Regularized unbalanced optimal transport as entropy minimization with respect to branching Brownian Motion

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Applied Probability Seminars, Warwick University

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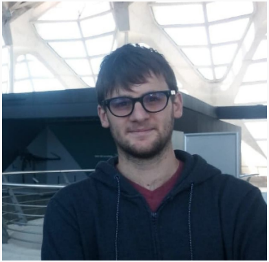
My coauthor

Joint work with **Aymeric Baradat** (Université Claude Bernard Lyon 1).

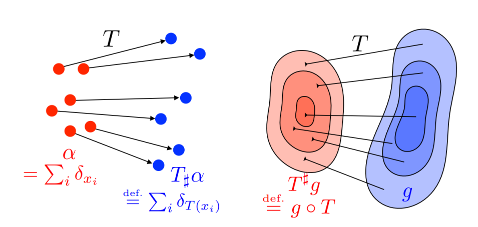


Disclaimer

He is the one who knows about probability!

What is this talk about?

Regularized (a.k.a. entropic) Optimal Transport...



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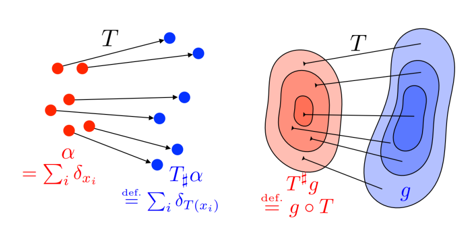

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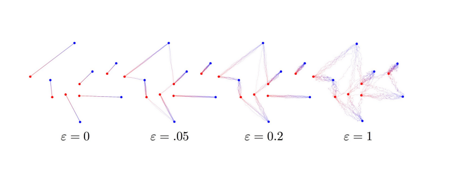

- Schrödinger, *Sur la théorie relativiste de l'électron et l'interprétation de la mécanique quantique* (1932).
- Léonard, *A survey of the Schrödinger problem and some of its connections with optimal transport* (2013).

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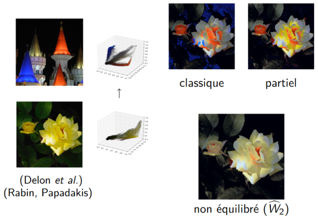

- Liero, Mielke, Savaré, *Optimal entropy-transport problems and a new Hellinger–Kantorovich distance between positive measures* (2018).
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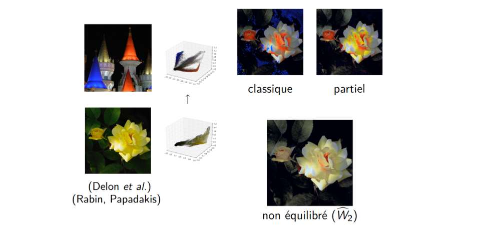

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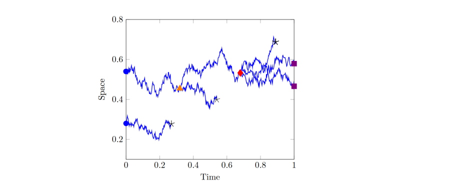
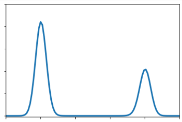
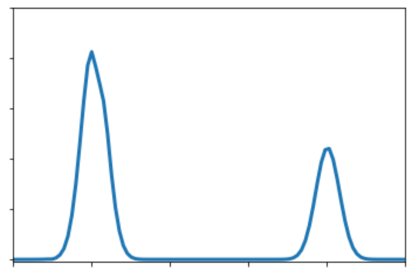


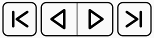
- Baradat and Lavenant, *Regularized unbalanced optimal transport as entropy minimization with respect to branching Brownian motion* (2021).

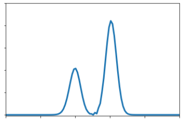
Goal: develop a probabilistic interpretation of RUOT.

Optimal Transport

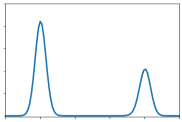


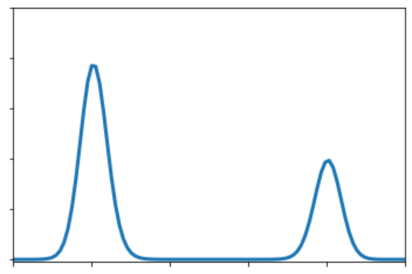


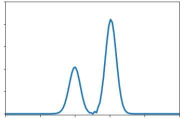




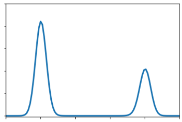
Regularized Optimal Transport

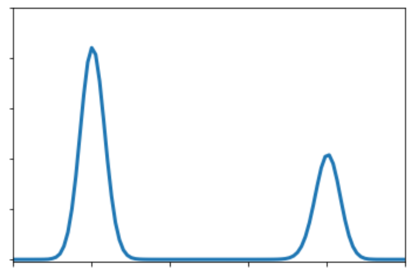


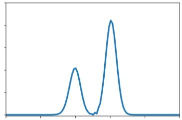




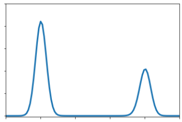
Unbalanced Optimal Transport

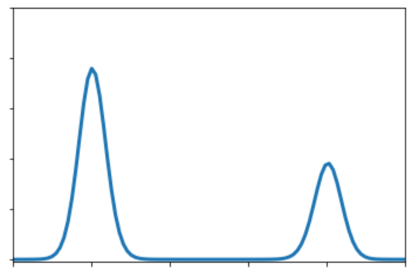


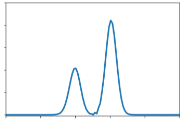




Regularized Unbalanced Optimal Transport







Outline

1. The Schrödinger problem

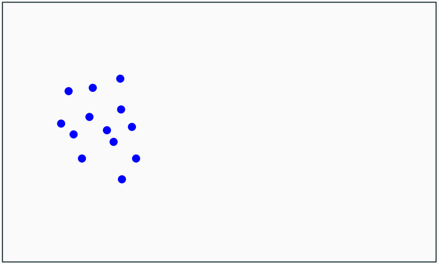
2. The branching Schrödinger problem

3. Equivalence of branching Schrödinger with regularized unbalanced optimal transport

1. The Schrödinger problem

A problem coming from Large deviation

N particles $\sim \alpha$ at time $t = 0$. They follow **Brownian motion**.



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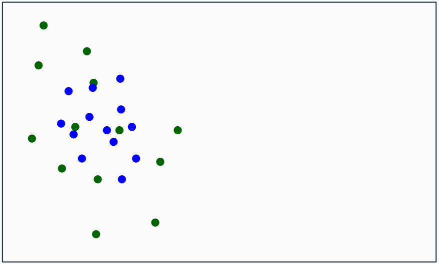

Expected distribution at time $t = 1$, $\sim \mathcal{N}(0,1) \star \alpha$.

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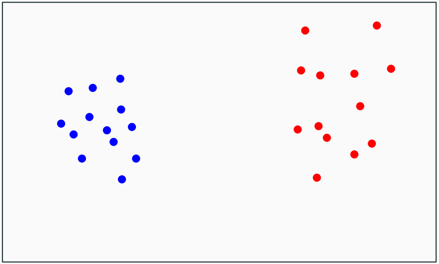

Observed distribution at time $t = 1$, $\beta \neq \mathcal{N}(0, 1) \star \alpha$.

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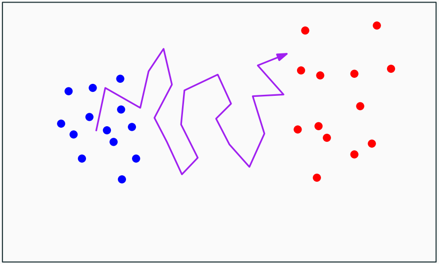

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The problem

If $N \gg 1$, given this unlikely event, what is the most likely evolution?

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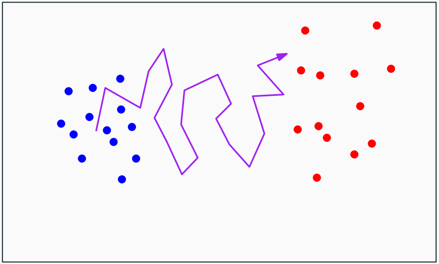

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Theory of Large Deviation: **entropy minimization** with respect to the law of Brownian motion.

Entropy minimization for the Schrödinger problem

State space $\mathbb{T}^d$ the d-dimensional torus, $\Omega = C([0,1], \mathbb{T}^d)$.

$R^\nu \in \mathcal{P}(\Omega)$ law of the Brownian motion with diffusivity ν and uniform initial distribution $\mathcal{L} = \mathrm{d}x$ (reversible Wiener measure).

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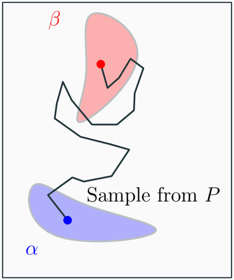
The Schrödinger problem

Given $\alpha, \beta \in \mathcal{P}(\mathbb{T}^d)$, find $P \in \mathcal{P}(\Omega)$ which minimizes

$$H(P|R^\nu) := \int_\Omega \log\left(\frac{\mathrm{d}P}{\mathrm{d}R^\nu}(X)\right) \mathrm{d}P(X).$$

with constraints $X_0 \sim \alpha$ and $X_1 \sim \beta$ under P.



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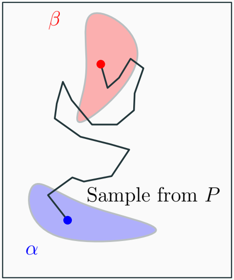

If $H(\alpha|\mathcal{L}), H(\beta|\mathcal{L}) < +\infty$, there exists a unique solution.

Structure of the solutions

Theorem (optimality conditions)

P optimal if and only if there exists $f, g : \mathbb{T}^d \to \mathbb{R}$ such that

$$\frac{\mathrm{d}P}{\mathrm{d}R^\nu}(X) = f(X_0)g(X_1).$$

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Under P, $(X_t)_{t\in[0,1]}$ follows:

the **forward** stochastic differential equation

$$\mathrm{d}X_t = v(t, X_t)\mathrm{d}t + \sqrt{\nu}\mathrm{d}B_t$$

with $v = \nabla[\tau_{\sqrt{\nu}t} * f]$

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the **backward** stochastic differential equation

$$\mathrm{d}X_{1-t} = w(1-t, X_{1-t})\mathrm{d}t + \sqrt{\nu}\mathrm{d}B_{1-t}$$

with $w = \nabla[\tau_{\sqrt{\nu}(1-t)} * g]$.

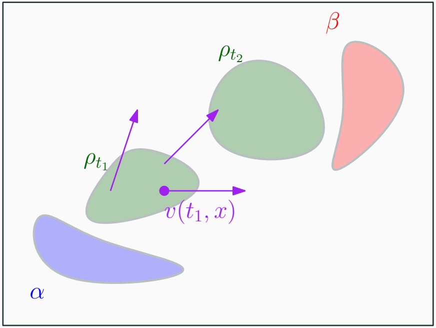
A "projection": regularized optimal transport

Regularized Optimal Transport

Look for ρ and v time-dependent density and velocity field which minimize

$$\mathcal{A}(\rho, v) = \int_0^1 \int_{\mathbb{T}^d} \frac{|v(t,x)|^2}{2} \rho(t,x) \, \mathrm{d}t\mathrm{d}x$$

under the constraint $\rho_0 = \alpha$, $\rho_1 = \beta$ and $\partial_t \rho + \nabla \cdot (\rho v) = \frac{\nu}{2} \Delta \rho$



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From Schrödinger to ROT

Given $P \in \mathcal{P}(\Omega)$ with $H(P|R^\nu) < +\infty$,
define $\rho_t := \mathrm{Law}_P(X_t)$,

$$v(t, X_t) := \lim_{h \to 0, h > 0} \mathbb{E}_P \left[\frac{X_{t+h} - X_t}{h} \middle| X_t \right].$$

Then (ρ, v) admissible and

$$\nu H(\alpha|\mathcal{L}) + \mathcal{A}(\rho, v) \leqslant \nu H(P|R^\nu).$$

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From ROT to Schrödinger

If (ρ, v) admissible with v smooth, P the law of the SDE

$$\mathrm{d}X_t = v(t, X_t) \, \mathrm{d}t + \sqrt{\nu} \, \mathrm{d}B_t.$$

Then P admissible and

$$\nu H(\alpha|\mathcal{L}) + \mathcal{A}(\rho, v) = \nu H(P|R^\nu).$$

Consequence: equality of the values

Theorem

For any α, β with $H(\alpha|\mathcal{L}), H(\beta|\mathcal{L}) < +\infty$, there holds

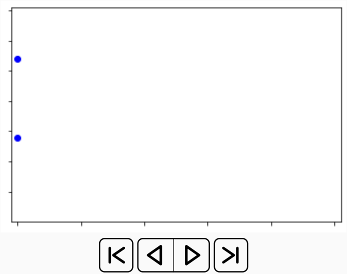
$$\nu H(\alpha|\mathcal{L}) + \min_{\rho,v} \left\{ \mathcal{A}(\rho, v) \ : \ \partial_t \rho + \nabla \cdot (\rho v) = \frac{\nu}{2} \Delta \rho, \ \rho_0 = \alpha, \rho_1 = \beta \right\}$$
$$= \min_{P} \{ \nu H(P|R^\nu) \ : \ X_0 \sim \alpha \text{ and } X_1 \sim \beta \text{ under } P \} .$$

Moreover, if (ρ, v) and P optimal then P is the law of the SDE with drift v.

2. The branching Schrödinger problem

The Branching Brownian motion

Parameters: diffusivity $\nu > 0$, branching rate $\lambda > 0$, law $(p_k)_{k=0,1,\ldots} \in \mathcal{P}(\mathbb{N})$.



Particles diffuse (ν), at temporal rate λ they “branch” and have a k offsprings, drawn from $(p_k)_{k=0,1,\ldots} \in \mathcal{P}(\mathbb{N})$.

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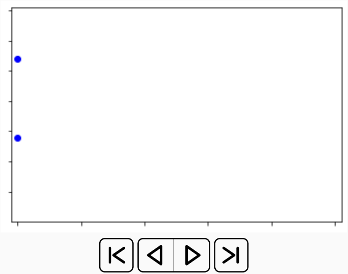

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At time t, random **measure** $M_t = \sum_{X \in \{\text{particles alive at time } t\}} \delta_X$.

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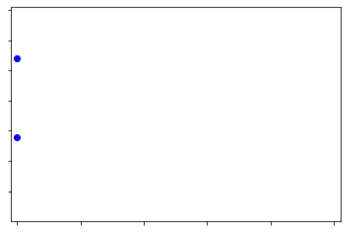

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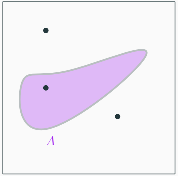
Description

The Branching Brownian Motion is a probability distribution on $\text{càdlàg}([0,1], \mathcal{M}_+(\mathbb{T}^d))$.

Assumptions: $0 < \nu, \lambda < \infty$ and $\sum k p_k < +\infty$.

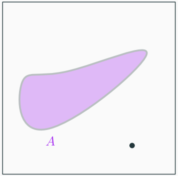
The Branching Schrödinger problem



$M_t(A) = 1$

$\mathbb{E}_P[M_t]$ is the deterministic measure $\mathbb{E}_P[M_t](A) = \mathbb{E}_P[M_t(A)]$.

The Branching Schrödinger problem



$M_t(A) = 0$

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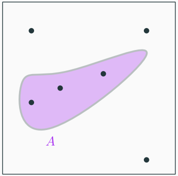
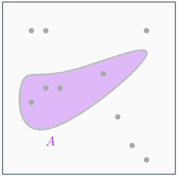


$M_t(A) = 3$

$\mathbb{E}_P[M_t]$ is the deterministic measure $\mathbb{E}_P[M_t](A) = \mathbb{E}_P[M_t(A)]$.

The Branching Schrödinger problem



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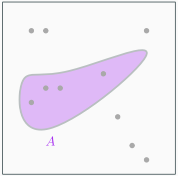

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R law of the Branching Brownian Motion with parameters ν, λ and (p_k).

Branching Schrödinger problem

Given $\alpha, \beta \in \mathcal{M}_+(\mathbb{T}^d)$, find $P \in \mathcal{P}(\text{càdlàg}([0,1], \mathcal{M}_+(\mathbb{T}^d)))$ which minimizes $H(P|R)$ under the constraints $\mathbb{E}_P[M_0] = \alpha$ and $\mathbb{E}_P[M_1] = \beta$.

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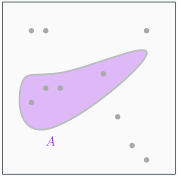

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Given $\alpha, \beta \in \mathcal{M}_+(\mathbb{T}^d)$, find $P \in \mathcal{P}(\text{càdlàg}([0,1], \mathcal{M}_+(\mathbb{T}^d)))$ which minimizes $H(P|R)$ under the constraints $\mathbb{E}_P[M_0] = \alpha$ and $\mathbb{E}_P[M_1] = \beta$.

Important remark. Ill-posed problem as the constraints are not closed:

$$\forall \varphi \in C(\mathbb{T}^d),\ \mathbb{E}_P[\langle \varphi, M_0 \rangle] := \mathbb{E}_P\left[\int \varphi(x)\,\mathrm{d}M_0(x)\right] = \int \varphi(x)\,\mathrm{d}\alpha(x)$$

3. Equivalence of branching Schrödinger with regularized unbalanced optimal transport

The regularized unbalanced optimal transport problem

Regularized Optimal Transport

Look for ρ, v time-dependent density, velocity field which minimize

$$\mathcal{A}(\rho, v) = \iint \frac{|v(t,x)|^2}{2}\rho(t,x)\,\mathrm{d}t\mathrm{d}x$$

under the constraint $\rho_0 = \alpha$, $\rho_1 = \beta$ and $\partial_t\rho + \nabla\cdot(\rho v) = \frac{\nu}{2}\Delta\rho$.

The regularized unbalanced optimal transport problem

$\Psi : \mathbb{R} \to [0, +\infty]$ convex function.

Regularized Unbalanced Optimal Transport

Look for ρ, v, r time-dependent density, velocity and scalar field which minimize

$$\mathcal{A}(\rho, v, r) = \iint \frac{|v(t,x)|^2}{2} \rho(t,x) \, \mathrm{d}t\mathrm{d}x \; + \iint \Psi(r(t,x))\rho(t,x) \, \mathrm{d}t\mathrm{d}x$$

under the constraint $\rho_0 = \alpha$, $\rho_1 = \beta$ and $\partial_t \rho + \nabla \cdot (\rho v) = \frac{\nu}{2} \Delta \rho + r\rho$.

The field $r = r(t,x)$ is the **growth rate**.

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The field $r = r(t,x)$ is the **growth rate**.

If Ψ grows polynomially at $+\infty$ and $H(\beta|\mathcal{L}) < +\infty$, then well posed.

$\mathrm{Ruot}(\alpha, \beta) := \min \left\{ \mathcal{A}(\rho, v, r) \; : \; \partial_t \rho + \nabla \cdot (\rho v) = \frac{\nu}{2} \Delta \rho + r\rho, \; \rho_0 = \alpha, \rho_1 = \beta \right\}$.

Equivalence of the values

Choose Ψ depending on λ, ν and (p_k) (see after).

Define $L : \varphi \to \log \mathbb{E}_R \left[\exp\left(\langle \varphi, M_0 \rangle\right)\right]$ log-Laplace transform of R_0.

We expect:

$$\nu L^*(\alpha) + \mathrm{Ruot}(\alpha, \beta) = \inf_P \{\nu H(P|R) \ : \ \mathbb{E}_P[M_0] = \alpha \text{ and } \mathbb{E}_P[M_1] = \beta\}$$

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Theorem (equivalence of the values)

The function

$$(\alpha, \beta) \mapsto \nu L^*(\alpha) + \mathrm{Ruot}(\alpha, \beta)$$

is the lower semi continuous envelope of

$$(\alpha, \beta) \mapsto \inf_P \{\nu H(P|R) \;:\; \mathbb{E}_P[M_0] = \alpha \text{ and } \mathbb{E}_P[M_1] = \beta\}$$

for the topology of weak convergence.

Equivalence of the competitors

Additional assumption: R_0 and $(p_k)_{k\in\mathbb{N}}$ have a finite exponential moment.

From Branching Schrödinger to RUOT

Given P with $H(P|R) < +\infty$ we build (ρ, v, r) competitor for RUOT with

$$\nu L^*(\alpha) + \mathcal{A}(\rho, v, r) \leqslant \nu H(P|R).$$

If $H(P|R) < +\infty$ then P is the law of BBM with random (predictable) space time dependent drift $\tilde{v}$, branching rate $\tilde{\lambda}$, law of offsprings $(\tilde{p}_k)_{k\in\mathbb{N}}$.

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From RUOT to Branching Schrödinger

Up to smoothing everything (including α, β) from (ρ, v, r) admissible we build a Branching Brownian Motion with drift v and branching rate, law of offsprings depending on r such that

$$\nu L^*(\alpha) + \mathcal{A}(\rho, v, r) \geqslant \nu H(P|R).$$

Choosing the right growth penalization

Definition (growth penalization)

Given ν, λ and (p_k) choose

$$\Psi(r) = \nu \inf_{\tilde{\lambda}, (\tilde{p}_k)} \left\{ H(\tilde{\lambda}(\tilde{p}_k) | \lambda(p_k)) \text{ such that } \sum_{k=0}^{+\infty} (k-1)\tilde{\lambda}\tilde{p}_k = r \right\}.$$

Equivalently with $\Phi_p(X) = \sum p_k X^k$ then $\Psi^*(s) = \nu\lambda \left(e^{-s/\nu} \Phi_p(e^{s/\nu}) - 1 \right)$.

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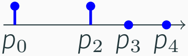
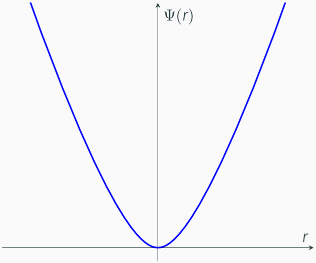
If $p_0 = p_2 = 1/2$ then



$$\Psi^*(s) = \lambda\nu \left(\cosh \left[\frac{s}{\nu} \right] - 1 \right),$$

Ψ convex, minimal for $r = 0$.



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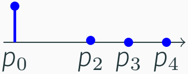
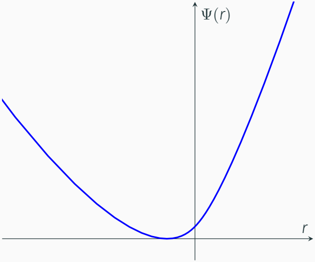
If $p_0 = 0.95$, $p_2 = 0.05$



then Ψ minimal for $\bar{r} < 0$.



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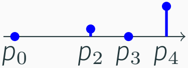
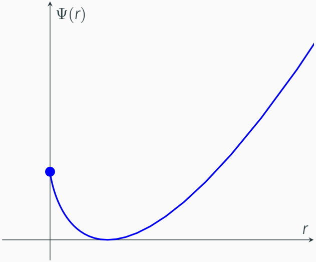
If $p_2 = 0.2$, $p_4 = 0.8$ (no killing allowed),



then $\Psi(r) = +\infty$ for $r < 0$.



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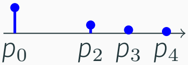
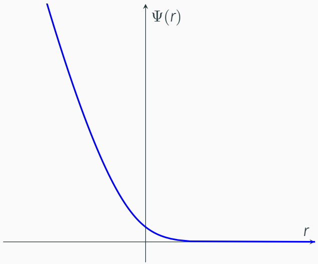
Equivalently with $\Phi_p(X) = \sum p_k X^k$ then $\Psi^*(s) = \nu\lambda \left(e^{-s/\nu}\Phi_p(e^{s/\nu}) - 1 \right)$.

If $p_k = 1/(k-1)^{2.2}$, and $p_0 = 1 - \sum_{k\geq 2} p_k$ (no exponential moment)



then $\Psi(r) = 0$ for $r \geq \bar r$.



Other measure valued processes?

Given a process R, need for the computation of $\mathbb{E}_R\left[\exp(\langle\theta, M_1\rangle) \middle| M_0\right]$.

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Example (Dawson-Watanabe)

If R Dawson-Watanabe superprocess then the associated PDE is

$$\partial_t\phi + \frac{1}{2}\Delta\phi + \frac{1}{2}\phi^2 = 0$$

as

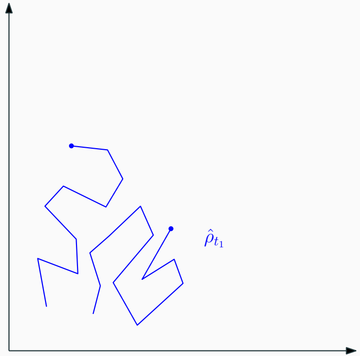
$$\mathbb{E}_R\left[\exp(\langle\phi(1,\cdot), M_1\rangle)\middle| M_0\right] = \exp(\langle\phi(0,\cdot), M_0\rangle).$$

We expect the value of the Schrödinger problem to coincide with

$$L^*(\alpha) + \min_{\rho,r}\left\{\iint r^2\rho \;:\; \partial_t\rho = \frac{\nu}{2}\Delta\rho + r\rho\right\}$$

(that is Ψ quadratic and $v = 0$).

One motivation: biology



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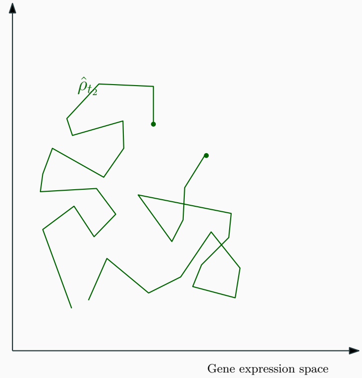

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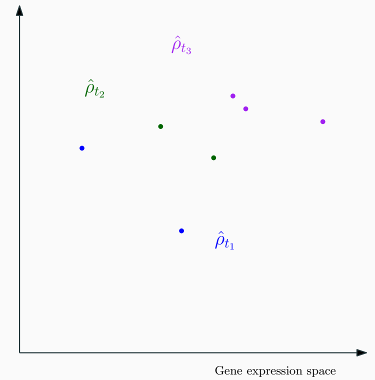

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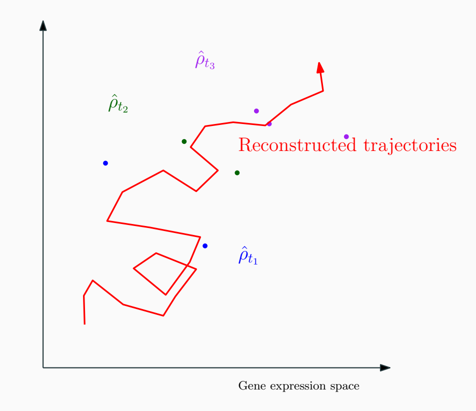

Idea: use the optimal transport to reconstruct the temporal couplings.

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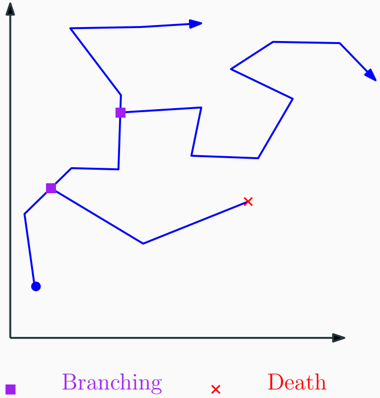

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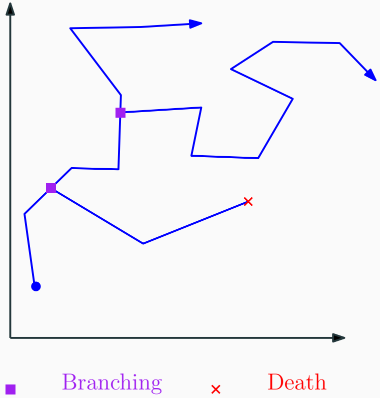

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Use **unbalanced** optimal transport to account for cell division.

Conclusion

What I have not presented:

- Proof of the equivalence (convex analysis, stochastic analysis).
- Small noise limit $\nu, \lambda \to 0$: partial optimal transport ($\Psi(r) = |r|$).
- Numerical simulations with the dynamical formulation of RUOT.

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Thank you for your attention