Geometric Numerical Integration
2. Symplectic integration

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Index course

1. Hamiltonian mechanics and numerical methods
2. **Symplectic integration**
3. Modified equations
4. Constrained mechanical systems
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We said yesterday...

We first recall the characterization of a Hamiltonian system:

Let us assume that the dimension D of

$$\frac{d}{dt}\mathbf{x} = f(\mathbf{x}) \tag{1}$$

is even, $D = 2d$, and let us write $\mathbf{x} = (\mathbf{q}, \mathbf{p})$ with $\mathbf{q}, \mathbf{p} \in \mathbb{R}^d$.

Then, the system (1) is said to be **Hamiltonian** if there is a function $H : \mathbb{R}^{2d} \to \mathbb{R}$ such that, for $i = 1, \ldots, d$, the scalar components f^i of f are given by

$$f^i(\mathbf{q}, \mathbf{p}) = \frac{\partial H}{\partial p^i}(\mathbf{q}, \mathbf{p}), \quad f^{d+i}(\mathbf{q}, \mathbf{p}) = -\frac{\partial H}{\partial q^i}(\mathbf{q}, \mathbf{p}).$$

We said yesterday...

Thus, the system is

$$\frac{d}{dt}q^i = \frac{\partial H}{\partial p^i}(\mathbf{q}, \mathbf{p}), \qquad \frac{d}{dt}p^i = -\frac{\partial H}{\partial q^i}(\mathbf{q}, \mathbf{p}),$$

or, in vector notation[1],

$$\frac{d}{dt}\begin{bmatrix}\mathbf{q}\\ \mathbf{p}\end{bmatrix} = J^{-1}\nabla H(\mathbf{q}, \mathbf{p}), \tag{2}$$

where

$$\nabla H = \left[\frac{\partial H}{\partial q^i}, \dots, \frac{\partial H}{\partial q^d}, \frac{\partial H}{\partial p^1}, \dots, \frac{\partial H}{\partial p^d}\right]^T$$

and

$$J = \begin{bmatrix} 0_{d\times d} & -I_{d\times d} \\ I_{d\times d} & 0_{d\times d}\end{bmatrix}.$$

The function H is called the **Hamiltonian**, $\mathbb{R}^{2d}$ is the **phase space**, and d is the **number of degrees of fredoom.**

[1] Sanz-Serna and Calvo, *Numerical Hamiltonian problems*, 1994

Symplecticness and preservation of oriented volume

Symplecticness and preservation of oriented volume

Definition

A mapping $\Phi : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ is said to be **symplectic** or **canonical** if, at each point $(\mathbf{q}, \mathbf{p}) \in \mathbb{R}^{2d}$,

$$\Phi'(\mathbf{q}, \mathbf{p})^T J \Phi'(\mathbf{q}, \mathbf{p}) = J, \tag{3}$$

where $\Phi'(\mathbf{q}, \mathbf{p})$ denotes the $2d \times 2d$ Jacobian matrix of Φ and

$$J = \begin{bmatrix} 0_{d\times d} & -I_{d\times d} \\ I_{d\times d} & 0_{d\times d} \end{bmatrix}.$$

[2] Arnold, *Mathematical methods of classical mechanics*, 1989

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$$J = \begin{bmatrix} 0_{d\times d} & -I_{d\times d} \\ I_{d\times d} & 0_{d\times d} \end{bmatrix}.$$

The (analytic) condition (3) has a geometric interpretation in terms of *preservation of two-dimensional areas*[2].

[2] Arnold, *Mathematical methods of classical mechanics*, 1989

Symplecticness and preservation of oriented volume

When $d = 1$, if we set $\Phi(\mathbf{q}, \mathbf{p}) = (\mathbf{q}^*, \mathbf{p}^*)$, the condition (3), after multiplying the matrices in the left-hand side, is seen to be equivalent to

$$\frac{\partial \mathbf{q}^*}{\partial \mathbf{q}} \frac{\partial \mathbf{p}^*}{\partial \mathbf{p}} - \frac{\partial \mathbf{q}^*}{\partial \mathbf{p}} \frac{\partial \mathbf{p}^*}{\partial \mathbf{q}} = 1.$$

The left-hand side is the **Jacobian determinant of Φ**.

[3] Preservation of the oriented area means that D and $\Phi(D)$ have the same orientation and (two-dimensional Lebesque) measure. The transformation (symmetry) $(\mathbf{q}, \mathbf{p}) \mapsto (\mathbf{q}, -\mathbf{p})$ preserves measure but not oriented area.

Symplecticness and preservation of oriented volume

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The left-hand side is the **Jacobian determinant of Φ**.

Therefore, **the transformation Φ is symplectic if and only if the mapping $(\mathbf{q},\mathbf{p}) \mapsto (\mathbf{q}^*,\mathbf{p}^*)$ preserves oriented area in the $(\mathbf{q},\mathbf{p})$-plane**, i.e., for any domain D the oriented area of the image $\Phi(D) \subset \mathbb{R}^2$ coincides with the oriented area of D.[3]

[3]Preservation of the oriented area means that D and $\Phi(D)$ have the same orientation and (two-dimensional Lebesque) measure. The transformation (symmetry) $(\mathbf{q},\mathbf{p}) \mapsto (\mathbf{q},-\mathbf{p})$ preserves measure but not oriented area.

Symplecticness and preservation of oriented volume

Example. Harmonic oscillator

For instance, for each t, the rotation

$$\varphi_t(\xi, \eta) = (\xi \cos t + \eta \sin t, -\xi \sin t + \eta \cos t)\,.$$

is a symplectic transformation in $\mathbb{R}^2$.

Symplecticness and preservation of oriented volume

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For instance, for each t, the rotation

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is a symplectic transformation in $\mathbb{R}^2$.
Using the same notation as before, $\varphi_t(\xi,\eta) = (\xi^*,\eta^*)$, we get

$$\frac{\partial\xi^*}{\partial\xi}\frac{\partial\eta^*}{\partial\eta} - \frac{\partial\xi^*}{\partial\eta}\frac{\partial\eta^*}{\partial\xi} = \cos t\cos t - \sin t(-\sin t) = 1.$$

Symplecticness and preservation of oriented volume

Differential forms provide an alternative language to express the preservation of area[4]

[4] Chapter 7 in Arnold, *Mathematical methods of classical mechanics*, 1989.

Symplecticness and preservation of oriented volume

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For the transformation $\Phi(\mathbf{q},\mathbf{p}) = (\mathbf{q}^*,\mathbf{p}^*)$, the differentials $d\mathbf{q}^*$ and $d\mathbf{p}^*$ are **differential 1-forms**:

$$d\mathbf{q}^* = \frac{\partial \mathbf{q}^*}{\partial \mathbf{q}} d\mathbf{q} + \frac{\partial \mathbf{q}^*}{\partial \mathbf{p}} d\mathbf{p}, \quad d\mathbf{p}^* = \frac{\partial \mathbf{p}^*}{\partial \mathbf{q}} d\mathbf{q} + \frac{\partial \mathbf{p}^*}{\partial \mathbf{p}} d\mathbf{p}.$$

Two differential 1-forms give rise, via the **exerior** or **wedge product** to a **differential 2-form.**

[4] Chapter 7 in Arnold, *Mathematical methods of classical mechanics*, 1989.

Symplecticness and preservation of oriented volume

The exterior product is

- **bilinear**:

$$\begin{aligned} d\mathbf{q}^* \wedge d\mathbf{p}^* =& \frac{\partial \mathbf{q}^*}{\partial \mathbf{q}} \frac{\partial \mathbf{p}^*}{\partial \mathbf{p}} d\mathbf{q} \wedge d\mathbf{q} + \frac{\partial \mathbf{q}^*}{\partial \mathbf{p}} \frac{\partial \mathbf{p}^*}{\partial \mathbf{q}} d\mathbf{p} \wedge d\mathbf{q} \\ &+ \frac{\partial \mathbf{q}^*}{\partial \mathbf{q}} \frac{\partial \mathbf{p}^*}{\partial \mathbf{p}} d\mathbf{q} \wedge d\mathbf{p} + \frac{\partial \mathbf{q}^*}{\partial \mathbf{p}} \frac{\partial \mathbf{p}^*}{\partial \mathbf{p}} d\mathbf{p} \wedge d\mathbf{p}; \end{aligned}$$

- and **skew-symmetric**:

$$d\mathbf{q} \wedge d\mathbf{q} = d\mathbf{p} \wedge d\mathbf{p} = 0, \quad d\mathbf{q} \wedge d\mathbf{p} = -d\mathbf{p} \wedge d\mathbf{q}.$$

Thus,

$$d\mathbf{q}^* \wedge d\mathbf{p}^* = \left(\frac{\partial \mathbf{q}^*}{\partial \mathbf{q}} \frac{\partial \mathbf{p}^*}{\partial \mathbf{p}} - \frac{\partial \mathbf{q}^*}{\partial \mathbf{p}} \frac{\partial \mathbf{p}^*}{\partial \mathbf{q}} \right) d\mathbf{q} \wedge d\mathbf{p}.$$

Symplecticness and preservation of oriented volume

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- and **skew-symmetric**:

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Thus,

$$d\mathbf{q}^* \wedge d\mathbf{p}^* = \left(\frac{\partial \mathbf{q}^*}{\partial \mathbf{q}} \frac{\partial \mathbf{p}^*}{\partial \mathbf{p}} - \frac{\partial \mathbf{q}^*}{\partial \mathbf{p}} \frac{\partial \mathbf{p}^*}{\partial \mathbf{q}} \right) d\mathbf{q} \wedge d\mathbf{p}.$$

Therefore, **conservation of area is equivalent to**

$$d\mathbf{q}^* \wedge d\mathbf{p}^* = d\mathbf{q} \wedge d\mathbf{p}.$$

Symplecticness and preservation of oriented volume

For general d the following result holds[5]:

Proposition

For a symplectic transformation the **determinant of Φ' equals 1**. Therefore, **symplectic transformations preserve the oriented volume in $\mathbb{R}^{2d}$**, i.e., $\Phi(D)$ and D have the same oriented volume for each domain $D \subset \mathbb{R}^{2d}$.

This result is often referred to as **Liouville's theorem**[6].

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[5] Section 38 in Arnold, *Mathematical methods of classical mechanics*, 1989.

[6] Hairer, Lubich, and Wanner, *Geometric Numerical Integration: Structure-Preserving Algorithms for Ordinary Differential Equations*, 2006.

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This result is often referred to as **Liouville's theorem**[6].

For $d > 1$, *preservation of oriented volume is a weaker property than symplecticness*. For instance, volume is preserved by the flow of differential equations with a divergence-free vector field.

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[5] Section 38 in Arnold, *Mathematical methods of classical mechanics*, 1989.

[6] Hairer, Lubich, and Wanner, *Geometric Numerical Integration: Structure-Preserving Algorithms for Ordinary Differential Equations*, 2006.

Symplecticness and preservation of oriented volume

Using $\Phi'(\mathbf{q},\mathbf{p})^T J \Phi'(\mathbf{q},\mathbf{p}) = J$, the proof of the following two results is easy.

Proposition

The composition $\Phi_1 \circ \Phi_2$ of two symplectic mappings is also symplectic.

Proposition

The change of variables $(\mathbf{q},\mathbf{p}) = \Phi(\bar{\mathbf{q}},\bar{\mathbf{p}})$ with Φ symplectic, transforms the Hamiltonian system of differential equations

$$\frac{d}{dt}\begin{bmatrix}\mathbf{q}\\ \mathbf{p}\end{bmatrix} = J^{-1}\nabla H(\mathbf{q},\mathbf{p}),$$

into a system for $(\bar{\mathbf{q}},\bar{\mathbf{p}})$ that is also Hamiltonian.
Moreover, the Hamiltonian function $\bar{H}$ of the transformed system is the result of changing variables in H, i.e., $\bar{H} = H \circ \Phi$.

Sympleticness and preservation of oriented volume

Theorem[7]

Let $D = 2d$. **An autonomous system**

$$\frac{d}{dt}\mathbf{x} = f(\mathbf{x}) \tag{4}$$

with flow φ_t **is Hamiltonian if and only if** φ_t **is a symplectic mapping** for each real t.

[7] Proposition 2.6.2 in Marsden and Ratiu, *Introduction to Mechanics and Symmetry*, 1999.

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Theorem[7]

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Symplecticness is a characteristic property that allows us to decide whether a differential system is Hamiltonian or otherwise in terms of its flow, without knowing the vector field f of the equation.

[7] Proposition 2.6.2 in Marsden and Ratiu, *Introduction to Mechanics and Symmetry*, 1999.

Symplecticness and preservation of oriented volume

In another words[8]...

[8] Sanz-Serna and Calvo, *Numerical Hamiltonian problems*, 1994.

Symplecticness and preservation of oriented volume

Symplecticness is a characterization of Hamiltonian systems in terms of their solutions, rather than in terms of the actual form of the differential equation.

Symplecticness and preservation of oriented volume

Example. The harmonic oscillator

Thus, the symplecticness of the rotation $\varphi_t(\xi, \eta) = (\xi \cos t + \eta \sin t, -\xi \sin t + \eta \cos t)$ is a **manifestation of the Hamiltonian character of the harmonic oscillator**.

Symplecticness and preservation of oriented volume

The behavior of the solutions of Hamiltonian problems is very different from that encountered in *general* systems; some features that are *the rule* in Hamiltonian systems are exceptional in non-Hamiltonian systems.
The special behaviour of Hamiltonian solutions may always be traced back to the symplecticness of the flow.

Symplecticness and preservation of oriented volume

Example. The harmonic oscillator

The origin is a center: a neutrally stable equilibrium surrounded by periodic trajectories. Small perturbations of the right-hand side of

$$\frac{d}{dt}q = p, \quad \frac{d}{dt}p = -q.$$

generically destroy the center.
After perturbation, the trajectories become spirals and the origin becomes either an asymptotically stable node (trajectories spiral in) or an unstable node (trajectories spiral out). However, if **the perturbation is such that the perturbed system is also Hamiltonian, then the center will not disappear under small perturbations**.

Symplecticness and preservation of oriented volume

A geometric integrator is a numerical method that preserves geometric properties of the exact flow of a differential equation[8].

[8] Hairer, Lubich, and Wanner, *Geometric Numerical Integration: Structure-Preserving Algorithms for Ordinary Differential Equations*, 2006.

Symplecticness and preservation of oriented volume

A geometric integrator is a numerical method that preserves geometric properties of the exact flow of a differential equation[8].

In particular, in the case of Hamiltonian problems, we are interested in **constructing integrators that preserve the symplectic structure.**

[8] Hairer, Lubich, and Wanner, *Geometric Numerical Integration: Structure-Preserving Algorithms for Ordinary Differential Equations*, 2006.

Symplecticness and preservation of oriented volume

Splitting integrators are *symplectic* in the following sense.

Assume that the system

$$\frac{d}{dt}\mathbf{x} = f(\mathbf{x}) = f^{(A)}(\mathbf{x}) + f^{(B)}(\mathbf{x})$$

is Hamiltonian, and that is split in such a way that both split systems

$$\frac{d}{dt}\mathbf{x} = f^{(A)}(\mathbf{x}), \qquad \frac{d}{dt}\mathbf{x} = f^{(B)}(\mathbf{x})$$

are also Hamiltonian with flows $\varphi_t^{(A)}$ and $\varphi_t^{(B)}$, respectively.
In the theorem above, we saw that *the flow associated to a Hamiltonian system is symplectic*.

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In the theorem above, we saw that *the flow associated to a Hamiltonian system is symplectic*.

Then, **the splitting integrator mapping ψ_h is symplectic, as a composition of flows that are individually symplectic**.

Symplecticness and preservation of oriented volume

Theorem

Assume that the Hamiltonian of the system

$$\frac{d}{dt}\begin{bmatrix}\mathbf{q}\\ \mathbf{p}\end{bmatrix} = J^{-1}\nabla H(\mathbf{q},\mathbf{p}),$$

is written as $H = H^{(A)} + H^{(B)}$ and split correspondingly:
$f = J^{-1}\nabla H$, $f^{(A)} = J^{-1}\nabla H^{(A)}$, $f^{(B)} = J^{-1}\nabla H^{(B)}$.
*For any splitting integrator, constructed as the composition of $\varphi_t^{(A)}$ and $\varphi_t^{(B)}$, and any h, **the mapping ψ_h is symplectic**.*
In particular, ψ_h conserves oriented volume.

Symplecticness and preservation of oriented volume

Remark

Note that *to have a symplectic* ψ_h *it is not enough that the system being integrated is Hamiltonian*.
If the split vector fields $f^{(A)}$ and $f^{(B)}$ are not Hamiltonian themselves, then ψ_h cannot be expected to be symplectic.

Symplecticness and preservation of oriented volume

Remark

Note that the n-fold composition ψ_h^n that advances the numerical solution over n time steps is then also symplectic.

Symplecticness and preservation of oriented volume

It would also be desirable to have integrators that preserved energy when applied to the Hamiltonian system (2), i.e., $H \circ \psi_h = H$.

Unfortunately, for realistic problems, such a requirement is incompatible with ψ_h being symplectic[9]. *It is standard practice to insist on symplecticness and sacrifice conservation of energy*:

[9] Section 10.3 in Sanz-Serna and Calvo, *Numerical Hamiltonian problems*.

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- **Symplecticness plays a key role in the Hamiltonian formalism** (*An autonomous system is Hamiltonian if and only if its associated t-flow is a symplectic mapping for each real t.*).

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- **Symplecticness plays a key role in the Hamiltonian formalism** (*An autonomous system is Hamiltonian if and only if its associated t-flow is a symplectic mapping for each real t.*).
- **While it is not difficult to find symplectic formulas, standard classes of integrators do not include energy-preserving schemes**, except if the energy is assumed to have particular forms.

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- **Symplecticness plays a key role in the Hamiltonian formalism** (*An autonomous system is Hamiltonian if and only if its associated t-flow is a symplectic mapping for each real t.*).
- **While it is not difficult to find symplectic formulas, standard classes of integrators do not include energy-preserving schemes**, except if the energy is assumed to have particular forms.
- **Symplectic schemes have small energy errors even when the integration interval is very long**.

[9] Section 10.3 in Sanz-Serna and Calvo, *Numerical Hamiltonian problems*.

Preservation of energy

Preservation of energy

If $(\mathbf{q}(t), \mathbf{p}(t))$ is a solution of a Hamiltonian system, then

$$\frac{d}{dt}H(\mathbf{q}(t), \mathbf{p}(t)) = \nabla H(\mathbf{q}(t), \mathbf{p}(t))^T J^{-1} \nabla H(\mathbf{q}(t), \mathbf{p}(t)) = 0.$$

Therefore, we may state:

Theorem

***The value of the Hamiltonian function is preserved by the flow of the corresponding Hamiltonian system**, i.e.,*
$H \circ \varphi_t = H$ for each real t.

In applications to physics, this result is the mathematical expression of the **principle of conservation of energy.**
Unlike symplecticness, which is a characteristic property, **conservation of energy on its own does not ensure that the underlying system is Hamiltonian.**

Preservation of the canonical probability measure

Preservation of the canonical probability measure

Let β denote a positive constant and assume that H is such that

$$Z = \int_{\mathbb{R}^{2d}} \exp\left(-\beta H(\mathbf{q}, \mathbf{p})\right) d\mathbf{q} d\mathbf{p} < \infty.$$

Then, we have the following result, which is a direct consequence of the fact that φ_t preserves both the volume element $d\mathbf{q}d\mathbf{p}$ and the value of $\exp(-\beta H)$ (because it preserves the value of H).

Theorem

The probability measure μ in $\mathbb{R}^{2d}$ with density (with respect to the ordinary Lebesgue measure) $Z^{-1} \exp\left(-\beta H(\mathbf{q}, \mathbf{p})\right)$ is preserved by the flow of the Hamiltonian system

$$\frac{d}{dt} \begin{bmatrix} \mathbf{q} \\ \mathbf{p} \end{bmatrix} = J^{-1} \nabla H(\mathbf{q}, \mathbf{p}), \tag{5}$$

i.e., $\mu(\varphi_t(D)) = \mu(D)$ for each domain $D \subset \mathbb{R}^{2d}$ and each real t.

Preservation of the canonical probability measure

In statistical mechanics[10], if (5) describes the dynamics of a physical system and β is the inverse of the absolute temperature[11], then μ is the **canonical measure** that governs the distribution of $(\mathbf{q}, \mathbf{p})$ over an **ensemble** of many copies of the given system when the system is in contact with a heat bath at constant temperature.

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[10] Allen and Tildesley, *Computer Simulation of Liquids*, 1989; Frenkel and Smit, *Understanding Molecular Simulation: From Algorithms to Applications*, 1996; Tuckerman, *Statistical Mechanics: Theory and Molecular Simulation*, 2010.

[11] It is also known as the *thermodynamic beta* and $\beta = 1/(k_B T)$, where k_B is the *Boltzmann constant* and T the temperature.

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That is, $Z^{-1} \exp\left(-\beta H(\mathbf{q}, \mathbf{p})\right) \, d\mathbf{q} d\mathbf{p}$ **represents the fraction of copies with momenta between $\mathbf{p}$ and $\mathbf{p} + d\mathbf{p}$, and positions between $\mathbf{q}$ and $\mathbf{q} + d\mathbf{q}$.**

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[10] Allen and Tildesley, *Computer Simulation of Liquids*, 1989; Frenkel and Smit, *Understanding Molecular Simulation: From Algorithms to Applications*, 1996; Tuckerman, *Statistical Mechanics: Theory and Molecular Simulation*, 2010.

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Preservation of the canonical probability measure

Under the canonical distribution, **(local) minima of the energy H correspond to (local) maxima of the probability density function**, i.e., to modes of the distribution.

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If the temperature decreases (β increases), **it is less likely to find the system at a location** $(\mathbf{q}, \mathbf{p})$ **with high energy.**

Preservation of the canonical probability measure

For Hamiltonian functions of the form $H(\mathbf{q}, \mathbf{p}) = K(\mathbf{p}) + U(\mathbf{q})$, we may factorize

$$\exp\left(-\beta H(\mathbf{q}, \mathbf{p})\right) = \exp\left(-\frac{1}{2}\beta \mathbf{p}^T M^{-1} \mathbf{p}\right) \times \exp\left(-\beta U(\mathbf{q})\right).$$

Therefore, under the canonical distribution, q **and** p **are stochastically independent.**

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Therefore, under the canonical distribution, q **and** p **are stochastically independent.**

The (marginal) **distribution of the positions $\mathbf{q}$ has probability density function proportional to** $\exp(-\beta U(\mathbf{q}))$**.**

The momenta $\mathbf{p}$ possess a Gaussian distribution with zero mean and covariance matrix equal to M**.**

Reversible systems

Reversible systems

Definition

Let S be a *linear involution* in $\mathbb{R}^D$, i.e., a linear map such that $S(S(\mathbf{x})) = \mathbf{x}$ for each $\mathbf{x}$.

A mapping $\Phi : \mathbb{R}^D \to \mathbb{R}^D$ is said to be **reversible** (with respect to S) if, for each $\mathbf{x}$, $S(\Phi(\mathbf{x})) = \Phi^{-1}(S(\mathbf{x}))$ or, more compactly,

$$S \circ \Phi = \Phi^{-1} \circ S. \tag{6}$$

Reversible systems

Proposition

If Φ is S-reversible, then, for each $\mathbf{x}$,

$$\left|\det \Phi'\left(S(\Phi(\mathbf{x}))\right)\right| = \left|\det \Phi'(\mathbf{x})\right|^{-1}.$$

Proposition

If Φ_1 is S-reversible, then $\Phi_1 \circ \Phi_1$ is S-reversible.
If Φ_1 and Φ_2 are S-reversible, then the symmetric composition $\Phi_1 \circ \Phi_2 \circ \Phi_1$ is S-reversible.

Theorem

Consider the system $\frac{d}{dt}\mathbf{x} = f(\mathbf{x})$ with flow φ_t. The following statements are equivalent:

- For each t, φ_t is an S-reversible mapping.
- For each $\mathbf{x} \in \mathbb{R}^D$, $S(f(\mathbf{x})) = -f(S(\mathbf{x}))$, i.e., $S \circ f = -f \circ S$.

Reversible systems

Systems of differential equations that satisfy the conditions in the previous theorem are said to be **reversible** (with respect to S).

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Systems of the particular form

$$\frac{d}{dt}\mathbf{q} = M^{-1}\mathbf{p}, \qquad \frac{d}{dt}\mathbf{p} = F(\mathbf{q}) \tag{7}$$

are reversible with respect to the **momentum flip** involution

$$S(\mathbf{q},\mathbf{p}) = (\mathbf{q}, -\mathbf{p}). \tag{8}$$

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Systems of differential equations that satisfy the conditions in the previous theorem are said to be **reversible** (with respect to S).

Systems of the particular form

$$\frac{d}{dt}\mathbf{q} = M^{-1}\mathbf{p}, \qquad \frac{d}{dt}\mathbf{p} = F(\mathbf{q}) \tag{7}$$

are reversible with respect to the **momentum flip** involution

$$S(\mathbf{q}, \mathbf{p}) = (\mathbf{q}, -\mathbf{p}). \tag{8}$$

If (7) describes a mechanical system, then $S \circ \Phi = \Phi^{-1} \circ S$ expresses the well-known **time-reversibility of mechanics**.

Reversible systems

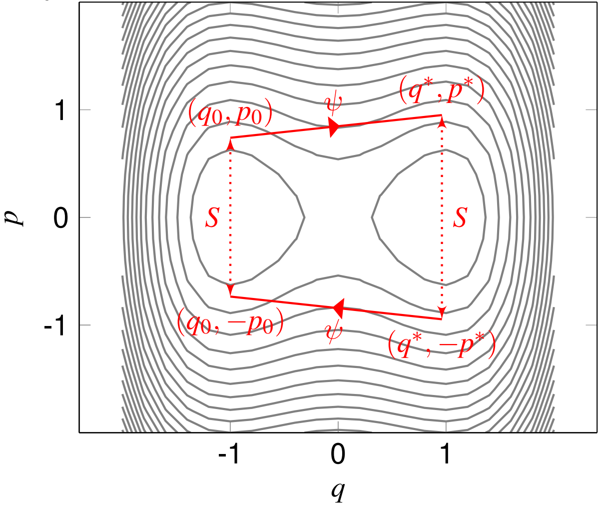
Proposition

The Hamiltonian system

$$\frac{d}{dt}\begin{bmatrix}\mathbf{q}\\ \mathbf{p}\end{bmatrix} = J^{-1}\nabla H(\mathbf{q},\mathbf{p}),$$

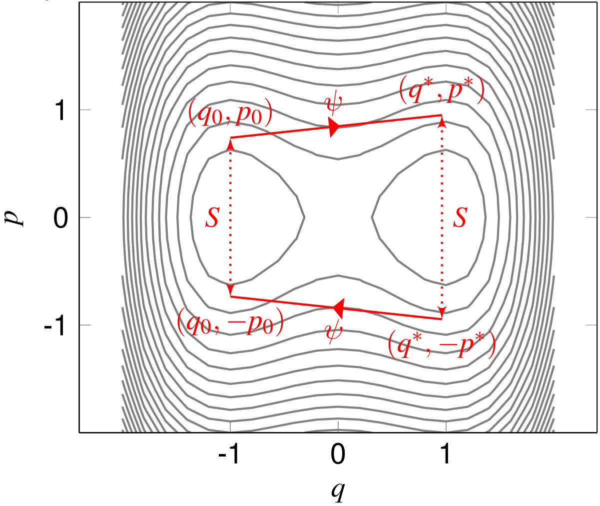
is reversible with respect to the momentum flip involution (8) if and only if H **is an even function of** $\mathbf{p}$, i.e., $H(\mathbf{q},-\mathbf{p}) = H(\mathbf{q},\mathbf{p})$ for all $\mathbf{q}$ and $\mathbf{p}$.

Reversible systems



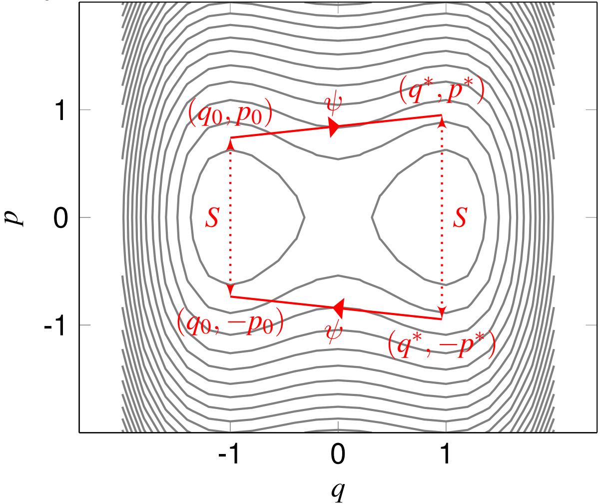
Reversibility of the Hamiltonian flow corresponding to a one-degree-of freedom double-well potential with probability modes at $q = \pm 1$ (cf. Sanz-Serna and Stuart, “Ergodicity of Dissipative Differential Equations Subject to Random Impulses”, 1999).

Reversible systems



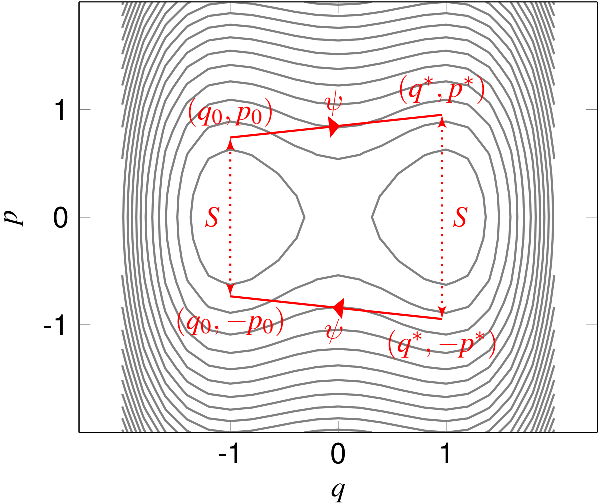
The continuous lines are contours of constant H. The symmetry of the contours with respect to the axis $p = 0$ is a consequence of the reversibility of the Hamiltonian flow.

Reversible systems



The solutions of Hamilton's equations move from left to right when $p > 0$ and from right to left when $p < 0$, so when contours are reflected over the horizontal axis the arrow of time is reversed.

Reversible systems



If a reversible ψ maps (q_0, p_0) into (q^*, p^*), it has to map $(q^*, -p^*)$ into (q_0, p_0), so as to preserve the symmetry of the figure. The transition $(q_0, p_0) \mapsto (q^*, p^*)$ has an increase in energy and $(q^*, -p^*) \mapsto (q_0, p_0)$ decreases energy in exactly the same amount.

Reversible systems

Theorem

Assume that

$$\frac{d}{dt}\mathbf{x} = f(\mathbf{x}) = f^{(A)}(\mathbf{x}) + f^{(B)}(\mathbf{x})$$

and the split systems

$$\frac{d}{dt}\mathbf{x} = f^{(A)}(\mathbf{x}), \quad \frac{d}{dt}\mathbf{x} = f^{(B)}(\mathbf{x})$$

are reversible with respect to the same involution S. If the system is integrated by means of a palindromic s-stage splitting integrator

$$(b_1, a_1, b_2, a_2, \ldots, a_{s'}, b_{s'+1}, a_{s'}, \ldots, a_2, b_2, a_1, b_1), \quad s = 2s',$$

or

$$(b_1, a_1, b_2, a_2, \ldots, b_{s'}, a_{s'}, b_{s'}, \ldots, a_2, b_2, a_1, b_1), \quad s = 2s' - 1,$$

then, for any h, **the mapping ψ_h will also be reversible.**

Reversible systems

Remark

The n-fold composition ψ_h^n that advances the numerical solution over n time steps is also reversible.

[12] Cano and Sanz-Serna, "Error Growth in the Numerical Integration of Periodic Orbits, with Application to Hamiltonian and Reversible Systems", 1997.

Reversible systems

Remark

The n-fold composition ψ_h^n that advances the numerical solution over n time steps is also reversible.

Remark

If variable time steps were taken, then the mapping $\psi_{h_n} \circ \cdots \circ \psi_{h_1}$, that advances the solution from t_0 to t_{n+1} would not be reversible. This is one of the reasons for not considering here variable time steps.

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The use of reversible integrators (with constant step sizes) **ensures that the numerical solution inherits relevant geometric properties of the true solution of the differential system.**[12]

[12] Cano and Sanz-Serna, "Error Growth in the Numerical Integration of Periodic Orbits, with Application to Hamiltonian and Reversible Systems", 1997.

Next session

- We will motivate why **modified equations** are useful and we will define them in detail.
- We will describe the most usual way of **finding modified equations explicitly**: the **Baker-Campbell-Haussdorff formula**.
- We will relate modified equations with the **order of numerical methods**.
- We will combine **modified equations and geometric integrators** using an example.

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