# What is a stochastic Hamiltonian process on finite graph? An optimal transport answer

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# Motivation

Can we define a stochastic process $X_t$ on graph that behaves like a Hamiltonian system?

1. Curiosity.
2. The notion of *gradient flow on graph* has been investigated extensively, Maas'11, Mielke'11, Chow-Huang-Li-Zhou'12, and many more.
3. Recent developments on **discrete** *optimal transport (OT)* (Gangbo-Li-Mou'19), *Schrödinger equations (SE)* (Chow-Li-Zhou'19) as well as *Schrödinger Bridge Problem (SBP)*(Leonard'14, Leonard'16) have demonstrated Hamiltonian principles on graph.

# Motivation

**Macroscopic:**

aggregate behavior

$$\partial_t \rho(x,t) + \nabla \cdot \left(\rho(x,t) \frac{\partial H}{\partial p}(x, \nabla S(x,t))\right) = 0,$$

$$\partial_t S(x,t) + H(x, \nabla S(x,t)) = 0.$$

Hamiltonian system on $\mathcal{T}^*\mathcal{P}(\mathbb{R}^d)$

Lift up to probability

Trace back to particle space

Two systems are equivalent in the sense of

$$\mathrm{Law}(\boldsymbol{X}_t) = \rho(\cdot, t), \quad \boldsymbol{p}_t = \nabla S(\boldsymbol{X}_t, t).$$

**Microscopic:**

particle behavior

$$\dot{\boldsymbol{X}}_t = \frac{\partial}{\partial p} H(\boldsymbol{X}_t, \boldsymbol{p}_t),$$

$$\dot{\boldsymbol{p}}_t = -\frac{\partial}{\partial x} H(\boldsymbol{X}_t, \boldsymbol{p}_t).$$

Hamiltonian system on $\mathcal{T}^*\mathbb{R}^d$

# Stochastic Hamiltonian process on a finite graph

## Definition

A stochastic process $\{X_t\}$ is called a **Hamiltonian process on the graph** $G = (V, E)$ if

1. The density $\rho$ of $X_t$ satisfies the following generalized Master equation,

$$\frac{d\rho}{dt} = \rho Q(S, \rho, t),$$

with

$$Q_{ij}(S, \rho, t) = 1_{(i,j)\in E} f_{ji}(S_j - S_i, \rho, t), \; Q_{ii}(S, \rho, t) = -\sum_{j\in N(i)} Q_{ij}(S, \rho, t).$$

2. The density $\rho$ and the potential $S$ form a Hamiltonian system on the cotangent bundle $\mathcal{T}^*\mathcal{P}(G)$ of the density space $\mathcal{P}(G)$.

A key concern is whether a Markov process $X_t$ exists for such a master equation or not.

# Stochastic Hamiltonian process on a finite graph

## Theorem

*Suppose that the stochastic process* $\{X_t\}_{t\geq 0}$ *with density* $\{\rho_t\}_{t\geq 0}$ *and potential* $\{S_t\}_{t\geq 0}$ *forms a Hamiltonian process on the graph* $G$*. In addition assume that* $F_{ij}$ *is the antiderivative of* $f_{ij}$*. Then the Hamiltonian always possesses the form*

$$\mathscr{H}(\rho, S) = \sum_{i\in V}\sum_{j\in N(i)} \rho_i F_{ji}(S_j - S_i, \rho, t) + \mathcal{V}(\rho, t), \tag{1}$$

*where* $\mathcal{V}$ *is a function depending* $\rho$ *and* $t$*. Moreover, the Hamiltonian system on* $\mathcal{T}^*\mathcal{P}(G)$ *is*

$$\frac{\partial}{\partial t}\rho_i(t) = \sum_{j\in N(i)} f_{ij}(S_i - S_j, \rho, t)\rho_j - f_{ji}(S_j - S_i, \rho, t)\rho_i,$$

$$\frac{\partial}{\partial t}S_i(t) = -\sum_{j\in N(i)}\left(F_{ji}(S_j - S_i, \rho, t) + \rho_j\frac{\partial}{\partial \rho_i}F_{ji}(S_j - S_i, \rho, t)\right) - \frac{\partial}{\partial \rho_i}\mathcal{V}(\rho, t).$$

$X_t$ must be a time-inhomogeneous Markov process.

# Example 1: OT on graph

The OT problem on graph $G$,

$$\min_{\rho, v} \left\{ \int_0^1 \langle v, v \rangle_{\theta(\rho)} dt \right\}, \tag{2}$$
$$\partial_t \rho + \mathrm{div}_G^\theta(\rho v) = 0, \ \rho(\cdot, 0) = \rho_a, \ \rho(\cdot, 1) = \rho_b,$$

where we define

$$\langle v, v \rangle_{\theta(\rho)} = \frac{1}{2} \sum_{(j,l) \in E} \theta_{jl}(\rho) v_{jl}^2, \quad (\mathrm{div}_G^\theta(\rho v))_j = - \sum_{l \in N(j)} \theta_{jl}(\rho) v_{jl},$$

with the upwind choice

$$\theta_{ij}^U(\rho) = \begin{cases} \rho_j & S_j < S_i \\ \rho_i & S_i < S_j \end{cases}$$

The Hamiltonian system is

$$\frac{d\rho_i}{dt} + \sum_{j \in N(i)} \theta_{ij}(\rho)(S_j - S_i) = 0, \quad \frac{dS_i}{dt} + \frac{1}{2} \sum_{j \in N(i)} \frac{\partial \theta_{ij}(\rho)}{\partial \rho_i} (S_i - S_j)^2 = 0. \tag{3}$$

# Example 2: SBP on graph

The Schrödinger Bridge Problem on $G$ can be expressed as

$$\min_{\rho, v} \left\{ \int_0^1 (\langle v, v \rangle_{\theta^U(\rho)} + \frac{1}{8} \mathcal{I}_G(\rho)) dt \right\}, \tag{4}$$

$$\partial \rho + \mathrm{div}_G^{\theta^U}(\rho v) = 0, \ \rho(\cdot, 0) = \rho_a, \ \rho(\cdot, 1) = \rho_b,$$

where the discrete Fisher Information is

$$\mathcal{I}_G(\rho) = \frac{1}{2} \sum_{(i,j) \in E} (\log(\rho_i) - \log(\rho_j))^2 \widetilde{\theta}_{ij}(\rho).$$

Here $\widetilde{\theta}$ is some weight function, not necessarily equal to $\theta^U$ before.

# Reference

Jianbo Cui, Shu Liu, and Haomin Zhou, *What is a stochastic Hamiltonian process on finite graph? An optimal transport answer*, Journal of Differential Equation, Vol. 305 (2021).

# Thank you!