Causal optimal transport and the Brownian transport map

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Joint work with Yair Shenfeld

Transport maps

Let $X \sim \mu$ be a measure on $\mathbb{R}^d$ and let $G \sim \gamma$ stand for the standard Gaussian.

If φ is such that $\varphi(G) \overset{law}{=} X$, we call φ a *transport map*.

The existence and properties of such maps are useful for:

- Generative models and sampling algorithms.

- Understanding analytic properties of μ.

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Optimal transport

> **Definition (Wasserstein distance between μ and γ)**
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> $$\mathcal{W}_2(\mu, \gamma) := \inf_{\pi} \left\{ \mathbb{E}_\pi \left[||x - y||^2 \right] \right\}^{1/2}$$
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> where π ranges over all possible couplings of μ and γ.

Brenier 87': There exists a transport map $\psi^{\mathrm{opt}} : \mathbb{R}^d \to \mathbb{R}^d$:

$$\mathbb{E} \left[||\psi^{\mathrm{opt}}(G) - G||^2 \right] = \mathcal{W}_2^2(\mu, \gamma).$$

Caffarelli 00': If μ is more log-concave than γ_d, ψ^{opt} is 1-Lipschitz.

(strong log-concavity: $-\nabla^2 \log \left(\frac{d\mu}{dx}(x) \right) \succeq \mathrm{Id}.$)

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Gaussian Poincaré inequality: For any test function f,

$$\mathrm{Var}(f(G)) \leq \mathbb{E}\left[\|\nabla f(G)\|^2\right].$$

In general, $X \sim \mu$ satisfies a Poincaré inequality with constant $C_{\mathrm{p}}(\mu) > 0$, if,

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Theorem (Brascamp-Lieb 76')

If μ is more log-concave than γ_d, then $C_{\mathrm{p}}(\mu) \leq 1$.

Proof (Cordero-Erausquin 02').

$$\mathrm{Var}_{\mu}(f) = \mathrm{Var}_{\gamma_d}(f \circ \psi^{\mathrm{opt}}) \leq \mathbb{E}_{\gamma_d}\left[\|\nabla\left(f \circ \psi^{\mathrm{opt}}\right)\|^2\right]$$
$$\leq \mathbb{E}_{\gamma_d}\left[\|\nabla\psi^{\mathrm{opt}}\|^2\|\nabla f(\psi^{\mathrm{opt}})\|^2\right] = \mathbb{E}_{\mu}\left[\|\nabla f\|^2\right].$$

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$\square$

If μ is log-concave, but compactly supported on a ball of diameter R, then $\mathrm{C_p}(\mu) \lesssim R^2$. Several proofs exists:

- Localization (Payne-Weinberger)
- Refined Brascamp-Lieb (Kolesnikov-Milman)
- Moment Maps (Klartag)

Question

For such μ is it necessarily true that there exists an R-Lipschitz φ with $\varphi_* \gamma_d = \mu$?

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A positive answer will not only recover known result but will also imply:

1. Dimension-free Φ-Sobolev inequalities (generalizing both Poincaré and log-Sobolev).
2. Bounds for higher eigenvalues of the weighted Laplacian.
3. Isoperimetric inequalities.
4. Improved rates of convergence for the CLT.

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We call $\mu = \gamma_d \star \nu$ a Gaussian mixture. It was recently proved by

Bardet, Gozlan, Malrieu and Zitt that if $\mathrm{diam}(\mathrm{supp}(\nu)) \leq R$, then

$$\mathrm{C_p}(\mu) \lesssim e^{R^2}.$$

Later, Chen,Chewi and Niles-Weed extended the result to the log-Sobolev inequality.

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Let μ be log-concave and isotropic,

$$\int_{\mathbb{R}^d} x\,d\mu(x) = 0 \quad \int_{\mathbb{R}^d} x \otimes x\,d\mu(x) = \mathrm{Id}.$$

A famous conjecture of Kannan-Lovász-Simonovits postulates,

$$C_{\mathrm{p}}(\mu) \leq C.$$

Current best bound, due to Klartag and Lehec (building upon Chen): $C_{\mathrm{p}}(\mu) \leq \mathrm{polylog}(d)$.

It seems natural to ask whether we can find a Lipschitz map φ with $\varphi_* \gamma_d = \mu$?

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- In general, one cannot find a Lipschitz transport map from γ_d to μ.

- The existence of such map implies sub-Gaussian tails of μ, which is not true for all isotropic log-concave measures.

- However, E. Milman showed that for KLS, it is enough to have map which is 'Lipschitz on average'.

Question

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By slightly altering our perspective, we give a positive answer to the previous questions.

Let $\Omega := C([0,1], \mathbb{R}^d)$ stand for the Wiener space with the Wiener measure γ. We will let $(B_t)_{t \in [0,1]}$ denote a Brownian motion.

We consider Lipschitz mappings $\Phi : \Omega \to \mathbb{R}^d$ with $D\Phi$ bounded almost surely.

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Theorem (M.-Shenfeld)

Let μ be a measure on $\mathbb{R}^d$. There exists map $\Phi : \Omega \to \mathbb{R}^d$, with $\Phi_* \gamma = \mu$ and

1. *If μ is log-concave with $\mathrm{diam}(\mathrm{supp}(\mu)) \leq R$,*

$$\|D\Phi\| \leq R.$$

2. *If $\mu = \gamma_d \star \nu$ and $\mathrm{diam}(\mathrm{supp}(\nu)) \leq R$,*

$$\|D\Phi\| \leq e^{R^2}.$$

3. *If μ is log-concave and isotropic,*

$$\mathbb{E}_\gamma \left[\|D\Phi\|^2 \right] \leq d^{o(1)} \, \mathrm{polylog}(d).$$

Recall the Cameron-Martin space

$$H := \{h \in \Omega | h_t = \int_0^t \dot{h}_s ds\}.$$

It is also characterized by the fact that $B_t + g$ is absolutely continuous with respect to γ, iff $g \in H$.

Heuristically, for a a random variable F we define the Malliavin derivative DF, as the Gateaux derivative in the H directions.

Malliavin calculus 101

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H has a natural inner product, $\langle h, h' \rangle_H := \int\limits_0^1 \dot{h}_t \dot{h}'_t dt$. Observe that $DF : \Omega \to H$ and we denote by DF_t, by $D_t F$.

We say that a map F is R-Lipschitz (in the H directions), if $\|DF\|_H \leq R$ almost surely. This definition is justified, since

$$\mathrm{Var}_\gamma(F) \leq \mathbb{E}_\gamma \left[\|DF\|_H^2 \right].$$

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We can mimic Caffareli's Euclidean optimal transport result. Two main issues to address:

- Need to define a Wasserstein metric on Ω.

- Need to embed μ in Ω.

First, define a metric, which is compatible with H:

$$d_H(\omega, \omega') = \begin{cases} \|\omega - \omega'\|_H & \text{if } \omega - \omega' \in H \\ \infty & \text{otherwise} \end{cases}.$$

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First attempt

Define a measure $\tilde{\mu}$ on Ω by

$$\frac{d\tilde{\mu}}{d\gamma}(\omega) = \frac{d\mu}{d\gamma_d}(\omega_1),$$

and consider,

$$\min_{\Psi_*\gamma=\tilde{\mu}} \mathbb{E}\left[d_H\left(\Psi(B.), B.\right)^2\right].$$

Equivalently,

$$\min_{u_t} \mathbb{E}\left[\int_0^1 \|u_t\|^2 dt\right],$$

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Define $v_t^{\mathrm{opt}} := \arg\min_{u_t} \mathbb{E}\left[\int\limits_0^1 \|u_t\|^2 dt\right]$.

Then, $v_t^{\mathrm{opt}}(\omega) = \psi^{\mathrm{opt}}(\omega_1) - \omega_1$, and $\Phi^{\mathrm{opt}}(\omega) = \omega + \int v_t dt$ satisfies,

- $\Phi_*^{\mathrm{opt}}\gamma = \tilde{\mu}$.

- $(\Phi_1^{\mathrm{opt}})_*\gamma = \mu$.

This is unsatisfactory.

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We consider an optimization problem adapted to the filtration of B_t.

Define $v_t := \arg \min_{u_t \text{ adapated}} \mathbb{E} \left[\int_0^1 \|u_t\|^2 dt \right]$ and $dX_t = dB_t + v_t dt$.

Facts:

- $X_1 \sim \mu$ (this is the transport map).

- $\text{Ent}(\mu\|\gamma) = \frac{1}{2} \int_0^1 \mathbb{E}[\|v_t\|^2] dt$.

- v_t is a martingale, with $v_t(X_t) = \nabla \ln \left(P_{1-t} \left(\frac{d\mu}{d\gamma_d}(X_t) \right) \right)$.

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The Föllmer Drift - (Some) History

- Analogous problems were already considered by in the 30's, by Schrödinger.

- The process itself was first studied by Föllmer, in 85', who used it to derive a variational expression for entropy.

- It appeared implicitly in the works of Feyel and Üstünel, from 2004, in their study of infinite dimensional transportation problems.

- In the context of functional inequalities, the use of the Föllmer process was pioneered by Lehec in 2012.

- Lassalle identified the process as the solution to a causal transportation problem in 2013.

Recall that $X_1 = B_1 + \int\limits_0^1 \nabla \ln \left(P_{1-t} \frac{d\mu}{d\gamma_d}(X_t) \right) dt$. It can be shown that

$$DX_t = \mathrm{I}_d + \int\limits_0^t \nabla^2 \ln \left(P_{1-s} \frac{d\mu}{d\gamma_d}(X_s) \right) DX_s ds.$$

We write $\nabla v_t := \nabla^2 \ln \left(P_{1-t} \frac{d\mu}{d\gamma_d}(X_t) \right)$ and for $h \in H$, we calculate,

$$f_h(t) := \langle DX_t, h \rangle_H = \int\limits_0^t \dot{h}_s ds + \int\limits_0^t \nabla v_t \langle DX_s, h \rangle_H ds.$$

In particular,

$$\frac{d}{dt} f_h(t) = \dot{h}_t - \nabla v_t f_h(t).$$

The Brownian transport map

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In particular,

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Solving this differential equation, we get, for every $h \in H$,

$$f_h(1) = \int_0^1 e^{\int_t^1 \nabla v_s ds} \cdot \dot{h}(t) dt.$$

So,

$$D_t X_1 = e^{\int_t^1 \nabla v_s ds},$$

and

$$\|DX_1\|_H^2 = \int_0^1 e^{2 \int_t^1 \nabla v_s ds} dt.$$

The Brownian transport map

Direct calculations show,

$$\nabla v_t := \nabla^2 \ln \left(P_{1-t} \frac{d\mu}{d\gamma}(X_t) \right) = \frac{\mathrm{Cov}(\mu_t)}{(1-t)^2} - \frac{1}{1-t} \mathrm{I}_d,$$

where

$$\frac{d\mu_t}{dx} \propto \frac{d\mu}{d\gamma_d}(x) e^{\frac{-(x-X_t)^2}{2(1-t)}}.$$

If $\mathrm{diam}(\mathrm{supp}(\mu)) \leq R$, clearly,

$$\nabla v_t \leq \frac{R^2}{(1-t)^2} - \frac{1}{1-t}.$$

Moreover, by Brascamp-Lieb, if μ is log-concave,

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The Brownian transport map

Direct calculations show,

$$\nabla v_t := \nabla^2 \ln \left(P_{1-t} \frac{d\mu}{d\gamma}(X_t) \right) = \frac{\mathrm{Cov}(\mu_t)}{(1-t)^2} - \frac{1}{1-t} \mathrm{I}_d,$$

where

$$\frac{d\mu_t}{dx} \propto \frac{d\mu}{d\gamma_d}(x) e^{\frac{-(x-X_t)^2}{2(1-t)}}.$$

If $\mathrm{diam}(\mathrm{supp}(\mu)) \leq R$, clearly,

$$\nabla v_t \leq \frac{R^2}{(1-t)^2} - \frac{1}{1-t}.$$

Moreover, by Brascamp-Lieb, if μ is log-concave,

$$\nabla v_t \leq \frac{1}{t}.$$

We apply the two inequalities to $\|DX_1\|_H^2 = \int\limits_0^1 e^{2\int_t^1 \nabla v_s ds} dt$

Theorem (M.- Shenfeld)

Consider X_1 as a map from $\Omega = C([0,1], \mathbb{R}^d)$ to $\mathbb{R}^d$.

1. *If μ is log-concave with $\mathrm{diam}(\mathrm{supp}(\mu)) \leq R$,*

$$\|DX_1\| \leq R.$$

2. *If $\mu = \gamma_d \star \nu$ and $\mathrm{diam}(\mathrm{supp}(\nu)) \leq R$,*

$$\|DX_1\| \leq e^{R^2}.$$

- The second result follows by showing $\nabla v_t \leq R^2$.

- Can be extended to semi-log concave measures.

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We have demonstrated a Lipschitz map $X_1 : \Omega \to \mathbb{R}^d$.

It seems natural to ask whether $X. : \Omega \to \Omega$ is Lipschitz as well?

It turns out that there exist strongly log-concave measures, for which $X.$ is not Lipschitz, for any constant. This is contrast to the optimal transport map Ψ^{opt}, which is provably 1-Lipschitz.

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Future directions

- Can the results be extended to larger classes of measures?

- What about similar, but different, constructions on the Wiener space?

- Can similar results be proved for maps between finite dimensional spaces?

- In particular, can the results be recovered for the Brenier map?

Thank You

The KLS connection

Instead of applying point-wise bounds, we could estimate

$$\mathbb{E}\left[\|DX_1\|_H^2\right] = \mathbb{E}\left[\int_0^1 e^{2\int_t^1 \nabla v_s(X_s)ds}\right].$$

For isotropic μ, define $\tau = \frac{1}{2} \wedge \inf\{t | \nabla v_t(X_t) \geq 2\}$.

$$\int_0^1 \nabla v_t(X_t) \leq 2 + \int_\tau^1 \frac{1}{t}dt = 2 + \log(\tau).$$

So,

$$\mathbb{E}\left[\|DX_1\|_H^2\right] \leq e^4 \mathbb{E}\left[\frac{1}{\tau^2}\right].$$

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The KLS connection

With the recent result of Yuansi Chen about the KLS constant, we prove:

<div>

Theorem

Let μ be an isotropic log-concave vector in $\mathbb{R}^d$. Then,

$$\mathbb{E}\left[\|DX_1\|_H^2\right] = d^{o(1)}.$$

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