_0,\) and

- if \(u_\varphi \neq 0\): \(x(t) = \left(\frac{u_\theta}{u_\varphi}\right) R \sin(\varphi(t)) + x_0, \ y(t) = -\left(\frac{u_\theta}{u_\varphi}\right) R \cos(\varphi(t)) + y_0\) (circle)
- If \(u_\varphi = 0\): \(x(t) = R \cos(\varphi_0) u_\theta t + x_0, \ y(t) = R \sin(\varphi_0) u_\theta t + y_0\) (line).
Associated second-order systems

The dynamics is a **mixed set of coupled first- and second-order eq.**:

\[
\ddot{\theta} = 0, \quad \ddot{\varphi} = 0, \quad \dot{x} = R \cos(\varphi)\dot{\theta}, \quad \dot{y} = R \sin(\varphi)\dot{\theta}.
\]

\[\Rightarrow\] There are, however, infinitely many systems of “associated” second-order equations (only), whose solution set **contains** the solutions of the nonhol. eq. □

**Examples. [1]** \(\ddot{\theta} = 0, \quad \ddot{\varphi} = 0, \quad \ddot{x} = -R \sin(\varphi)\dot{\theta}\dot{\varphi}, \quad \ddot{y} = R \cos(\varphi)\dot{\theta}\dot{\varphi}.

\[\Rightarrow\] If \(u_\varphi \neq 0\), its solutions are \(\theta(t) = u_\theta t + \theta_0\), \(\varphi(t) = u_\varphi t + \varphi_0\)

\[x(t) = \left(\frac{u_\theta}{u_\varphi}\right) R \sin(\varphi(t)) + u_x t + x_0,
\]

\[y(t) = -\left(\frac{u_\theta}{u_\varphi}\right) R \cos(\varphi(t)) + u_y t + y_0.
\]

\[\Rightarrow\] By restricting to those for which \(\dot{x} = \cos(\varphi)\dot{\theta}\) and \(\dot{y} = \sin(\varphi)\dot{\theta}\) (i.e. \(u_x = u_y = 0\)), we get back the solutions of the non-holonomic eq. (and similarly for solutions with \(u_\varphi = 0\)).
The constraints are $\dot{x} = R \cos(\varphi) \dot{\varphi}$ and $\dot{y} = R \sin(\varphi) \dot{\varphi}$

\[ \begin{align*}
\dot{\varphi} &= 0, & \ddot{x} &= -R \sin(\varphi) \dot{\varphi} \dot{\varphi}, & \ddot{y} &= R \cos(\varphi) \dot{\varphi} \dot{\varphi}. \\
\dot{\varphi} &= 0, & \ddot{x} &= -\frac{\sin(\varphi)}{\cos(\varphi)} \dot{x} \dot{\varphi}, & \ddot{y} &= \frac{\cos(\varphi)}{\sin(\varphi)} \dot{y} \dot{\varphi}. \\
\dot{\varphi} &= 0, & \ddot{x} &= -\dot{y} \dot{\varphi}, & \ddot{y} &= \ddot{x} \dot{\varphi}. \\
\end{align*} \]

[4] Given that $\sin(\varphi) \dot{x} - \cos(\varphi) \dot{y} = 0,$

\[ 
\begin{align*}
J \ddot{\varphi} &= -mR(\sin(\varphi) \dot{x} - \cos(\varphi) \dot{y}) \dot{\varphi}, \\
(I + mR^2) \ddot{\varphi} &= mR(\sin(\varphi) \dot{x} - \cos(\varphi) \dot{y}) \dot{\varphi}, \\
(I + mR^2) \ddot{x} &= -R(I + mR^2) \sin(\varphi) \dot{\varphi} \dot{\varphi} + mR^2 \cos(\varphi)(\sin(\varphi) \dot{x} - \cos(\varphi) \dot{y}) \dot{\varphi}, \\
(I + mR^2) \ddot{y} &= R(I + mR^2) \cos(\varphi) \dot{\varphi} \dot{\varphi} + mR^2 \sin(\varphi)(\sin(\varphi) \dot{x} - \cos(\varphi) \dot{y}) \dot{\varphi}. \\
\end{align*} \]

[5] Many more ....

Is any of these ‘associated’ second-order equations equivalent to the Euler-Lagrange equations of some regular Lagrangian $\tilde{L}$?
Problems. There is **no systematic way** to catalogue the second-order systems that are associated to a nonholonomic system.

If no regular Lagrangian exists for one assoc. system, it may still exist for one of the infinitely many other assoc. systems.

Method. We use techniques developed for the so-called ‘Inverse problem of Lagrangian mechanics’ to answer such questions.
The inverse problem of Lagrangian mechanics

Problem. When are $\ddot{q}^i = f^i(q, \dot{q})$ equivalent to the Euler-Lagrange equations of a (yet to be determined) regular Lagrangian $L$?

$\leadsto$ Find multipliers $g_{ij}(q, \dot{q})$ such that $g_{ij}(\ddot{q}^j - f^j) = \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}^i} \right) - \frac{\partial L}{\partial q^i}$.

Solution. The multipliers must satisfy the Helmholtz conditions

$$\det(g_{ij}) \neq 0, \quad g_{ji} = g_{ij}, \quad \frac{\partial g_{ij}}{\partial \dot{q}^k} = \frac{\partial g_{ik}}{\partial \dot{q}^j},$$

$$\frac{d}{dt}(g_{ij}) - \nabla_j g_{ik} - \nabla_i g_{kj} = 0,$$

$$g_{ik} \Phi^k_j = g_{jk} \Phi^k_i, \quad \nabla^k_j(q, \dot{q}), \Phi^k_j(q, \dot{q}) \text{ made up from derivatives of } f^j.$$

Conversely: if the above has a solution, $\ddot{q}^i = f^i$ is derivable from a Lagrangian.

$\leadsto$ If a Lagrangian exists, then its Hessian w.r.t. fibre coord. $\ddot{q}^i$ is a multiplier!

$\leadsto$ This is a mixed set of algebraic eq. and PDE for $g_{ij}$ (in $2n$-variables $(q^i, \dot{q}^i)$).
Some Lagrangians

[1] There is no regular Lagrangian.

[2] $\tilde{L} = \frac{1}{2} \dot{\phi}^2 + \sqrt{I + mR^2} \left( \frac{\dot{\theta}^2}{\phi} + \frac{\dot{x}^2}{\cos(\phi) \phi} + \frac{\dot{y}^2}{\sin(\phi) \phi} \right)$ and

$\tilde{L} = \frac{1}{2} \dot{\phi}^2 + \frac{1}{2} \dot{\theta}^2 - \frac{\sqrt{I + mR^2}}{2} \left( \frac{\dot{x}^2}{\cos(\phi) \phi} + \frac{\dot{y}^2}{\sin(\phi) \phi} \right)$ are two Lagrangians.

[3] $\tilde{L} = \frac{1}{2} \dot{\phi}^2 + \frac{1}{2} \dot{\theta}^2 \frac{1}{2\phi} \left( (\dot{x}^2 - \dot{y}^2) \cos \varphi + 2 \dot{x} \dot{y} \sin \varphi \right)$ is a regular Lagrangian.

[4] $\tilde{L} = -\frac{1}{2} m (\dot{x}^2 + \dot{y}^2) + \frac{1}{2} I \dot{\theta}^2 + \frac{1}{2} J \dot{\phi}^2 + mR \dot{\theta} (\cos(\varphi) \dot{x} + \sin(\varphi) \dot{y})$ is a regular Lagrangian.
Original motivation


⇝ For some of the well-known classical examples, they propose a Hamiltonian, whose Hamilton equations, when restricted to a certain subset of phase space, reproduce the nonholonomic dynamics.

⇝ Problem: To apply their method one needs to know beforehand the solutions in explicit form!

⇝ Our method (1. Find a regular Lagrangian via the conditions of the Inverse Problem; 2. Use the Legendre transformation to obtain a Hamiltonian) does not depend on knowing the solutions!
Numerical integrators

To compute a numeric approximation of the solution of the nonholonomic system we can use either a nonholonomic integrator for the original Lagrangian and the constraint, or a variational integrator for the new found Lagrangians.

1. For a variational integrator of a system with Lagrangian $\tilde{L}$, one needs to choose a discrete Lagrangian $\tilde{L}_d(q_1, q_2)$ (a function on $Q \times Q$ which resembles as close as possible the continuous Lagrangian).

A solution $q(t)$ is then discretised by an array $q_k$ which are solutions of the so-called discrete Euler-Lagrange equations

$$D_1 \tilde{L}_d(q_k, q_{k+1}) + D_2 \tilde{L}_d(q_{k-1}, q_k) = 0.$$
2. On the other hand, for a **nonholonomic integrator** of a nonholonomic system with Lagrangian $L$ and constraints $a_{\alpha j}(q)\dot{q}^j = 0$, we need to choose both a discrete Lagrangian $L_d$ and a discrete constraint functions $a_{\alpha d}$ on $Q \times Q$.

The nonholonomic discrete equations are

$$D_1 L_d(q_k, q_{k+1}) + D_2 L_d(q_{k-1}, q_k) = \sum_{\beta=1}^{m} (\lambda_k)_{\beta} a_{\beta}(q_k), \quad a_{\alpha}(q_k, q_{k+1}) = 0.$$ 

Usually one takes the discretization as (for certain $\epsilon$ and certain $h$):

$$L_d(q_1, q_2) = L\left( q = (1 - \epsilon)q_1 + \epsilon q_2, \dot{q} = \frac{q_2 - q_1}{h} \right),$$

$$a_{\alpha}(q_1, q_2) = a_{\alpha i}(q = (1 - \epsilon)q_1 + \epsilon q_2) \frac{q_2^i - q_1^i}{h}.$$ 

It seems reasonable that if a free Lagrangian for the nonholonomic system exists, the Lagrangian integrator may perform better than a nonholonomic integrator with badly chosen discrete constraints.
The vertically rolling disk

A solution with a variational integrator and nonholonomic integrator with $\epsilon = 0$.

The conservation of the (continuous) energy.

The (discrete) constraints are preserved for both the nonholonomic integrator (by construction) and for the variational integrator (by theorem).
solution with $\epsilon = 1/3$  solution with $\epsilon = 1/2$  solution with $\epsilon = 1$
The nonholonomic particle

The nonholonomic Lagrangian and the constraint are

\[ L = \frac{1}{2}(\dot{x}^2 + \dot{y}^2 + \dot{z}^2) \quad \text{and} \quad \dot{z} + x\dot{y} = 0. \]

The function

\[ \tilde{L} = \frac{1}{2}\dot{x}^2 + \frac{\sqrt{1 + x^2}}{2} \left( \frac{\dot{y}^2}{\dot{x}} + \frac{\dot{z}^2}{x\ddot{x}} \right) \]

is a Lagrangian for an ‘associated’ system.
$xy$-solution with $\epsilon = 0$

$xy$-solution with $\epsilon = 1/5$

$xy$-solution with $\epsilon = 1/3$

$xy$-solution with $\epsilon = 1/2$

$xy$-solution with $\epsilon = 2/3$

$xy$-solution with $\epsilon = 4/5$