Concepts and Algorithms of Scientific and Visual Computing

–Symplecticity–

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Hamiltonian vs. Total Energy

From the homogeneity of time follows, that the Lagrangian of an isolated system is not explicitly dependent on time and therefore

$$\partial_t H = -\partial_t L = 0.$$

Furthermore for potentials, which are independent from the velocity, it follows by calculation that

$$H = T + V.$$

Hence for isolated systems, the Hamiltonian corresponds to the total energy and is a conserved quantity. There is a deep connection between such characteristics of Hamiltonian systems and their underlying geometry in the phase space.

Hamiltonian Flow and Symplectic Mapping

The flow of a Hamiltonian system is defined by the mapping $\varphi_t : \mathcal{U} \to \mathbb{R}^{6N}$, which maps $\mathbf{U}_0$ to $\varphi_t(\mathbf{U}_0) := \mathbf{U}(t)$ if and only if $\mathbf{U}_0 = \mathbf{U}(t_0)$.

A differentiable mapping $\mathbf{g} : \mathcal{U} \to \mathbb{R}^{6N}$ acting on an open subset $\mathcal{U} \subseteq \mathbb{R}^{6N}$ is called symplectic if and only if

$$\omega(\mathbf{g}'(\mathbf{U})\boldsymbol{\xi}, \mathbf{g}'(\mathbf{U})\boldsymbol{\mu}) = \omega(\boldsymbol{\xi}, \boldsymbol{\mu})$$

holds for all $\boldsymbol{\xi}, \boldsymbol{\mu} \in \mathbb{R}^{6N}$.

Here, $\mathbf{g}'$ denotes the Jacobian of $\mathbf{g}$, whereas the mapping $\omega : \mathbb{R}^{6N} \to \mathbb{R}^{6N}$ maps the pair $(\boldsymbol{\xi}, \boldsymbol{\mu})$ to

$$\omega(\boldsymbol{\xi}, \boldsymbol{\mu}) := \boldsymbol{\xi}^{\mathsf{T}} \mathbf{J} \boldsymbol{\mu}$$

with $\mathbf{J} := \operatorname{adiag}(\mathbf{1}, -\mathbf{1})$.[1]

[1] To motivate the definition of ω, consider a single particle moving in the one-dimensional space $\mathbb{R}$. Let $\boldsymbol{\xi}, \boldsymbol{\mu} \in \mathcal{U}$ be two-dimensional vectors of the phase space $\mathcal{U} \subseteq \mathbb{R}^2$. The area of the parallelogram spanned by $\boldsymbol{\xi}$ and $\boldsymbol{\mu}$ is given by $\det(\boldsymbol{\xi}, \boldsymbol{\mu}) = \boldsymbol{\xi}^{\mathsf{T}} \mathbf{J} \boldsymbol{\mu} = \omega(\boldsymbol{\xi}, \boldsymbol{\mu})$.

Symplectic Mapping

One can think about a symplectic mapping as one which preserves the structure of the phase space in the sense that it preserves the surface areas resulting from the projections onto planes of momenta and positions.

In order to make this statement clear, consider a two-dimensional submanifold M of a set $\mathcal{U} \subseteq \mathbb{R}^2$ given by the image $M = \zeta(C)$ of a compact set $C \subseteq \mathbb{R}^2$ under a continuous differentiable function $\zeta : \mathbb{R}^2 \to \mathbb{R}^2$.

One can regard M as the limit of the unions of the parallelograms, which are spanned by the vectors $\partial_p \zeta(p,q)\,\mathrm{d}p$ and $\partial_q \zeta(p,q)\,\mathrm{d}q$ with areas $\omega(\partial_p \zeta(p,q)\,\mathrm{d}p, \partial_q \zeta(p,q)\,\mathrm{d}q)$.

Symplectic Mapping

Integration over all parallelograms leads to the area

$$\Omega(M) = \int_{\mathbf{C}} \omega\Big(\partial_p \zeta(p,q), \partial_q \zeta(p,q)\Big)\, \mathrm{d}p\, \mathrm{d}q \tag{1}$$

of the whole surface of M. After applying a mapping $\mathbf{g} : \mathcal{U} \to \mathbb{R}^2$ on M, the surface area reads

$$\Omega(\mathbf{g}(M)) = \int_{\mathbf{C}} \omega\Big(\partial_p (\mathbf{g} \circ \zeta)(p,q), \partial_q (\mathbf{g} \circ \zeta)(p,q)\Big)\, \mathrm{d}p\, \mathrm{d}q. \tag{2}$$

With $(\mathbf{g} \circ \zeta)'(p,q) = (\mathbf{g}' \circ \zeta)(p,q)\, \zeta'(p,q)$, it can be easily proven that the integrands in Eq. (1) and Eq. (2) are equal and hence

$$\Omega(\mathbf{g}(M)) = \Omega(M)$$

holds if and only if $\mathbf{g}$ is symplectic.

Symplectic Mapping

Furthermore, it can also be proven that for each fixed $t \in \mathbb{R}_{\geq 0}$, the flow φ_t of a Hamiltonian system is a symplectic transformation.

This statement was proved by J. Henri Poincaré in the 19th century, if the Hamiltonian is twice continuously differentiable. It follows for the case $t = 0$ directly and for all $t \in \mathbb{R}_{>0}$ by calculation with

$$\mathrm{d}_t \omega \left(\partial_{\mathbf{U}_0} \varphi_t(\mathbf{U}_0), \partial_{\mathbf{U}_0} \varphi_t(\mathbf{U}_0) \right) = 0$$

using the fact, that

$$\partial_{\mathbf{U}_0} \varphi_t(\mathbf{U}_0)$$

is a solution of the variational equation

$$\mathbf{J}\dot{\mathbf{V}} = \nabla^2 H(\varphi_t(\mathbf{U}_0))\mathbf{V}.$$

Symplectic Mapping

Conversely, it can be shown that a system is locally Hamiltonian if its flow is symplectic.

A system $\mathbf{U} = \mathbf{F}(\mathbf{U})$ is called locally Hamiltonian if and only if for every $\mathbf{U}_0 \in \mathcal{U}$ there exists a neighborhood with

$$\mathbf{F}(\mathbf{U}) = \mathbf{J}^{-1} \nabla H(\mathbf{U})$$

for some analytical function H.

Moreover, the set of all Hamiltonian systems is closed under transformations of coordinates with symplectic functions, and every function which maps a Hamiltonian system to a Hamiltonian system is symplectic. Therefore, the notions of canonical transformations and symplectic transformations are equivalent.

This is known as Theorem X proven by Carl G. Jacobi in the 19th century.

Symplectic Integrators

Therefore it is evident that integration methods for Hamiltonian systems, which are structure preserving in the sense of symplecticity, are naturally of special interest.

By definition, an integration method is symplectic if and only if the discrete flow

$$\Phi_{\Delta t} : \mathbf{U}_0 = \mathbf{U}(t_0) \mapsto \mathbf{U}_1 \approx \mathbf{U}(\Delta t)$$

with fixed temporal step size Δt is symplectic.

Such methods accurately preserve linear and angular momentum, and energy does not drift, but oscillates instead around the initial energy.

Of course, the intensity of this oscillations depends on the temporal step size Δt used for the integration.

Variational Integrators

A popular way for the construction of symplectic integration algorithms is based on the assumption, that if the numerical method optimizes a discrete trajectory, then it will have similar geometric properties.

The key idea here is a discrete treatment of the traditional continuous models. For that we define a discrete analog of the Lagrangian given by

$$L^d(q_n, q_{n+1}) \approx \int_{t_n}^{t_{n+1}} L(q, \dot{q}) \mathrm{d}t,$$

which can be approximated with the use of an appropriate quadrature rule.

Similarly, a discrete version of Hamilton's principle is given by

$$S^d(n') = \sum_{n=0}^{n'-1} L^d(q_n, q_{n+1}) \xrightarrow{!} \text{ext.}$$

Variational Integrators

As in the continuous case we carry out a variation of S^d with constant q_0 and q_N and obtain

$$\begin{aligned} \mathrm{d}S^d &= \mathrm{d}\sum_{n=0}^{n'-1} L^d(q_n, q_{n+1}) \\ &= \sum_{n=0}^{n'-1} \Big(\mathcal{D}_{q_n} L^d(q_n, q_{n+1}) \mathrm{d}q_n + \mathcal{D}_{q_{n+1}} L^d(q_n, q_{n+1}) \mathrm{d}q_{n+1} \Big) \\ &= \sum_{n=1}^{n'-1} \Big(\mathcal{D}_{q_n} \Big(L^d(q_n, q_{n+1}) + L^d(q_{n-1}, q_n) \Big) \mathrm{d}q_n \Big) \stackrel{!}{=} 0, \end{aligned}$$

so that the discrete Euler-Lagrange equation is then given by

$$\mathcal{D}_{q_n} \Big(L^d(q_n, q_{n+1}) + L^d(q_{n-1}, q_n) \Big) = 0.$$

Variational Integrators

Applying the Legendre transformation

$$p_{n+1} = \mathcal{D}_{q_{n+1}} L^d(q_n, q_{n+1})$$

leads to the so-called right discrete Hamiltonian

$$H^d_+(q_n, p_{n+1}) = p_{n+1} q_{n+1} - L^d(q_n, q_{n+1})$$

and the corresponding right discrete canonical equations

$$q_{n+1} = \mathcal{D}_{p_{n+1}} H^d_+(q_n, p_{n+1}), \quad p_n = \mathcal{D}_{q_n} H^d_+(q_n, p_{n+1}).$$

Variational Integrators

Similarly the application of the Legendre transformation

$$p_n = -\mathcal{D}_{q_n} L^d(q_n, q_{n+1})$$

leads to the so-called left discrete Hamiltonian

$$H^d_-(p_n, q_{n+1}) = -p_n q_n - L^d(q_n, q_{n+1})$$

and the corresponding left discrete canonical equations

$$q_n = -\mathcal{D}_{p_n} H^d_-(p_n, q_{n+1}), \quad p_{n+1} = -\mathcal{D}_{q_{n+1}} H^d_-(p_n, q_{n+1}).$$

Variational Integrators

The discrete Euler-Lagrange formalism and the discrete Hamilton formalism are defined analogously to their continuous counterparts and can be extended to higher dimensions in a similar way.

The application of the first one leads to a two-step method

$$(q_{n-1}, q_n) \mapsto q_{n+1}$$

analogously to the second-order continuous Euler-Lagrange equation, whereas applying the latter one leads to a one-step method

$$(q_n, p_n) \mapsto (q_{n+1}, p_{n+1})$$

analogously to the first-order continuous canonical equations. Both resulting systems of recurrence equations are equivalent and can be easily transformed into each other.

Variational Integrators

We will illustrate their application for the simple scenario of a free particle with mass m in a gravitation field with gravity constant g.

Its continuous Lagrangian is given by

$$L(q, \dot{q}) = \frac{m}{2}\dot{q}^2 - mgq$$

which leads to the equation of motion $\ddot{q} = -g$. In the discrete case, the application of the midpoint quadrature rule leads to the discrete Lagrangian

$$L^d(q_n, q_{n+1}) = \Delta t \left(\frac{m}{2} \left(\frac{q_{n+1} - q_n}{\Delta t} \right)^2 - mg \frac{q_n + q_{n+1}}{2} \right).$$

Substitution into the discrete Euler-Lagrange equation leads to the two-step recurrence scheme

$$\frac{q_{n+1} - 2q_n + q_{n-1}}{\Delta t^2} = -g,$$

which corresponds to the well-known second-order central difference quotient.