A probabilistic view on unbalanced optimal transport

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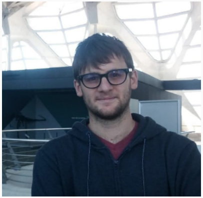
My coauthor

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



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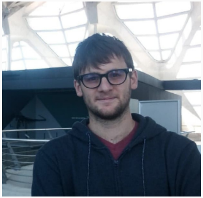
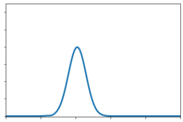
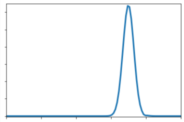


Disclaimer

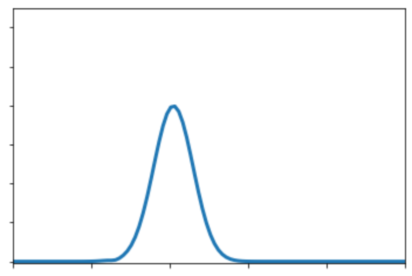
He is the one who knows about probability!

Optimal Transport

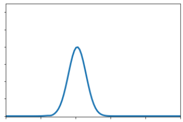




initial final



Regularized Optimal Transport



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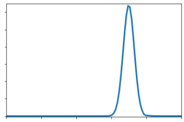
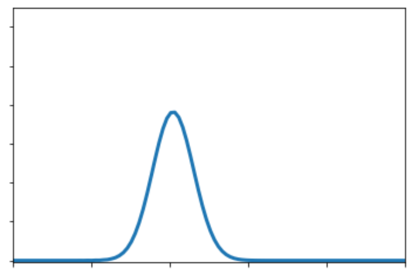
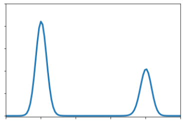
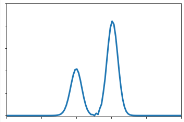


final



With bimodal inputs





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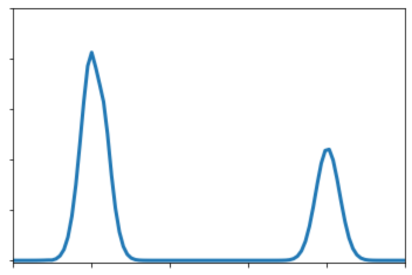
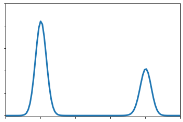
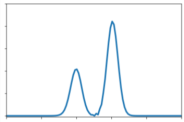


Solution: Unbalanced Optimal Transport





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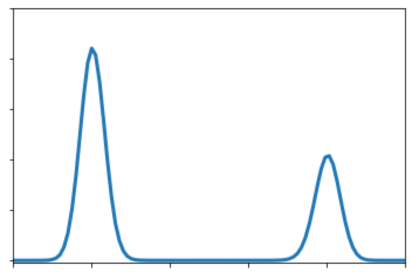
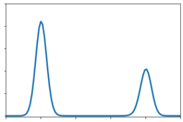
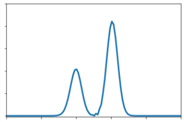


Today: Regularized Unbalanced Optimal Transport





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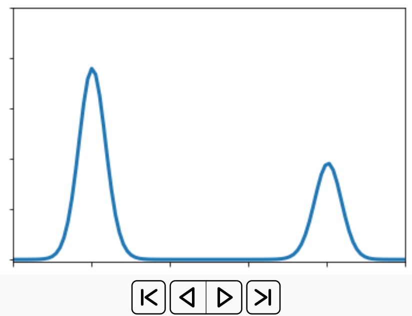
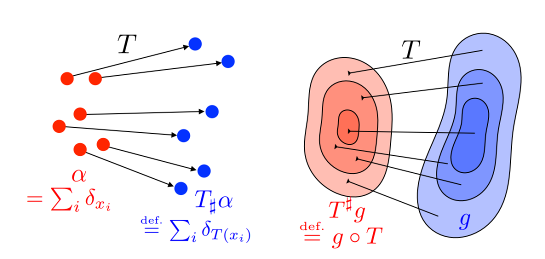


What is this talk about?

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



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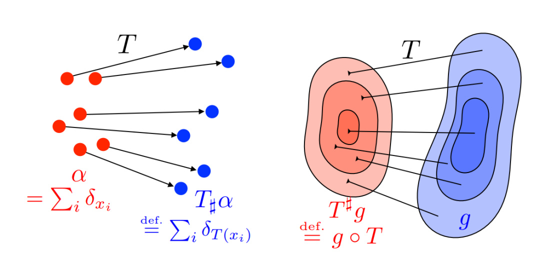
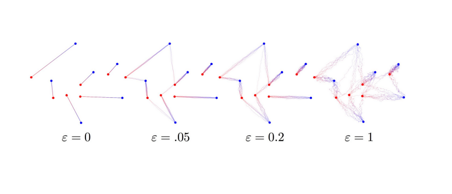


... as entropy minimization w.r.t. the law of Brownian Motion



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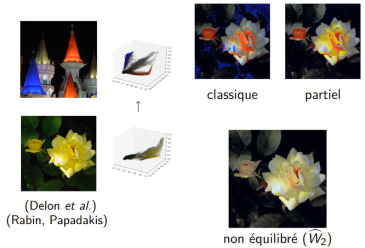

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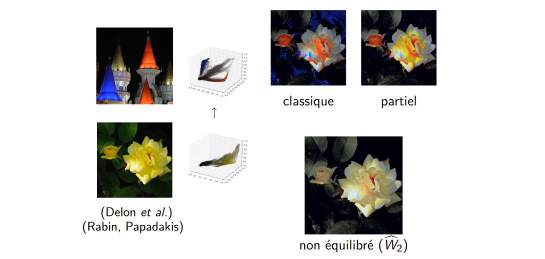
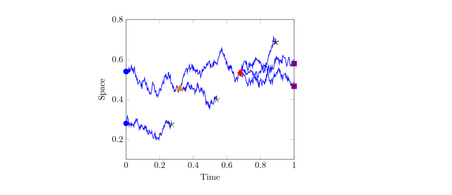


... as entropy minimization w.r.t. the law of Branching Brownian Motion



Today

Goal of this presentation

Show an **equivalence** between two problems of calculus of variations:

- The dynamical formulation (a.k.a Benamou Brenier formulation) of **regularized unbalanced optimal transport**.
- Entropy minimization with respect to the law of **branching Brownian Motion** (“Branching Schrödinger problem”).

Outline

1. The Schrödinger problem

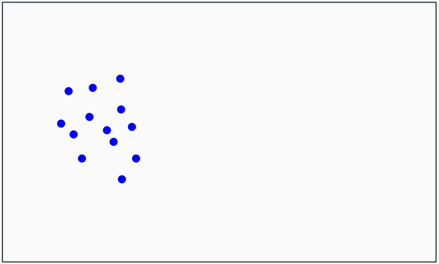
2. The branching Schrödinger problem

1. The Schrödinger problem

- Léonard (2013): A survey of the Schrödinger problem and some of its connections with optimal transport;
- Gentil, Léonard, and Ripani (2017): About the analogy between optimal transport and minimal entropy.

A problem coming from Large deviation

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



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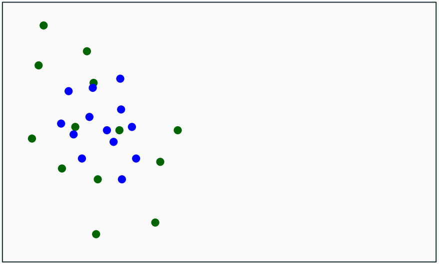

Expected distribution at time $t = 1$, $\sim \mathcal{N}(0,1) \star \alpha$.

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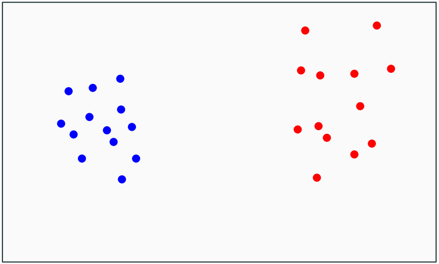

Observed distribution at time $t = 1$, $\beta \neq \mathcal{N}(0,1) \star \alpha$.

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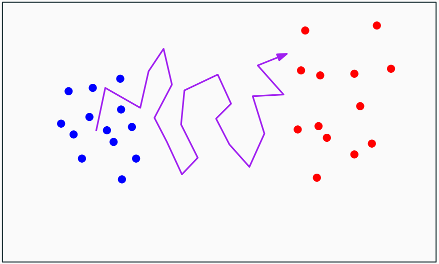

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The problem

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

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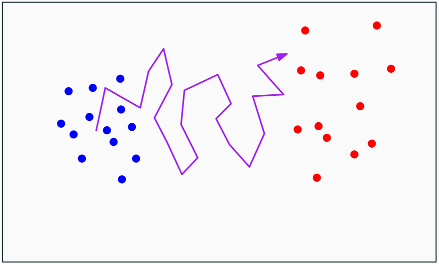

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Theory of Large Deviation: **entropy minimization** with respect to the law of Brownian motion.

Schrödinger problem and Regularized Optimal Transport

State space $\mathbb{T}^d$ the d-dimensional torus, $\alpha, \beta \in \mathcal{P}(\mathbb{T}^d)$ and $\nu > 0$.

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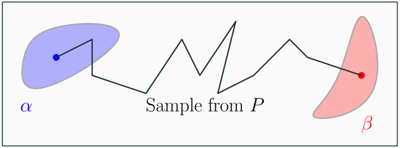
Space $\Omega = C([0,1], \mathbb{T}^d)$. $R^\nu \in \mathcal{P}(\Omega)$ Wiener measure with diffusivity ν and $X_0 \sim \mathcal{L} = \mathrm{d}x$ under R^ν.

The Schrödinger problem

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

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

such that $X_0 \sim \alpha$ and $X_1 \sim \beta$ under P.



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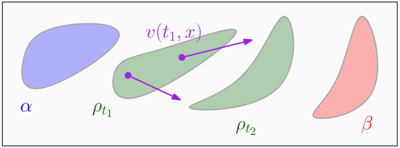
Regularized Optimal Transport

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

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

such that $\rho_0 = \alpha$, $\rho_1 = \beta$ and

$$\partial_t \rho + \mathrm{div}(\rho v) = \frac{\nu}{2} \Delta \rho$$



Equivalence between the problems

Both problems are well-posed if $H(\alpha|\mathcal{L}), H(\beta|\mathcal{L}) < +\infty$.

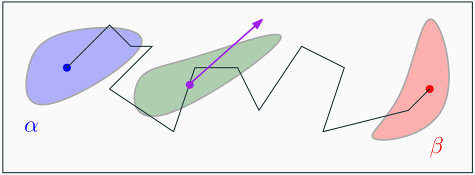
From Schrödinger to ROT

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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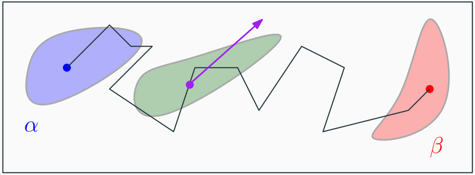
From ROT to Schrödinger

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

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

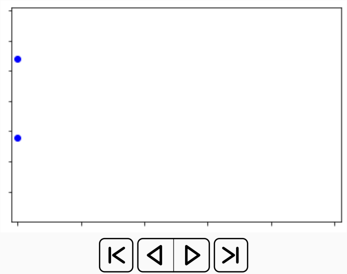
Moreover, if (ρ, v) and P optimal then P is the law of the SDE with drift v.

2. The branching Schrödinger problem

- Liero, Mielke, and Savaré (2018): Optimal entropy-transport problems and a new Hellinger–Kantorovich distance between positive measures;
- Chizat (2017): Unbalanced optimal transport: Models, numerical methods, applications;
- Kondratyev, Monsaingeon, and Vorotnikov (2016): A new optimal transport distance on the space of finite Radon measures;
- Baradat and Lavenant (2021): Arxiv 2111.01666.

The Branching Brownian motion

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



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

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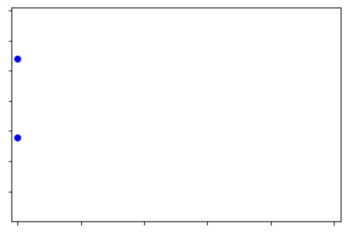

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At time t, random **measure** $M_t = \sum_{X \in \{\text{particles alive at time } t\}} \delta_X$.

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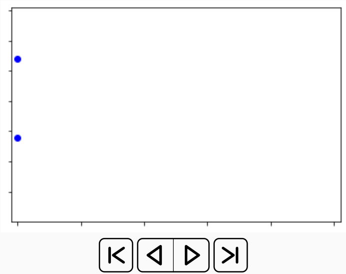

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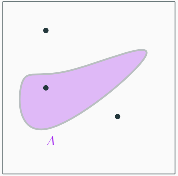
Description

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

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

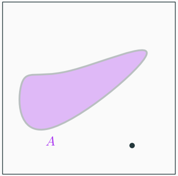
The Branching Schrödinger problem



$M_t(A) = 1$

$\mathbb{E}_P[M_t]$ 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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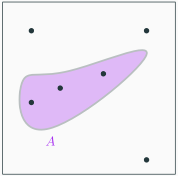
The Branching Schrödinger problem



$M_t(A) = 3$

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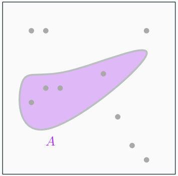
The Branching Schrödinger problem



$\mathbb{E}[M_t](A) = 4/3$

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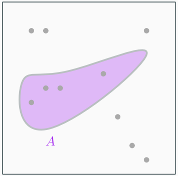
The Branching Schrödinger problem



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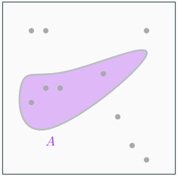
R law of the Branching Brownian Motion with parameters ν, λ and (p_k).

Branching Schrödinger problem

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

The Branching Schrödinger problem



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

$$\{P \ : \ \mathbb{E}_P[M_0] = \alpha \text{ and } \mathbb{E}_P[M_1] = \beta\}$$

is not closed for a topology making $H(\cdot|R)$ continuous.

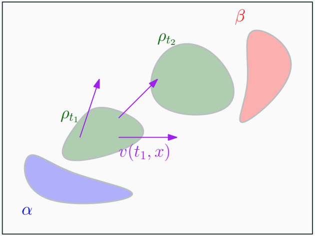
The regularized unbalanced optimal transport problem

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 $\partial_t \rho + \mathrm{div}(\rho v) = \frac{\nu}{2} \Delta \rho$.



The regularized unbalanced optimal transport problem

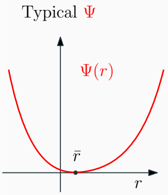
$\Psi : \mathbb{R} \to [0, +\infty]$ convex function. The field $r = r(t,x)$ is the **growth rate**.

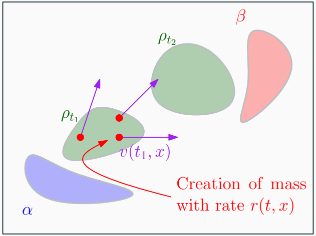
Regularized Unbalanced Optimal Transport

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 $\partial_t \rho + \mathrm{div}(\rho v) = \frac{\nu}{2} \Delta \rho + r\rho$.





The regularized unbalanced optimal transport problem

$\Psi : \mathbb{R} \to [0, +\infty]$ convex function. The field $r = r(t, x)$ is the **growth rate**.

Regularized Unbalanced Optimal Transport

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

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

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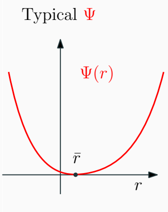

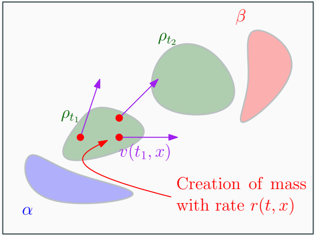

If Ψ grows polynomially at $+\infty$ and $H(\beta|\mathcal{L}) < +\infty$, then well posed.

Equivalence of the values

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

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

$$\mathrm{BrSch}(\alpha, \beta) := \inf_{P} \{ \nu H(P|R) \ : \ \mathbb{E}_P[M_0] = \alpha \text{ and } \mathbb{E}_P[M_1] = \beta \} .$$

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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:

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

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The function $(\alpha, \beta) \mapsto \nu L^*(\alpha) + \mathrm{Ruot}(\alpha, \beta)$ is the lower semi continuous envelope of $(\alpha, \beta) \mapsto \mathrm{BrSch}(\alpha, \beta)$ for the topology of weak convergence.

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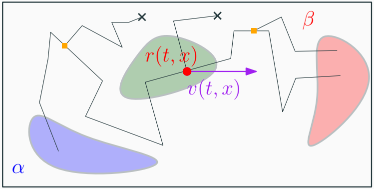
Idea of the proof: **duality**.

Equivalence of the competitors

Additional assumption: one finite exponential moment for M_0 and (p_k).



Intuition: as before v drift, $r = \sum_{k=0}^{+\infty}(k-1)\tilde{\lambda}\tilde{p}_k$ for modified branching rate $\tilde{\lambda}$, modified law of offsprings $(\tilde{p}_k)_{k\in\mathbb{N}}$.

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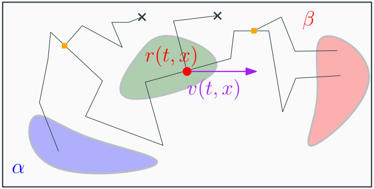

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From Branching Schrödinger to RUOT

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 $\tilde{v}$, $\tilde{\lambda}$ and $(\tilde{p}_k)_{k\in\mathbb{N}}$.

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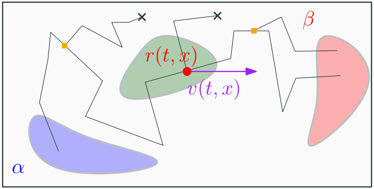

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From RUOT to Branching Schrödinger

Up to smoothing everything (including α, β) from (ρ, v, r) admissible we build a BBM with drift v and $\tilde{\lambda}$, $(\tilde{p}_k)_{k\in\mathbb{N}}$ 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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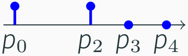
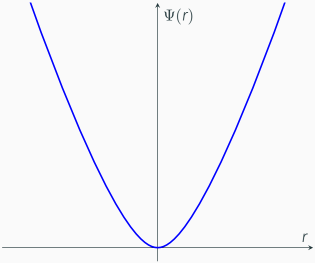
If $p_0 = p_2 = 1/2$ then



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

Ψ convex, minimal for $r = 0$.



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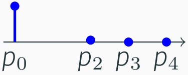
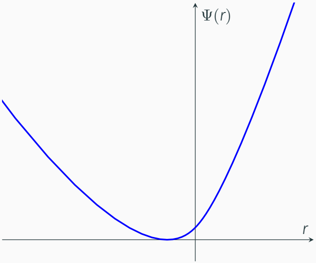
If $p_0 = 0.95$, $p_2 = 0.05$



then Ψ minimal for $\bar{r} < 0$.



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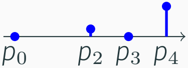
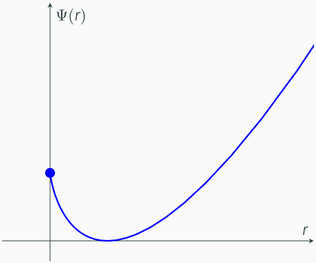
If $p_2 = 0.2$, $p_4 = 0.8$ (no killing allowed),



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



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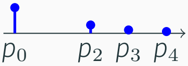
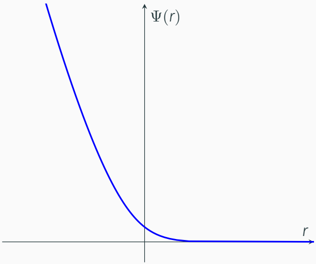
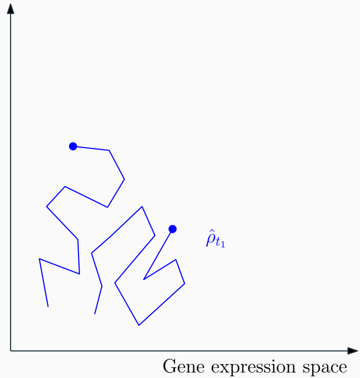
If $p_k = 1/(k-1)^{2.2}$, and $p_0 = 1 - \sum_{k \geq 2} p_k$ (no exponential moment)



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



One motivation: biology



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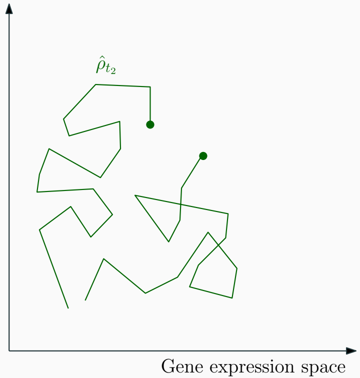

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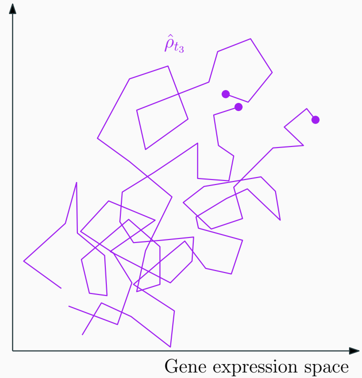

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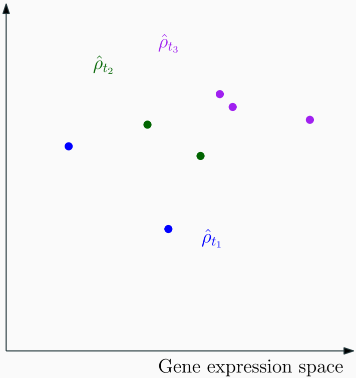

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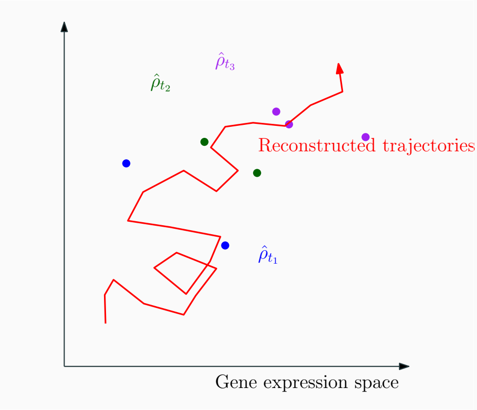

Idea: use the optimal transport to reconstruct the temporal couplings.

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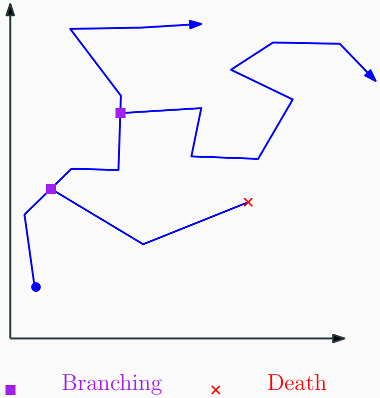

In reality cells divided and die.

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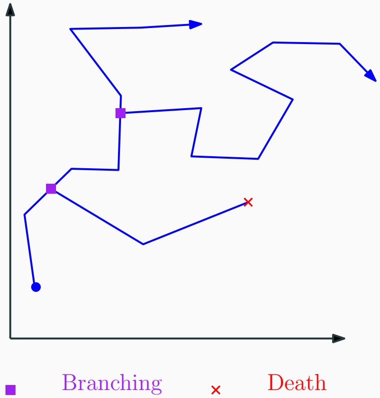

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Use **unbalanced** optimal transport to account for cell division.

Conclusion

What I have not presented:

- Proofs 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.
- Formal computations for other measure valued processes.

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Thank you for your attention

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 $v = 0$).