

# The discrete Herglotz variational principle

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1 Contact Hamiltonian systems

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# Contact Hamiltonian mechanics

Contact geometry: odd-dimensional analogue to symplectic geometry.

Contact Hamiltonian mechanics: allows dissipation of energy

## Variational principle

[Herglotz. *Berührungstransformationen*. 1930.]

[Georgieva, Guenther, Bodurov. *Generalized variational principle of Herglotz for several independent variables. First Noether-type theorem*. 2003]

[León, Lainz, Muñoz-Lecanda. *The Herglotz principle and vakonomic dynamics*. 2021]

[Gaset, Lainz, Mas, Rivas. *The Herglotz variational principle for dissipative field theories*. 2024]

## Discretisation

[V, Bravetti, Seri. *Contact variational integrators*. 2019.]

[Bravetti, Seri, V, Zadra. *Numerical integration in celestial mechanics: a case for contact geometry*. 2020.]

[Bravetti, Seri, Zadra. *New directions for contact integrators*. 2021.]

[Anahory Simoes, Martín de Diego, Lainz Valcázar, de León. *On the Geometry of Discrete Contact Mechanics*. 2021]

# 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  $n$ .

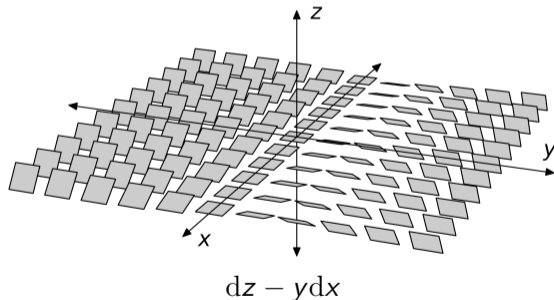
Locally, such a distribution is given by the kernel of a **1-form**  $\eta$  satisfying

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

called a contact form.

Multiplying  $\eta$  by a non-vanishing function does not change the contact structure.

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



## 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

$$\eta = dz - p dx = dz - \sum_i p_i dx_i.$$

### Contact Hamiltonian vector field

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

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

For comparison with symplectic mechanics, note that

$$\iota_{X_H}(d\eta) = -d(\iota_{X_H}\eta) + \mathcal{L}_{X_H}\eta = dH + f_H\eta.$$

In Darboux coordinates the contact Hamiltonian equations are

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

## Damped mechanical systems

Contact Hamiltonian systems satisfy  $\frac{dH}{dt} = -H \frac{\partial H}{\partial z}$  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:

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

(Meaning of  $z$  will be discussed later.)

## Other applications

Thermodynamics [Bravetti. Contact geometry and thermodynamics. International Journal of Geometric Methods in Modern Physics, 2018.]

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

Optimal control [Ohsawa T. Contact geometry of the Pontryagin maximum principle. Automatica, 2015.]

Liénard Systems (e.g. van der Pol oscillator) [Zadra, Bravetti, Seri. Geometric Numerical Integration of Liénard Systems via a Contact Hamiltonian Approach. MDPI Mathematics, 2021.]

Scaling reductions [Bravetti, Jackman, Sloan. Scaling symmetries, contact reduction and Poincaré's dream. J Phys A, 2023.]

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## Herglotz' variational principle

The contact Hamiltonian equation for  $z$  is

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

### Herglotz' variational principle

[Herglotz, 1930]

Lagrangian  $\mathcal{L} : TQ \times \mathbb{R} \rightarrow \mathbb{R}$ .

Given a curve  $x : [0, T] \rightarrow Q$ , define  $z : [0, T] \rightarrow \mathbb{R}$  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:

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

## Direct approach (aka implicit approach)

A variation  $\delta x$  of  $x$  induces a variation  $\delta z$  of  $z$ :

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

The solution of  $\delta \dot{z}(t) = A(t) + \frac{dB(t)}{dt} \delta z(t)$  is

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

## Direct approach (aka implicit approach)

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

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

Generalized Euler-Lagrange equations 
$$\frac{\partial \mathcal{L}}{\partial x} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{x}} + \frac{\partial \mathcal{L}}{\partial z} \frac{\partial \mathcal{L}}{\partial \dot{x}} = 0$$

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 
$$\phi_T^*(dz - p dx) = e^{B(T)}(dz - p dx)$$

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

## Vakonomic approach

Consider  $\dot{z} = \mathcal{L}$  as a constraint, so the action becomes

$$S = z(T) + \int_0^T \lambda(\dot{z} - \mathcal{L}(x, \dot{x}, z))dt = z(0) + \int_0^T \dot{z} + \lambda(\dot{z} - \mathcal{L}(x, \dot{x}, z))dt$$

Vary  $x, z$  with fixed endpoints:

$$0 = \frac{\delta S}{\delta x} = \lambda \frac{\partial \mathcal{L}}{\partial x} - \lambda \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{x}} - \dot{\lambda} \frac{\partial \mathcal{L}}{\partial \dot{x}}$$
$$0 = \frac{\delta S}{\delta z} = -\dot{\lambda} - \lambda \frac{\partial \mathcal{L}}{\partial z}$$

Hence 
$$\dot{\lambda} = -\lambda \frac{\partial \mathcal{L}}{\partial z} \quad \frac{\partial \mathcal{L}}{\partial x} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{x}} + \frac{\partial \mathcal{L}}{\partial z} \frac{\partial \mathcal{L}}{\partial \dot{x}} = 0$$

If we restrict to solution curves, but vary the endpoints, we get  $\delta S = \left[ \lambda(\delta z - p\delta x) \right]_0^T$ .

[León, Lainz, Muñoz-Lecanda. *The Herglotz principle and vakonomic dynamics*. 2021]

## Nonholonomic (chetaev) approach

Consider  $S = \int_0^T \mathcal{L}$  and impose two separate constraints:

► Dynamical constraint:  $\dot{z} = \mathcal{L}$

► Constraint on the variations considered:  $\delta z = \frac{\partial \mathcal{L}}{\partial \dot{x}} \delta x$

Then

$$\begin{aligned} \delta S &= \int_0^T \frac{\partial \mathcal{L}}{\partial x} \delta x + \frac{\partial \mathcal{L}}{\partial \dot{x}} \delta \dot{x} + \frac{\partial \mathcal{L}}{\partial z} \delta z \, dt \\ &= \int_0^T \left( \frac{\partial \mathcal{L}}{\partial x} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{x}} + \frac{\partial \mathcal{L}}{\partial z} \frac{\partial \mathcal{L}}{\partial \dot{x}} \right) \delta x \, dt + \left[ \frac{\partial \mathcal{L}}{\partial \dot{x}} \delta x \right]_0^T \end{aligned}$$

### Warning

In generalisation to field theory, nonholonomic and vakonomic principles are not equivalent!

[Gaset, Lainz, Mas, Rivas. [The Herglotz variational principle for dissipative field theories](#). 2024]

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## Discrete Herglotz variational principle

Variational integrator:

$$\text{approximate } \int_t^{t+h} \mathcal{L}(x, \dot{x}, z) dt \quad \text{by} \quad hL(x_j, x_{j+1}, z_j; h),$$

where  $h > 0$  is the step size.

### Discrete Herglotz variational principle

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

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

Look for a discrete curve  $x$  such that

$$\frac{dz_N}{dx_j} = 0 \quad \forall j \in \{1, \dots, N-1\}.$$

Idea: variations of  $x$  do not affect the final value of  $z$ .

## Direct (implicit) approach

Denote by  $D_i$  the partial derivative wrt  $i$ -th entry.

From

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

it follows that variations wrt  $x_i$  evolve as

$$\begin{aligned}\frac{\partial z_j}{\partial x_i} &= \frac{\partial z_{j-1}}{\partial x_i} + hD_1L(x_{j-1}, x_j, z_{j-1})\frac{\partial x_{j-1}}{\partial x_i} + hD_2L(x_{j-1}, x_j, z_{j-1})\frac{\partial x_j}{\partial x_i} + hD_3L(x_{j-1}, x_j, z_{j-1})\frac{\partial z_{j-1}}{\partial x_i} \\ &= (1 + hD_3L(x_{j-1}, x_j, z_{j-1}))\frac{\partial z_{j-1}}{\partial x_i} + hD_1L(x_{j-1}, x_j, z_{j-1})\delta_{j-1}^i + hD_2L(x_{j-1}, x_j, z_{j-1})\delta_j^i\end{aligned}$$

This implies that

### Lemma

For  $h$  sufficiently small:  $\frac{\partial z_N}{\partial x_i} = 0 \quad \forall i \quad \Leftrightarrow \quad \frac{\partial z_{i+1}}{\partial x_i} = 0 \quad \forall i$

## Direct (implicit) approach

$z_i = z_{i-1} + hL(x_{i-1}, x_i, z_{i-1})$  implies

$$\frac{\partial z_i}{\partial x_i} = hD_2L(x_{i-1}, x_i, z_{i-1})$$

$z_{i+1} = z_i + hL(x_i, x_{i+1}, z_i)$  implies

$$\begin{aligned}\frac{\partial z_{i+1}}{\partial x_i} &= \frac{\partial z_i}{\partial x_i} + hD_1L(x_i, x_{i+1}, z_i) + hD_3hL(x_i, x_{i+1}, z_i)\frac{\partial z_i}{\partial x_i} \\ &= hD_2L(x_{i-1}, x_i, z_{i-1}) + hD_1L(x_i, x_{i+1}, z_i) + h^2D_3hL(x_i, x_{i+1}, z_i)D_2L(x_{i-1}, x_i, z_{i-1})\end{aligned}$$

### Discrete generalized Euler-Lagrange equation

$$0 = D_2L(x_{j-1}, x_j, z_{j-1}) + D_1L(x_j, x_{j+1}, z_j) + hD_2L(x_{j-1}, x_j, z_{j-1})D_3L(x_j, x_{j+1}, z_j).$$

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

# Discrete Herglotz equations

## Discrete generalized Euler-Lagrange equation

$$0 = D_2L(x_{j-1}, x_j, z_{j-1}) + D_1L(x_j, x_{j+1}, z_j) + hD_2L(x_{j-1}, x_j, z_{j-1})D_3L(x_j, x_{j+1}, z_j).$$

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

$$hL \approx \int_t^{t+H} \mathcal{L} \quad \text{so} \quad L \approx \mathcal{L}$$

$$D_2L(x_{j-1}, x_j, z_{j-1}) + D_1L(x_j, x_{j+1}, z_j) \approx \frac{\partial \mathcal{L}}{\partial x} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{x}}$$

$$hD_2L(x_{j-1}, x_j, z_{j-1}) \approx \frac{\partial \mathcal{L}}{\partial \dot{x}}$$

$$D_3L(x_j, x_{j+1}, z_j) \approx \frac{\partial \mathcal{L}}{\partial z}$$

## Allowing dependence on $z_j$ and $z_{j+1}$

### Discrete generalized Euler-Lagrange equation

$$0 = D_2 L(x_{j-1}, x_j, z_{j-1}, z_j) + D_1 L(x_j, x_{j+1}, z_j, z_{j+1}) \\ + \frac{h D_2 L(x_{j-1}, x_j, z_{j-1}, z_j)}{1 - h D_4 L(x_{j-1}, x_j, z_{j-1}, z_j)} (D_3 L(x_j, x_{j+1}, z_j, z_{j+1}) + D_4 L(x_{j-1}, x_j, z_{j-1}, z_j)).$$

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

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

$$D_2 L(x_{j-1}, x_j, z_{j-1}, z_j) + D_1 L(x_j, x_{j+1}, z_j, z_{j+1}) \approx \frac{\partial \mathcal{L}}{\partial x} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{x}} \\ \frac{h D_2 L(x_{j-1}, x_j, z_{j-1}, z_j)}{1 - h D_4 L(x_{j-1}, x_j, z_{j-1}, z_j)} \approx \frac{\partial \mathcal{L}}{\partial \dot{x}} \\ D_3 L(x_j, x_{j+1}, z_j, z_{j+1}) + D_4 L(x_{j-1}, x_j, z_{j-1}, z_j) \approx \frac{\partial \mathcal{L}}{\partial z}$$

## Contact structure

The discrete generalized Euler-Lagrange equation can be written as

$$\frac{hD_2L(x_{j-1}, x_j, z_{j-1}, z_j)}{1 - hD_4L(x_{j-1}, x_j, z_{j-1}, z_j)} + \frac{hD_1L(x_j, x_{j+1}, z_j, z_{j+1})}{1 + hD_3L(x_j, x_{j+1}, z_j, z_{j+1})} = 0$$

### 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

$$p_j^- = \frac{hD_2L(x_{j-1}, x_j, z_{j-1}, z_j)}{1 - hD_4L(x_{j-1}, x_j, z_{j-1}, z_j)},$$
$$p_j^+ = -\frac{hD_1L(x_j, x_{j+1}, z_j, z_{j+1})}{1 + hD_3L(x_j, x_{j+1}, z_j, z_{j+1})}.$$

The map  $F$  is a contact transformation with respect to the 1-form  $dz - p dx$ .

## Vakonomic approach

$$\begin{aligned} S &= z_N + \lambda_j(z_{j+1} - z_j - hL(x_j, x_{j+1}, z_j)) \\ &= z_0 + \sum_j (z_{j+1} - z_j) + \lambda_j(z_{j+1} - z_j - hL(x_j, x_{j+1}, z_j)) \end{aligned}$$

Vary both  $x$  and  $z$ :

$$0 = \frac{\partial S}{\partial x_i} = -\lambda_i h D_1 L(x_i, x_{i+1}, z_i) - \lambda_{i-1} h D_2 L(x_{i-1}, x_i, z_{i-1})$$

$$0 = \frac{\partial S}{\partial z_i} = \lambda_{i-1} - \lambda_i - \lambda_i h D_3 L(x_i, x_{i+1}, z_i)$$

So

$$-\lambda_i h D_1 L(x_i, x_{i+1}, z_i) - (\lambda_i + \lambda_i h D_3 L(x_i, x_{i+1}, z_i)) h D_2 L(x_{i-1}, x_i, z_{i-1}) = 0$$

and again we find

$$D_1 L(x_i, x_{i+1}, z_i) + D_2 L(x_{i-1}, x_i, z_{i-1}) + h D_3 L(x_i, x_{i+1}, z_i) D_2 L(x_{i-1}, x_i, z_{i-1}) = 0$$

## Nonholonomic approach

$$S = \sum_i hL(x_i, x_{i+1}, z_i)$$

Consider only those variations satisfying

$$\delta z_j = D_2 L(x_{j-1}, x_j, z_{j-1}) \delta x_j$$

Then

$$\begin{aligned} \delta S &= \sum_i h D_1 L(x_i, x_{i+1}, z_i) \delta x_i + D_2 L(x_i, x_{i+1}, z_i) \delta x_{i+1} + D_3 L(x_i, x_{i+1}, z_i) \delta z_i \\ &= \sum_i h (D_1 L(x_i, x_{i+1}, z_i) + D_2 L(x_{i-1}, x_i, z_{i-1}) + D_3 L(x_i, x_{i+1}, z_i) D_2 L(x_{i-1}, x_i, z_{i-1})) \delta x_i \end{aligned}$$

and again we find

$$D_1 L(x_i, x_{i+1}, z_i) + D_2 L(x_{i-1}, x_i, z_{i-1}) + h D_3 L(x_i, x_{i+1}, z_i) D_2 L(x_{i-1}, x_i, z_{i-1}) = 0$$

## Backward error analysis

Solutions of the difference equations

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

are formally interpolated by solutions of the **modified equations**

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

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

## Conclusions

- ▶ There are (at least) three implementations of the Herglotz variational principle:
  - ▶ direct (implicit)
  - ▶ vakonomic
  - ▶ nonholonomic (Chetaev)

In mechanics (discrete/continuous), they are all equivalent.

- ▶ Options for discrete Lagrangians
  - ▶  $L(x_j, x_{j+1}, z_j)$ : more explicit difference equations
  - ▶  $L(x_j, x_{j+1}, z_j, z_{j+1})$ : more symmetric difference equations
- ▶ Hamiltonian (splitting) integrators are also available for contact Hamiltonian systems.
- ▶ Structure-preserving discretizations for contact systems can be obtained using many of the same ideas as for symplectic systems.

But relevance of long-time conservation properties is not as obvious.

## Selected references

### References: Herglotz principle

[Herglotz. *Berührungstransformationen*. University of Gottingen, 1930.]

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