Concepts and Algorithms of Scientific and Visual Computing

–Variational Principles–

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Variational Principles

The simulation of natural phenomena requires an accurate mathematical model of the underlying physics, usually given by the equations of motion. Deriving such differential equations for complex systems is often hard using the approaches of traditional Newtonian physics.

A different view is given by Hamilton's principle:

Nature selects from all possible behaviors of a mechanical system, that one which leads to an extremal well-defined action.

An example is given by Fermat's law:

The path between two points taken by a light ray, is always the one which can be traversed in the least time.

Variational Principles

More specifically, let $(q, \dot{q})^{\mathsf{T}} \in \mathcal{V}$ describe the configuration of a mechanical system with one degree of freedom in the time interval $[t_i, t_f] \subseteq \mathbb{R}$. Furthermore, let T be the kinetic energy and V the overall potential. The corresponding so-called Lagrangian L is defined by

$$L(q(t), \dot{q}(t), t) := T(q(t), \dot{q}(t), t) - V(q(t), \dot{q}(t), t).$$

Hamilton's principle states, that nature selects from all possible mappings

$$[t_i, t_f] \ni t \mapsto (q(t), \dot{q}(t)) \in \mathcal{V} \subseteq \mathbb{R}^2$$

that one, which makes the action S extremal, i.e.

$$S[q] := \int_{t_i}^{t_f} L(q(t), \dot{q}(t), t)\, \mathrm{d}t \to \mathrm{ext}.$$

Furthermore, we assume, that the solution q is continuously differentiable:

"Natura non facit saltus."

Variational Principles

Hamilton principle can be transformed into an ordinary differential equation, whose solution minimizes S. We will derive the so-called Euler-Lagrange equation using calculus of variations.

For that, we assume, that the optimal solution q is known and create a family of continuously differentiable curves

$$\tilde{q}(t, \epsilon) = q(t) + \epsilon\alpha(t)$$

using an arbitrary function

$$[t_i, t_f] \ni t \mapsto \alpha(t) \in \mathbb{R}$$

with fix boundary values

$$\alpha(t_i) = \alpha(t_f) = 0$$

and $\epsilon \in \mathbb{R}$.

Variational Principles

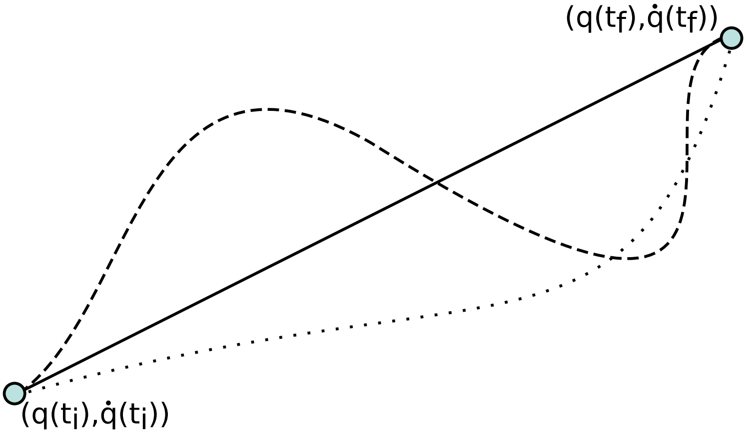


Figure : Illustration of the curve $t \mapsto (q(t), \dot{q}(t))$ as a straight line and possible variations.

Variational Principles

We define

$$S_\alpha(\epsilon) := \int_{t_i}^{t_f} L(\tilde{q}(t), \dot{\tilde{q}}(t), t)\,\mathrm{d}t,$$

which is called the variation of S. The curve q makes S extremal if and only if the integrals $S_\alpha(\epsilon)$ for all continuously differentiable functions α have an extrema at $\epsilon = 0$. Hence it is necessary, that

$$\mathrm{d}_\epsilon S_\alpha(\epsilon) = \int_{t_i}^{t_f} \Big(\partial_{\tilde{q}}(L)\,\alpha(t) + \partial_{\dot{\tilde{q}}}(L)\,\dot{\alpha}(t)\Big)\,\mathrm{d}t \stackrel{!}{=} 0.$$

for $\epsilon = 0$. Partial integration of the second summand of the integrand leads to

$$\begin{aligned} \mathrm{d}_\epsilon S_\alpha(\epsilon) \quad &= \quad \int_{t_i}^{t_f} \partial_{\tilde{q}}(L)\,\alpha(t)\,\mathrm{d}t + \Big[\partial_{\dot{\tilde{q}}}(L)\,\alpha(t)\,\mathrm{d}t\Big]_{t=t_i}^{t=t_f} \\ &- \quad \int_{t_i}^{t_f} \mathrm{d}_t\Big(\partial_{\dot{\tilde{q}}} L\Big)\,\alpha(t)\,\mathrm{d}t = 0. \end{aligned}$$

Because of $\alpha(t_i) = \alpha(t_f) = 0$, the second summand vanishes.

Variational Principles

The results can be expressed by

$$\mathrm{d}_\epsilon S_\alpha(\epsilon) = \int_{t_i}^{t_f} \left(\partial_{\tilde{q}}(L) - \mathrm{d}_t\left(\partial_{\dot{\tilde{q}}} L\right)\right)\alpha(t)\,\mathrm{d}t = 0$$

for $\epsilon = 0$. Since this has to be fulfilled for all possible functions α, the integral vanishes, if and only if the left factor of the integrand is identical zero (fundamental lemma of variational calculus). This leads with $\epsilon = 0$ to the Euler-Lagrange equation

$$\partial_q(L) - \mathrm{d}_t\left(\partial_{\dot{q}} L\right) = 0.$$

The left part is usually denoted as the Euler-Lagrange derivative

$$\delta_q L := \partial_q(L) - \mathrm{d}_t(\partial_{\dot{q}} L)$$

which simplifies the Euler-Lagrange equation to $\delta_q L = 0$.

Example: Double Pendulum

The functional S can be minimized in a similar way for a vector-valued function $\mathbf{q}$.

We illustrate this using the concrete example of a double pendulum with

$$2N - k = 2 \cdot 2 - 2 = 2 \text{ degrees of freedom.}$$

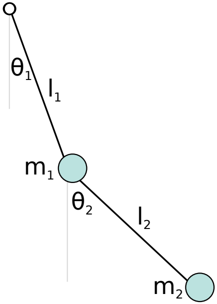
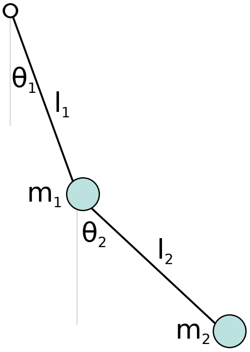


Figure : Double pendulum with particle masses m_1, m_2 and stiff rods with lengths l_1, l_2.

Example: Double Pendulum

We introduce generalized coordinates θ_1, θ_2 and velocities $\dot{\theta}_1, \dot{\theta}_2$, so that the Cartesian coordinates can be expressed as follows:

$$
\begin{aligned}
x1 &= l_1 \sin \theta_1, \\
y1 &= -l_1 \cos \theta_1, \\
x2 &= l_1 \sin \theta_1 + l_2 \sin \theta_2, \\
y2 &= -l_1 \cos \theta_1 - l_2 \cos \theta_2.
\end{aligned}
$$



Example: Double Pendulum

Therefore the kinetic energy is given by

$$
\begin{aligned}
T(\theta_1, \theta_2, \dot{\theta}_1, \dot{\theta}_2) &= \frac{1}{2} m_1 (\dot{x}_1^2 + \dot{y}_1^2) + \frac{1}{2} m_1 (\dot{x}_2^2 + \dot{y}_2^2) \\
&= \frac{1}{2} m_1 l_1^2 \dot{\theta}_1^2 + \frac{1}{2} m_2 \Big(l_1^2 \dot{\theta}_1^2 + l_2^2 \dot{\theta}_2^2 + 2 l_1 l_2 \dot{\theta}_1 \dot{\theta}_2 \cos(\theta_1 - \theta_2) \Big)
\end{aligned}
$$

and the potential by

$$
\begin{aligned}
V(\theta_1, \theta_2) &= m_1 g y_1 + m_2 g y_2 \\
&= -(m_1 + m_2) g l_1 \cos\theta_1 - m_2 g l_2 \cos\theta_2
\end{aligned}
$$

leading to the Lagrangian

$$
\begin{aligned}
L(\theta_1, \theta_2, \dot{\theta}_1, \dot{\theta}_2) &= T(\theta_1, \theta_2, \dot{\theta}_1, \dot{\theta}_2) - V(\theta_1, \theta_2) \\
&= \frac{1}{2} (m_1 + m_2) l_1^2 \dot{\theta}_1^2 + \frac{1}{2} m_2 l_2^2 \dot{\theta}_2^2 + m_2 l_1 l_2 \dot{\theta}_1 \dot{\theta}_2 \cos(\theta_1 - \theta_2) \\
&\quad + (m_1 + m_2) g l_1 \cos\theta_1 + m_2 g l_2 \cos\theta_2 .
\end{aligned}
$$

Example: Double Pendulum

For θ_1, this leads to

$$\begin{aligned}
\partial_{\dot\theta_1} L &= (m_1+m_2) l_1^2 \dot\theta_1 + m_2 l_1 l_2 \dot\theta_2 \cos(\theta_1-\theta_2), \\
\mathrm{d}_t \partial_{\dot\theta_1} L &= (m_1+m_2) l_1^2 \ddot\theta_1 + m_2 l_1 l_2 \ddot\theta_2 \cos(\theta_1-\theta_2) - m_2 l_1 l_2 \dot\theta_2 \sin(\theta_1-\theta_2)(\dot\theta_1-\dot\theta_2), \\
\partial_{\theta_1} L &= -l_1 g (m_1+m_2) \sin\theta_1 - m_2 l_1 l_2 \dot\theta_1 \dot\theta_2 \sin(\theta_1-\theta_2)
\end{aligned}$$

and the equation of motion

$$(m_1+m_2) l_1 \ddot\theta_1 + m_2 l_2 \ddot\theta_2 \cos(\theta_1-\theta_2) + m_2 l_2 \dot\theta_2^2 \sin(\theta_1-\theta_2) + g(m_1+m_2)\sin\theta_1 = 0.$$

Similarly, for θ_2 we finally obtain

$$m_2 l_2 \ddot\theta_2 + m_2 l_1 \ddot\theta_1 \cos(\theta_1-\theta_2) - m_2 l_1 \dot\theta_1^2 \sin(\theta_1-\theta_2) + m_2 g \sin\theta_2 = 0.$$