Hamiltonian mechanics

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A Hamiltonian is a smooth function

$$H : T^*Q \times \mathbb{R} \to \mathbb{R}.$$

In standard mechanical systems

$$H(q, p, t) = T(q, p) + V(q, t)$$

though in general H need not be energy. In canonical coordinates (q^i, p_i) Hamilton's equations are

$$\dot{p}_i = -\frac{\partial H}{\partial q^i} \quad \dot{q}^i = \frac{\partial H}{\partial p_i}.$$

Thus H defines a vector field $X_H \in \Gamma(TT^*Q)$ that generates a (local) one-parameter group of symplectomorphisms.

The cotangent bundle carries a canonical 1-form (Liouville / tautological form)

$$\theta := p_i dq^i.$$

Its exterior derivative gives the canonical symplectic form

$$\omega := -d\theta = dq^i \wedge dp_i.$$

The Hamiltonian vector field is defined implicitly by

$$\iota_{X_H}\omega = dH.$$

Because ω is nondegenerate, this uniquely determines X_H.

Symplectic structure induces a Poisson bracket

$$\{F, G\} := \omega(X_F, X_G)$$

that is handy for instance for calculating the total derivative of an observable

$$\frac{dF}{dt} = \{F, H\} + \frac{\partial F}{\partial t}.$$

This implies that if $\{F, H\} = 0$ and $\frac{\partial F}{\partial t} = 0$ then an observable F is conserved along the flow.

Insights for Operator Learning

The natural object is the flow generated by a symplectic vector field on the phase space. This converts dynamics into an operator semigroup acting on states.

By providing surrogate H_θ and defining $X_{H_\theta} \coloneqq J\nabla H_\theta$ we get a surrogate for X_H whose continuous flow preserves H_θ and the symplectic form.