Generating functions for variational integrators

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Symplectic vector spaces

V a real vector space, $\dim V = 2d$.

Definition (Symplectic form)

It is a skew-symmetric non-degenerate bilinear form $< .,. >$ on V.

Example (Position-momenta phase space)

X any vector space, $V = X \times X^*$, $< (a_1, a_2), (b_1, b_2) >= b_2(a_1) - a_2(b_1)$.

Set $J = \begin{pmatrix} 0_{d\times d} & I_d \\ -I_d & 0_{d\times d} \end{pmatrix}$ its matrix: $< a, b >= a^T \cdot J \cdot b$.

Example (Graph of a map $V \to V$)

(V, J) symplectic vector space $\Rightarrow (V \times \overline{V}, J \times -J)$ again symplectic.

Definition (Symplectomorphism $\phi\colon (V_1, < .,. >_1) \to (V_2, < .,. >_2)$)

It is a linear map $\phi\colon V_1 \to V_2$ s.t. $\forall a, b \in V_1, < \phi(a), \phi(b) >_2 = < a, b >_1$.

Proposition (Symplectomorphy)

$$X \times X \times (X \times X)^* \simeq X \times X^* \times \overline{X \times X^*}$$

Lagrangian subspaces, В. И. Арнольд[1], 1967

Definition

A Lagrangian subspace L of $(V, <.,.>)$ is a vector subspace that is isotropic and of dimension d.

Example ($V = X \times X^*$, generating functions)

- $L = X \times \{0_{X^*}\}$
- $L = \{(x, \Psi(x)) \in X \times X^*, x \in X\}$, $\Psi \colon X \to X^*$ symmetric.

Example ($V \times \overline{V}$, symplectomorphisms)

- the diagonal $L = \{(v, v) \in V \times V, v \in V\}$
- $L = \{(v, \phi(v)) \in V \times V\}$, $\phi \colon (V, <.,.>) \to (V, <.,.>)$.

Remark (Hamiltonian dynamics = generating functions)

Those examples relate to one another through the symplectomorphy (1).

[1] Characteristic class entering in quantization condition, Arnol'd, 1967

Newton's second law, 1687

$(F_i)_i \colon \mathbb{R}^d \to \mathbb{R}^d$ a force admitting a potential $V \colon \mathbb{R}^d \to \mathbb{R}$ and $m > 0$ the mass of the particule.

$$
\begin{aligned}
m\ddot{q}_i = F_i(q_1, \ldots, q_d) &\Leftrightarrow \dot{\begin{pmatrix} q \\ v \end{pmatrix}} = \begin{pmatrix} v \\ \frac{1}{m}\nabla V(q) \end{pmatrix} \\
&\Leftrightarrow \dot{\begin{pmatrix} q \\ p \end{pmatrix}} = \begin{pmatrix} \frac{p}{m} \\ \nabla V(q) \end{pmatrix} \\
&\Leftrightarrow \dot{x} = J \cdot \nabla_x H
\end{aligned} \tag{1}
$$

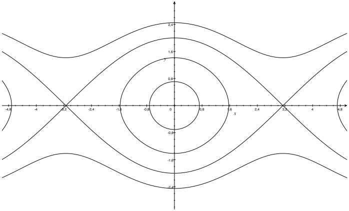
where

- $x = (q, p) \in \mathbb{R}^d \times (\mathbb{R}^d)^*$ a point of the phase space,
- $J = \begin{pmatrix} 0_{d\times d} & Id \\ -Id & 0_{d\times d} \end{pmatrix}$ is the symplectic form,
- $H(q, p) = \frac{1}{2m} \sum_{i=1}^{d} p_i^2 - V(q)$ the Hamiltonian.

Symplecticity

Proposition (Energy conservation)

$$\frac{\partial}{\partial t} H(q(t), p(t)) = 0.$$



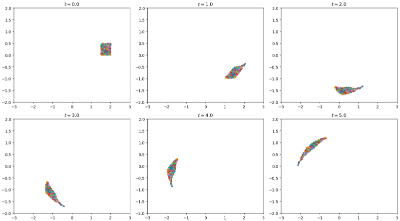
Phase plan of $\ddot{q} = -\frac{g}{L} sin(q)$
$H(q,p) = \frac{p^2}{2mL^2} + mgL(1 - \cos q)$

$$\phi_t^H : \begin{array}{ccc} \mathbb{R}^d \times (\mathbb{R}^d)^* & \rightarrow & \mathbb{R}^d \times (\mathbb{R}^d)^* \\ (q(0), p(0)) & \mapsto & ((q(t), p(t)) \end{array}$$

Proposition

Any Hamiltonian flow is symplectic:

$$Jac(\phi_t^H)^T \cdot J \cdot Jac(\phi_t^H) = J$$



$d = 1$: volume preservation

source : furnstahl.github.io

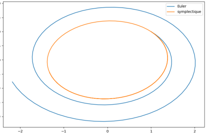
Symplectic integrators

Definition (An integrator)

It is a family $\varphi_{\Delta t}: x_n \mapsto x_{n+1}$ parametrized by the time-step Δt.
$\varphi_{\Delta t}$ is symplectic if $\mathbf{Jac}(\varphi_{\Delta t})^T \cdot J \cdot \mathbf{Jac}(\varphi_{\Delta t}) = J$.

Example (Symplectic Euler method, DeVogelaere, 1956)

$$\begin{pmatrix} q_{n+1} \\ p_{n+1} \end{pmatrix} = \begin{pmatrix} q_n + \Delta t \frac{\partial H}{\partial p}(q_n, p_{n+1}) \\ p_n - \Delta t \frac{\partial H}{\partial q}(q_n, p_{n+1}) \end{pmatrix}$$



$H(q,p) = \frac{p^2+q^2}{2}$,
$\Delta t = 0.1$, $n = 100$ itérations

Theorem (Quasi-first integral, Benettin et Giorgilli, 1994)

Under some assumptions, $\exists (H_\epsilon)_\epsilon$, $C > 0$, $\epsilon^* > 0$ *s.t.*

$$\forall n \in \mathbb{N}, \forall \epsilon < \epsilon^*, \ |H_\epsilon(\varphi_\epsilon^n(q,p)) - H_\epsilon(q,p)| \leq C n \epsilon \exp\left(-\frac{\epsilon^*}{\epsilon}\right) \qquad (2)$$

Euler-Lagrange equations, $1750's$

Starting again from Newtonian mechanics (1):

$$m\ddot{q}_i = F_i(q_1, \dots, q_d) \Leftrightarrow \dot{\begin{pmatrix} q \\ v \end{pmatrix}} = \begin{pmatrix} v \\ \frac{1}{m}\nabla V(q) \end{pmatrix}$$
$$\Leftrightarrow \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial v} = \frac{\partial L}{\partial q}$$
$$\Leftrightarrow \delta \int L = 0$$

where

- (q, v) position and velocity of the particule,
- $L(q, v) = \frac{1}{2m}\sum_{i=1}^{d} v_i^2 + V(q)$ the Lagrangian.

Generating functions

Definition (The action)

$$S_t : \begin{array}{ccc} \mathbb{R}^d \times \mathbb{R}^d & \to & \mathbb{R} \\ (q_0, q_1) & \mapsto & \int_0^t L(q(s), \dot{q}(s)) \mathrm{d}s \end{array} \tag{3}$$

where $s \in [0, t] \mapsto q(s)$ the extremal path s.t. $\left\{ \begin{array}{ll} q(0) & = q_0, \\ q(t) & = q_1 \end{array} \right.$.

Remark

t is small, q_1 close to q_0.

The graph of the generating function (3) is the graph of the Hamiltonian flow !

$$\begin{array}{ccccc} \mathrm{Graph}(dS_t) & \mapsto & & \mathrm{Graph}(\phi_t^H) & \\ \cap & & & \cap & \\ T^*(\mathbb{R}^d \times \mathbb{R}^d) & \tilde{\rightarrow} & T^*\mathbb{R}^d & \times & T^*\mathbb{R}^d \\ (q_0, q_1, \frac{\partial S_t}{\partial q_0}(q_0, q_1), \frac{\partial S_t}{\partial q_1}(q_0, q_1)) & \mapsto & (q_0, p_0), & & \phi_t^H(q_0, p_0) \end{array}$$

Variational integrators[2]

Discretize S_t:

$$\int_0^t L(q(s), \dot{q}(s))\mathrm{d}s \approx \int_0^t L(q_0, \frac{q_1 - q_0}{t})\mathrm{d}s$$

and obtain the discrete action

$$\hat{S}_t \colon (q_0, q_1) \mapsto tL(q_0, \frac{q_1 - q_0}{t}).$$

Then, start from, e.g, (q_0, q_1) and iterate:

$$\begin{aligned} p_0 = & \quad \partial_1 \hat{S}_t(q_0, q_1) & \\ p_1 = & \quad \partial_2 \hat{S}_t(q_0, q_1) & = \partial_1 \hat{S}_t(q_1, q_2) \\ & \dots & \end{aligned} \tag{4}$$

Symplectic tools $\Rightarrow$ the numerical method (4) has the same stability theory than with symplectic integrators, estimates (2) etc...

[2] Discrete mechanics and variational integrators, Marsden and West, 2001

Composition of Lagrangian spaces and consequences

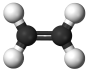
Hamiltonian flows	$\phi^{H_3} = \phi^{H_1} \circ \phi^{H_2}$
Trajectories	Concatenation of paths
Generating functions	$S_3(q_0, q_2) = \underset{q_1}{\text{extr}}\big(S_1(q_0, q_1) + S_2(q_1, q_2)\big)$

Composition of Lagrangian spaces in mechanics

$\Rightarrow$ **This provides a geometric framework towards:**

Symplectic multi-step methods:

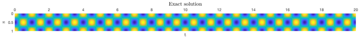
- vibration of molecules
- delayed ODEs



Ethylene
fig.: Wikipedia

Variational integrators for field theories:

- wave equation,
- Poisson equation,
- Geometrically exact beam theory on $SO(3)$



An oscillation mode of the wave equation
fig.: R. Sato

Multisymplectic Hamiltonian variational integrators, Tran, Leok, 2021
Special Symplectic Spaces, Tulczyjew, Lawruk, 1975

Conclusion and perspectives

- Hamiltonian and variational structures of an equation provide time discretizations with long run stability and large time steps.
- For continuous media, the study of those structure is a prerequisite to the use of such methods.

Symplectic methods in beam theory with L. Le Marrec, V. Carlier, A. Patel :

- *Timoshenko beam under finite and dynamic transformations: Lagrangian coordinates and Hamiltonian structures*, C., Le Marrec, CAM, 2025
- ongoing: energetic exchanges between vibration modes and study of bifurcations

Variational integrators for field theories with S. Leyendecker, D. M. de Diego, R. Sato, T. Wang :

- ongoing: boundary Lagrangians and application to field theories