Discretization of contact Hamiltonian systems using Herglotz' variational principle

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Contact geometry

$(2n+1)$-dimensional manifold M.

Contact structure

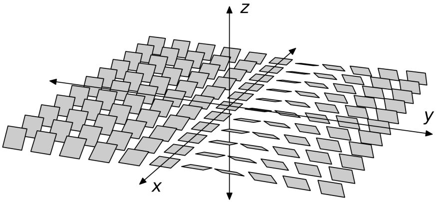
A distribution of hyperplanes $\xi \subset TM$ that is maximally non-integrable: a submanifold that is always tangent to the distribution has dimension at most n.

Locally, such a distribution is given by the kernel of a 1-form η satisfying

$$\eta \wedge (\mathrm{d}\eta)^n \neq 0,$$

called a contact form.

Multiplying η by a non-vanishing function does not change the contact structure.



$\mathrm{d}z - y\mathrm{d}x$

$f : M \to M$ is a contact transformation if $f^*\eta = g\eta$ for some $g : M \to \mathbb{R}$.

Contact geometry

There exist Darboux local coordinates $(x_1, \dots, x_n, p_1, \dots, p_n, z)$ such that the contact 1-form can be written as

$$\eta = \mathrm{d}z - p\,\mathrm{d}x \qquad = \mathrm{d}z - \sum_i p_i\,\mathrm{d}x_i.$$

Contact Hamiltonian vector field

$$\mathcal{L}_{X_H}\eta = f_H \eta \qquad \text{and} \qquad \eta(X_H) = -H,$$

where $\mathcal{L}$ is the Lie derivative and $f_H : M \to \mathbb{R}$.
(In terms of the Reeb vector field, $f_H = -R_\eta(H)$.)

For comparison with symplectic mechanics, note that

$$\iota_{X_H}(\mathrm{d}\eta) = -\mathrm{d}(\iota_{X_H}\eta) + \mathcal{L}_X \eta = \mathrm{d}H + f_H \eta.$$

In Darboux coordinates the contact Hamiltonian equations are

$$\dot{x} = \frac{\partial H}{\partial p}, \qquad \dot{p} = -\frac{\partial H}{\partial x} - p\frac{\partial H}{\partial z}, \qquad \dot{z} = p\frac{\partial H}{\partial p} - H.$$

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Damped mechanical systems

Contact Hamiltonian systems satisfy

$$\frac{\mathrm{d}H}{\mathrm{d}t} = -H\frac{\partial H}{\partial z}$$

so dissipation can occur!

Example. A Hamiltonian of the form

$$H = \frac{1}{2}p^2 + V(x) + \alpha z$$

describes a mechanical system with linear damping:

$$\begin{cases} \dot{x} = p \\ \dot{p} = -V'(x) - \alpha p \\ \dot{z} = p^2 - H. \end{cases}$$

Written as a second order ODE:

$$\ddot{x} = -V'(x) - \alpha \dot{x}.$$

The physical meaning of z will be discussed later.

Contact geometry in thermodynamics

First law for of thermodynamics can be written as

$$\mathrm{d}U - T\mathrm{d}S + P\mathrm{d}V - \mu\mathrm{d}N = 0$$

i.e. states are constrained within a manifold with tangent spaces in the kernel of

$$\eta = \mathrm{d}U - T\mathrm{d}S + P\mathrm{d}V - \mu\mathrm{d}N$$

Various thermodynamical process can be written as Hamiltonian flows with respect to the contact structure defined by η.

[Mrugała, Nulton, Schön, Salamon. Contact structure in thermodynamic theory. Rep. Math. Phys. 1991]

[Bravetti. Contact Hamiltonian dynamics: the concept and its use. Entropy, 2017]

Contact geometry in integrable systems

Background: symplectic Hamiltonian vector fields and integrable $(2+1)$-dimensional PDEs.

Integrable PDEs of "hydrodynamic type" (aka "dispersionless")

$$A(u)u_x + B(u)u_y + D(u)u_t = 0$$

have several kinds of Lax pairs:

- Non-linear: compatibility of

$$\psi_y = F(\psi_x, u) \quad \text{and} \quad \psi_t = G(\psi_x, u)$$

- Linear non-isospectral: compatibility of

$$\psi_y = X_f \psi \quad \text{and} \quad \psi_t = X_g \psi$$

  Where X_f, X_g denote the (symplectic) Hamiltonian vector fields of $f(x, p)$ and $g(x, p)$ (related to F and G) and p is a spectral parameter.

Contact geometry in integrable systems

This can be generalized to $(3+1)$-dimensional PDEs

$$A(u)u_x + B(u)u_y + C(u)u_z + D(u)u_t = 0.$$

But then we need Hamiltonian vector field in a 3-dimensional space.

- Non-linear Lax pair: compatibility of

$$\psi_y = \psi_z F(\psi_x/\psi_z, u) \quad \text{and} \quad \psi_t = \psi_z G(\psi_x/\psi_z, u)$$

- Linear non-isospectral Lax pair: compatibility of

$$\psi_y = X_f \psi \quad \text{and} \quad \psi_t = X_g \psi$$

  Where X_f, X_g denote the contact Hamiltonian vector fields of $f(x, p, z)$ and $g(x, p, z)$ and p is a spectral parameter.

Hence $(3+1)$-dimensional integrable PDEs can be found by looking for suitable contact Hamiltonian functions f and g.

[Sergyeyev. New integrable $(3+1)$-dimensional systems and contact geometry. Letters in Mathematical Physics, 2018.]

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Herglotz' variational principle

The contact Hamiltonian equation for z is

$$\dot{z} = p\frac{\partial H}{\partial p} - H \qquad \stackrel{?}{=} \mathcal{L}$$

Herglotz' variational principle

Lagrangian $\mathcal{L} : TQ \times \mathbb{R} \to \mathbb{R}$.
Given a curve $x : [0, T] \to Q$, define $z : [0, T] \to \mathbb{R}$ by $z(0) = z_0$ and

$$\dot{z}(t) = \mathcal{L}(x(t), \dot{x}(t), z(t))$$

We look for a curve x such that every variation of x that vanishes at the boundary of $[0, T]$ leaves the action $z(T)$ invariant.

If $\mathcal{L}$ does not depend on z we find the classical variational principle:

$$z(T) = \int_0^T \mathcal{L}(x(t), \dot{x}(t))\, \mathrm{d}t.$$

[Herglotz. Berührungstransformationen Lecture notes, Göttingen, 1930.]

Herglotz' variational principle

A variation δx of x induces a variation δz of z:

$$\dot z(t) = \mathcal{L}(x(t), \dot x(t), z(t)) \quad \Rightarrow \quad \delta \dot z = \underbrace{\frac{\partial \mathcal{L}}{\partial x}\delta x + \frac{\partial \mathcal{L}}{\partial \dot x}\delta \dot x}_{A(t)} + \underbrace{\frac{\partial \mathcal{L}}{\partial z}}_{\frac{\mathrm{d}B(t)}{\mathrm{d}t}} \delta z.$$

The solution of $\delta \dot z(t) = A(t) + \frac{\mathrm{d}B(t)}{\mathrm{d}t}\delta z(t)$ is

$$\begin{aligned}
\delta z(T) &= e^{B(T)} \left[\int_0^T A(\tau) e^{-B(\tau)} \,\mathrm{d}\tau + \delta z(0) \right] \\
&= e^{B(T)} \left[\int_0^T \left(\frac{\partial \mathcal{L}}{\partial x}\delta x + \frac{\partial \mathcal{L}}{\partial \dot x}\delta \dot x \right) e^{-B(\tau)} \,\mathrm{d}\tau + \delta z(0) \right] \\
&= e^{B(T)} \bigg[\int_0^T \left(\frac{\partial \mathcal{L}}{\partial x} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathcal{L}}{\partial \dot x} + \frac{\partial \mathcal{L}}{\partial z}\frac{\partial \mathcal{L}}{\partial \dot x} \right) \delta x \, e^{-B(\tau)} \,\mathrm{d}\tau \\
&\qquad + \frac{\partial \mathcal{L}}{\partial \dot x}(T)\delta x(T)\, e^{-B(T)} - \frac{\partial \mathcal{L}}{\partial \dot x}(0)\delta x(0) + \delta z(0) \bigg].
\end{aligned}$$

Herglotz' variational principle

$$\delta z(T) = e^{B(T)} \left[\int_0^T \left(\frac{\partial \mathcal{L}}{\partial x} - \frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial \mathcal{L}}{\partial \dot{x}} + \frac{\partial \mathcal{L}}{\partial z} \frac{\partial \mathcal{L}}{\partial \dot{x}} \right) \delta x \, e^{-B(\tau)} \, \mathrm{d}\tau \right.$$
$$\left. + \frac{\partial \mathcal{L}}{\partial \dot{x}}(T) \delta x(T) \, e^{-B(T)} - \frac{\partial \mathcal{L}}{\partial \dot{x}}(0) \delta x(0) + \delta z(0) \right].$$

Variations satisfy $\delta x(0) = \delta x(T) = \delta z(0) = 0$.

Generalized Euler-Lagrange equations

$$\frac{\partial \mathcal{L}}{\partial x} - \frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial \mathcal{L}}{\partial \dot{x}} + \frac{\partial \mathcal{L}}{\partial z} \frac{\partial \mathcal{L}}{\partial \dot{x}} = 0$$

If instead we restrict to solution curves, but vary the endpoints, we obtain

$$\delta z(T) = \frac{\partial \mathcal{L}}{\partial \dot{x}}(T) \delta x(T) - e^{B(T)} \left[\frac{\partial \mathcal{L}}{\partial \dot{x}}(0) \delta x(0) + \delta z(0) \right]$$

Contact structure

$$\phi_T^*(\mathrm{d}z - p \, \mathrm{d}x) = e^{B(T)} (\mathrm{d}z - p \, \mathrm{d}x)$$

where $p = \frac{\partial \mathcal{L}}{\partial \dot{x}}$ and ϕ_T denotes the flow over the time interval $[0, T]$.

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Discrete Herglotz variational principle

Variational integrator: approximate $\mathcal{L}(x, \dot{x}, z)$ by $L(x_j, x_{j+1}, z_j, z_{j+1}; h)$, where $h > 0$ is the step size.

discrete Herglotz variational principle

Given $x = (x_0, \ldots, x_N) \in Q^{N+1}$ we define $z = (z_0, \ldots, z_N) \in \mathbb{R}^{N+1}$ by $z_0 = 0$ and

$$z_{j+1} - z_j = hL(x_j, x_{j+1}, z_j, z_{j+1}; h)$$

Look for a discrete curve x such that

$$\frac{\mathrm{d}z_{j+1}}{\mathrm{d}x_j} = 0 \qquad \forall j \in \{1, \ldots, N-1\}.$$

Then in particular, $\dfrac{\mathrm{d}z_N}{\mathrm{d}x_j} = 0$ for all $j \in \{1, \ldots, N-1\}$:

variations of x do not affect the final value of z.

Discrete Herglotz variational principle

Discrete generalized Euler-Lagrange equation

$$0 = \mathrm{D}_2 L(x_{j-1}, x_j, z_{j-1}, z_j) + \mathrm{D}_1 L(x_j, x_{j+1}, z_j, z_{j+1}) + \frac{h\mathrm{D}_2 L(x_{j-1},x_j,z_{j-1},z_j)}{1-h\mathrm{D}_4 L(x_{j-1},x_j,z_{j-1},z_j)}\left(\mathrm{D}_3 L(x_j, x_{j+1}, z_j, z_{j+1}) + \mathrm{D}_4 L(x_{j-1}, x_j, z_{j-1}, z_j)\right).$$

where D_i is the partial derivative w.r.t. the i-th variable.

If L a consistent discretization of a continuous Lagrangian $\mathcal{L}$,

$$\mathrm{D}_2 L(x_{j-1}, x_j, z_{j-1}, z_j) + \mathrm{D}_1 L(x_j, x_{j+1}, z_j, z_{j+1}) \approx \frac{\partial \mathcal{L}}{\partial x} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathcal{L}}{\partial \dot{x}}$$

$$\frac{h\mathrm{D}_2 L(x_{j-1}, x_j, z_{j-1}, z_j)}{1 - h\mathrm{D}_4 L(x_{j-1}, x_j, z_{j-1}, z_j)} \approx \frac{\partial \mathcal{L}}{\partial \dot{x}}$$

$$\mathrm{D}_3 L(x_j, x_{j+1}, z_j, z_{j+1}) + \mathrm{D}_4 L(x_{j-1}, x_j, z_{j-1}, z_j) \approx \frac{\partial \mathcal{L}}{\partial z}$$

Contact structure

The discrete generalized Euler-Lagrange equation can be written as

$$\frac{h\mathrm{D}_2 L(x_{j-1}, x_j, z_{j-1}, z_j)}{1 - h\mathrm{D}_4 L(x_{j-1}, x_j, z_{j-1}, z_j)} + \frac{h\mathrm{D}_1 L(x_j, x_{j+1}, z_j, z_{j+1})}{1 + h\mathrm{D}_3 L(x_j, x_{j+1}, z_j, z_{j+1})} = 0$$

Position-momentum formulation

$$F : T^*Q \times \mathbb{R} \mapsto T^*Q \times \mathbb{R} : (x_{j-1}, p_{j-1}, z_{j-1}) \mapsto (x_j, p_j, z_j),$$

where $p_j = p_j^- = p_j^+$ and

$$p_j^- = \frac{h\mathrm{D}_2 L(x_{j-1}, x_j, z_{j-1}, z_j)}{1 - h\mathrm{D}_4 L(x_{j-1}, x_j, z_{j-1}, z_j)},$$

$$p_j^+ = -\frac{h\mathrm{D}_1 L(x_j, x_{j+1}, z_j, z_{j+1})}{1 + h\mathrm{D}_3 L(x_j, x_{j+1}, z_j, z_{j+1})}.$$

The map F is a contact transformation with respect to the 1-form

$$\mathrm{d}z - p\,\mathrm{d}x.$$

All contact maps are variational

Theorem

Iterations of any contact transformation

$$(x_0, p_0, z_0) \mapsto (x_1, p_1, z_1)$$

yield a discrete curve $x = (x_0, \dots, x_N)$ that solves the discrete Herglotz variational principle for some discrete Lagrangian $L(x_j, x_{j+1}, z_j)$.

Proof idea. Like in the symplectic case, every contact transformation has a generating function, which can be used as a discrete Lagrangian. ■

In practice it is beneficial to take L symmetric in z_j and z_{j+1}, but from this Theorem it follows that there is always an equivalent Lagrangian independent of z_{j+1}.

Backward error analysis

Solutions of the difference equations

$$\begin{cases} \dfrac{z_{j+1} - z_j}{h} = L(x_j, x_{j+1}, z_j, z_{j+1}; h) \\ \dfrac{x_{j+1} - 2x_j + x_{j-1}}{h^2} = F(x_{j-1}, x_j, x_{j+1}, z_{j-1}, z_j, z_{j+1}; h). \end{cases}$$

are formally interpolated by solutions of the modified equations

$$\begin{cases} \dot{z} = \mathcal{L}_{\mathrm{mod}}(x, \dot{x}, z, h) = \mathcal{L}(x, \dot{x}, z) + h\mathcal{L}_1(x, \dot{x}, z) + h^2\mathcal{L}_2(x, \dot{x}, z) + \dots \\ \ddot{x} = f_{\mathrm{mod}}(x, \dot{x}, z; h) = f(x, \dot{x}, z) + hf_1(x, \dot{x}, z) + h^2 f_2(x, \dot{x}, z) + \dots \end{cases}.$$

(The power series are usually not convergent. Truncations need to be used to make rigorous statements.)

The modified equations are also a contact system

In particular, $\ddot{x} = f_{\mathrm{mod}}(x, \dot{x}, z; h)$ is the generalized Euler-Lagrange equation of $\mathcal{L}_{\mathrm{mod}}(x, \dot{x}, z, h)$.

Hamiltonian integrators

In many examples, $H(x,p,z) = A(p) + B(x) + Cz$. Then

$$\begin{aligned} X_A &= A'(p)\partial_x + (pA(p) - A(p))\partial_z \\ X_B &= -B'(x)\partial_p - B(x)\partial_z \\ X_{Cz} &= -pC\partial_p - Cz\partial_z, \end{aligned}$$

which are all explicitly integrable:

$$\begin{aligned} \exp(tX_A)(x,p,z) &= (x + tA'(p), p, z + t(pA(p) - A(p))) \\ \exp(tX_B)(x,p,z) &= (x, p - t(B'(x) + B(x)), z + t(pA(p) - A(p))) \\ \exp(tX_C)(x,p,z) &= (x, p - tpC, \exp(Ct)z) \end{aligned}$$

Splitting integrator

$$S_2(h) = \exp\left(\frac{h}{2}X_C\right)\exp\left(\frac{h}{2}X_B\right)\exp(hX_A)\exp\left(\frac{h}{2}X_B\right)\exp\left(\frac{h}{2}X_C\right).$$

As a composition of contact maps, $S_2(h)$ is itself a contact map.

Since it is symmetric, S_2 is a second order integrator.

Hamiltonian integrators

Given a second order contact integrator S_2, higher order contact integrators can be obtained recursively by "Yoshida's trick":

$$S_{2n+2}(h) = S_{2n}(\alpha_n h) S_{2n}(\beta_n h) S_{2n}(\alpha_n h)$$

where $\alpha_n = \frac{1}{2 - 2^{\frac{1}{2n+1}}}$ and $\beta_n = -\frac{2^{\frac{1}{2n+1}}}{2 - 2^{\frac{1}{2n+1}}}$.

A more complicated but similar construction for S_2 applies for Hamiltonians

$$H(t, x, p, z) = A(t, p) + B(t, x) + C(t) z$$

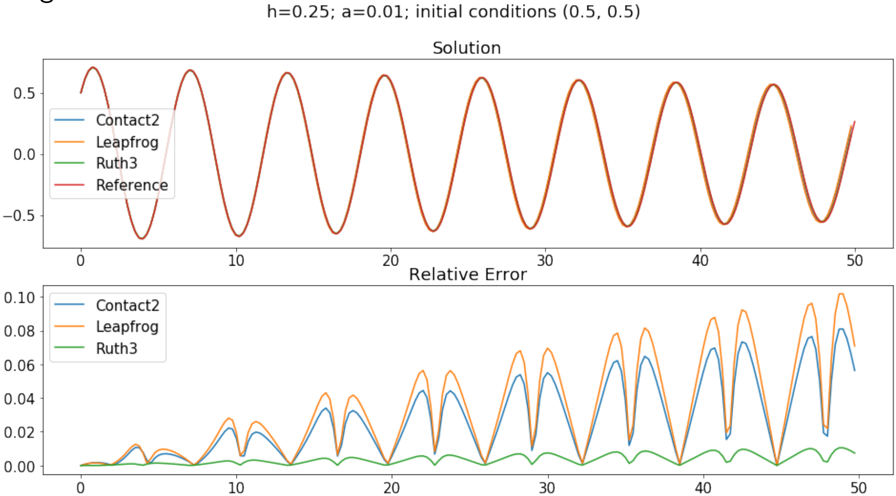
depending explicitly on time.

[Yoshida. Construction of higher order symplectic integrators. Physics letters A, 1990]

Numerical example: harmonic oscillator

$$\mathcal{L} = \frac{1}{2}\dot{x}^2 - V(x) - az \qquad \Rightarrow \qquad \ddot{x} = -V'(x) - \alpha\dot{x}$$

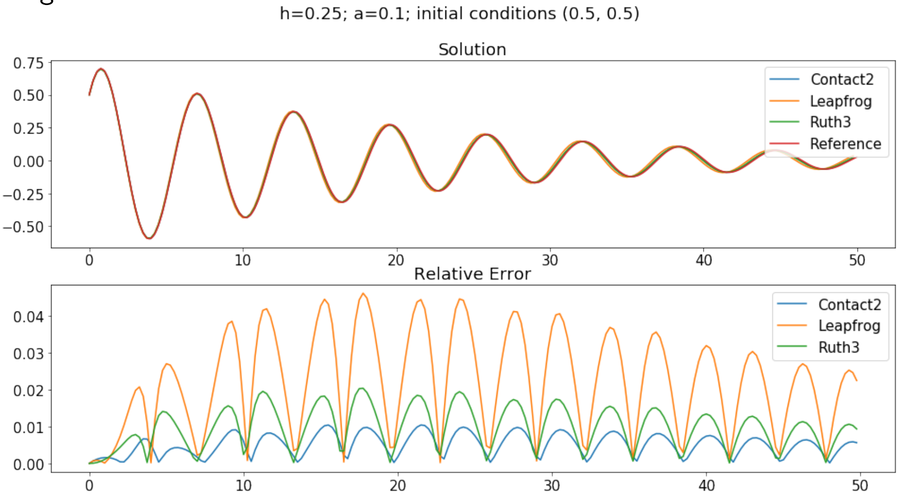
Very small damping: contact integrators comparable to symplectic integrators



Numerical example: harmonic oscillator

$$\mathcal{L} = \frac{1}{2}\dot{x}^2 - V(x) - az \qquad \Rightarrow \qquad \ddot{x} = -V'(x) - \alpha\dot{x}$$

Slightly larger damping: contact integrators better than symplectic integrators



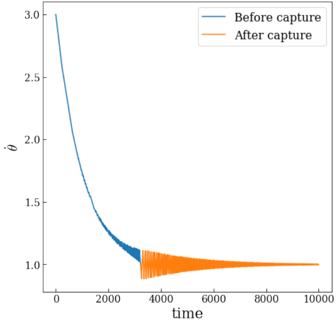
Time-depenent example: spin-orbit mechanics

Flexible satellite in a fixed orbit, experiencing torque from gravity.

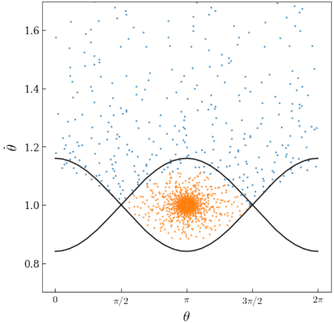
The torque is a time-dependent linear dissipation:

$$H = \frac{p^2}{2} + \frac{N_z(\theta,t)}{C} + \frac{dC}{dt}\frac{1}{C}z \quad \Rightarrow \quad \ddot{\theta} + \frac{dC}{dt}\frac{\dot{\theta}}{C} - \frac{N_z(\theta,t)}{C} = 0.$$

Example: capture into resonance.



Angular velocity decreasing



Poincaré section: angle and angular velocity at fixed point in the orbit

Conclusions

- Contact mechanics is less known than symplectic mechanics, but has significant applications in physics and a similarly rich structure.

- Structure-preserving discretizations for contact systems can be obtained using many of the same ideas as for symplectic systems.

References:

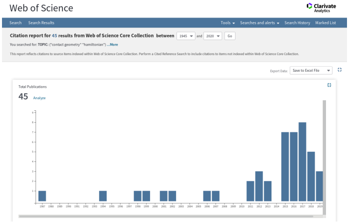
[V, Bravetti, Seri. Contact variational integrators. arXiv:1902.00436]

[Bravetti, Seri, V, Zadra. Numerical integration in celestial mechanics: a case for contact geometry. arXiv:1909.02613]

Conclusions

- Contact mechanics is less known than symplectic mechanics, but has significant applications in physics and a similarly rich structure.

  Though it's getting more attention recently...



Number op papers mentioning "contact geometry" and "Hamiltonian" 1987-2019

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