New estimates on the matching problem[1]

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[1] Joint work with Federico Stra and Dario Trevisan

Outline

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Matching problems

Generally speaking, matching problems deal with families of random M points, independent and identically distributed in a given d-dimensional domain D.

The problem is then to estimate (since exact computations are basically impossible, except in some 1-d cases) the cost, for M large, of the optimal matching (optimal transport).

The results depend in a very sensitive way on d and on the power p of the cost function $c = \mathrm{dist}^p$. Typical domains: $D = [0,1]^d$, $D = \mathbb{T}^d$.

Our result, based on semigroup techniques, covers also more general domains, with $d = 1, 2$.

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Matching problems

• **Bipartite problem:** $M = 2N$, with N blue points, N red points, and we want to match each red point to a blue point, so that the problem is about the rate of convergence to 0 of

$$\mathbb{E}\Big(W_2^2\big(\tfrac{1}{N}\sum_i \delta_{X_i}, \tfrac{1}{N}\sum_i \delta_{Y_i}\big)\Big).$$

• **Monopartite problem:** $M = 2N$, but the points are not coloured (or coloured, but free to marry another point with the same colour).

• **Optimal matching to the common law.** If $\boldsymbol{m}$ is the common law of the X_i, we want to know the rate of convergence to 0 of

$$\mathbb{E}\Big(W_2^2\big(\tfrac{1}{N}\sum_i \delta_{X_i}, \boldsymbol{m}\big)\Big).$$

• **Grid matching problem.** Given a deterministic grid of "equally spaced" points, $Y_1, \ldots, Y_N$, estimate

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Three level of investigation

(1) Find tight upper and lower bounds:

$$C^{-1}\phi_{p,d}(N) \le \mathbb{E}(W_p^p) \le C\phi_{p,d}(N);$$

(2) Prove the existence of the limit of renormalized expectations, possibly computing/characterizing the limit:

$$\exists \ell_{p,d} := \lim_{N\to\infty} \frac{\mathbb{E}(W_p^p)}{\phi_{p,d}(N)};$$

(3) Find the second term in the expansion:

$$\mathbb{E}(W_p^p) \sim \ell_{p,d}\phi_{p,d}(N) + \phi^*_{p,d}(N) + o\big(\phi^*_{p,d}(N)\big).$$

Heuristics

Since we have N points in a d-dimensional domain, say $(0,1)^d$, we expect an average distance $\sim N^{-1/d}$, and so the naive guess is

$$\mathbb{E}\Big(W_p^p\big(\frac{1}{N}\sum_{i=1}^N \delta_{X_i}, \boldsymbol{m}\big)\Big) \sim \frac{1}{N^{p/d}}.$$

Using the random 1-Lipschitz function $\phi(z) := \min_i |z - X_i|$, Kantorovich duality gives indeed

$$\mathbb{E}\Big(W_p^p\big(\frac{1}{N}\sum_{i=1}^N \delta_{X_i}, \boldsymbol{m}\big)\Big) \gtrsim \frac{1}{N^{p/d}}.$$

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However, this lower bound is tight for $d > 2$, but *not* tight for $d = 2$, where a logarithmic correction appears:

Theorem. (Ajtai-Komlos-Turnady, Combinatorica, 1984) *For* $D = (0,1)^2$ *and all* $p \geq 1$, *there exists* $c_p \in (0, \infty)$ *such that*

$$c_p^{-1} \frac{(\log N)^{p/2}}{N^{p/2}} \leq \mathbb{E}\big(W_p^p(\frac{1}{N}\sum_{i=1}^N \delta_{X_i}, \boldsymbol{m})\big) \leq c_p \frac{(\log N)^{p/2}}{N^{p/2}}.$$

In physicist's words, *this is due to the fluctuations in the number of points, in small regions, which imply the necessity of "long distance pairings".*

If $d = 1$ we have even a larger deviation: $N^p \mathbb{E}(W_p^p) \sim N^{p/2}$. In the 1-d case many explicity computations are possible (Bobkov-Ledoux), for instance $\mathbb{E}(W_2^2(\mu^N, \boldsymbol{m})) = \frac{1}{6N}$ for any N if $D = (0,1)$.

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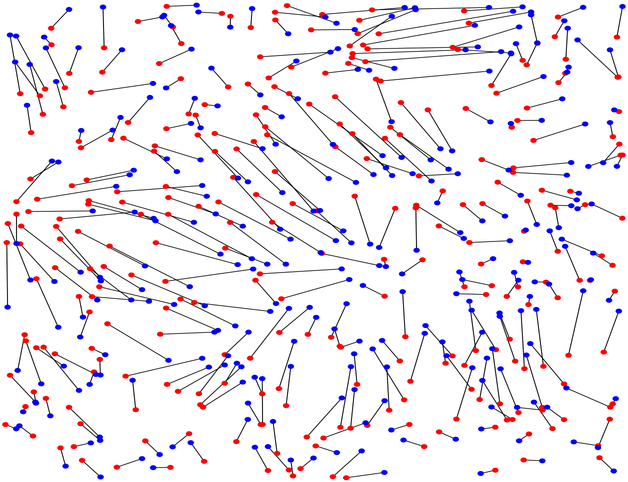

Convergence of empirical measures

By the law of large numbers, for any nice test function f one has

$$\frac{1}{N}\sum_i f(X_i) - \int f\, d\boldsymbol{m} \to 0 \quad \text{almost surely,}$$

which means that $\frac{1}{N}\sum_i \delta_{X_i} \to \boldsymbol{m}$ weakly as $N \to \infty$. Obviously we need a quantitative version of this fact, for instance the central limit theorem tells that

$$\sqrt{N}\Big(\frac{1}{N}\sum_i f(X_i) - \int f\, d\boldsymbol{m}\Big) \quad \text{weakly converge to a centered Gaussian.}$$

Another information comes from Sanov's theorem, which gives

$$\mathbb{E}\Big(W_p\big(\frac{1}{N}\sum_i \delta_{X_i}, \boldsymbol{m}\big) > \epsilon\Big) \sim e^{-N\alpha(\epsilon)} \qquad \alpha(\epsilon) := \inf\Big\{\mathrm{Ent}_{\boldsymbol{m}}(\nu) :\ W_p(\nu, \boldsymbol{m}) \geq \epsilon\Big\}.$$

However these estimates are valid, for $\epsilon > 0$ fixed, for $N \geq N(\epsilon)$, and therefore useless to estimate $\mathbb{E}\big(W_p^p(\frac{1}{N}\sum_i \delta_{X_i}, \boldsymbol{m})\big)$.

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Some results

Theorem. (Talagrand, Annals Appl. Prob., 1992) For $D = [0,1]^d$ and $d \geq 3$,

$$\limsup_{N\to\infty} N^{1/d}\mathbb{E}\big(W_1(\frac{1}{N}\sum_{i=1}^{N}\delta_{X_i}, \boldsymbol{m})\big) \leq \omega_d^{-1/d}\big(1 + K\frac{\log d}{d}\big).$$

Theorem. (Dobric-Yukich, J. Th. Prob., 1995) *If $d \geq 3$, $D = (0,1)^d$ and $\boldsymbol{m} = \rho\mathscr{L}^d$, then*

$$\lim_{N\to\infty} N^{1/d}\,\mathbb{E}\big(W_1(\frac{1}{N}\sum_{i=1}^{N}\delta_{X_i}, \boldsymbol{m})\big) = \beta(d)\int_D \rho^{1-1/d}\,dx$$

for some constant $\beta(d)$.

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More probabilistic techniques

This topic is well illustrated in the 2014 monograph "Upper and lower bounds for stochastic processes" by Talagrand, particularly in the case $p = 1$.

The general idea, first developed in the Gaussian setting, is to estimate the expectation of the supremum

$$V := \sup_{u \in U} Z_u$$

of a centered stochastic process $\{Z_u\}_{u \in U}$ knowing the law of the random variables Z_u and the "metric" information

$$\left(\mathbb{E}(|Z_u - Z_v|^2)\right)^{1/2} \leq \rho(u, v).$$

This leads to bounds of the form (Dudley)

$$\mathbb{E}\big(\sup_{v \in B_\delta(u)} |Z_v - Z_u|\big) \leq C \int_0^\delta \sqrt{\log n(U, \rho, \epsilon)}\, d\epsilon \qquad \forall \delta > 0,$$

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where $n(U, \rho, \epsilon)$ is the minimum number n of balls with radius ϵ needed to cover U, so the geometry of the space of parameters (U, ρ) comes into play.

More probabilistic techniques

Using Kantorovich duality, this technique can be applied with $U = \mathrm{Lip}_1(D)$, and

$$Z_u(\omega) := \int_D u\, d\boldsymbol{m} - \sum_{i=1}^N \frac{u(X_i(\omega))}{N}.$$

This technique is very general and powerful, but it does not seem to provide more than tight upper and lower bounds. Indeed, Talagrand raises (Research problem 4.3.3) the question about the existence of the limit

$$\lim_{N\to\infty} \sqrt{\frac{N}{\log N}}\, \mathbb{E}\big(W_1(\sum_{i=1}^N \frac{1}{N}\delta_{X_i}, \boldsymbol{m})\big)$$

in the 2-d case.

Moreover, when we consider W_2, we are forced to consider, as space of parameters U, the space of $d^2/2$-concave functions, and these arguments do not seem to be applicable, because the "geometry" of this space is harder.

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In a recent work (*Scaling hypothesis for the Euclidean bipartite matching problem*, Physical Review E, 2014), Caracciolo-Lucibello-Parisi-Sicuro used a specific ansatz to make predictions on the expansion of $\mathbb{E}\big(W_p^p(\rho_0, \rho_1)\big)$, in the case $D = \mathbb{T}^d$.

Predictions:

$$\frac{\mathbb{E}\big(W_p^p(\rho_0,\rho_1)\big)}{N^{-p/d}} \sim \begin{cases} \text{for } d = 1,\ O(N^{p/2}) \text{ and } \frac{N}{6} \text{ for } p = 2; \\ \text{for } d = 2,\ O((\log N)^{p/2}), \text{ and } \frac{1}{2\pi}\log N + e_{2,2} \text{ for } p = 2; \\ \text{for } d > 2,\ e_{p,d} + O(N^{(2-d)/d}); \\ \text{for } d > 2 \text{ and } p = 2,\ e_{2,d} + \frac{\zeta_d(1)}{2\pi^2} N^{(2-d)/d}. \end{cases}$$

The correctedness of the constants in blue, relative to W_2 and computed with the ansatz, has also been validated numerically (ζ_d is the so-called Epstein function). However, the method does not predict the constant in the leading order term with $d > 2$!

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These predictions are obtained by linearizing *in C^1 topology* the Monge-Ampére equation

$$\det \nabla^2 \psi = \frac{\rho_0}{\rho_1 \circ \nabla \psi}$$

(which describes the optimal map from ρ_0 to ρ_1) around $\rho_0 = \rho_1 = 1$, thus writing $\psi = Id + \nabla \phi$ one obtains

$$-\Delta \phi = \rho_1 - \rho_0.$$

The ansatz says that $\nabla \phi$ should be "close" to the optimal displacement map and the predictions come from the computation of $\mathbb{E}(|\nabla \phi|^2)$, in discrete Fourier variables:

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But, the empirical measures ρ_0 and ρ_1 *do not* belong to $H^{-1}(\mathbb{T}^d)$ as soon as $d > 1$, hence this energy is infinite for every ω!

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By mathematical standards, the proof of these predictions is not rigorous, first of all because of the appearence of divergent quantities, but also because in any case the ansatz does not provide a coupling between ρ_0 and ρ_1, only an approximate one, in some sense.

In any case, even if this were an exact coupling, the necessity of *lower* bounds (or the necessity to estimate how close it is to being optimal) remains.

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Main result

Theorem. *Let D be a smooth, closed, 2-dimensional Riemannian manifold with finite volume. Then, if $\boldsymbol{m}$ is the normalization of Riemannian volume measure, one has*

$$\lim_{N\to\infty} \frac{N}{\log N}\, \mathbb{E}\Big(W_2^2\big(\sum_{i=1}^N \frac{1}{N}\delta_{X_i}, \boldsymbol{m}\big)\Big) = \frac{\boldsymbol{m}(D)}{4\pi}.$$

An analogous result is proved in the 1-d case.

The case $D = \mathbb{T}^2$ is included, our "PDE" proof use semigroup techniques and spectral analysis, for this reason it works for general domains. We also cover the case $D = (0,1)^2$, with a *ad hoc* comparison argument.

Standard techniques related to the phenomenon of concentration of measure (Gaussian concentration due to Ricci lower bounds) then give also that the random variables

$$\frac{N}{\log N} W_2^2\big(\sum_{i=1}^N \frac{1}{N}\delta_{X_i}, \boldsymbol{m}\big)$$

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$$c_p^{-1} \frac{(\log N)^{p/2}}{N^{p/2}} \leq \mathbb{E}\Big(W_p^p\big(\frac{1}{N}\sum_{i=1}^N \delta_{X_i}, \boldsymbol{m}\big)\Big) \leq c_p \frac{(\log N)^{p/2}}{N^{p/2}}.$$

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Ideas from the proof: upper bound

The heuristic idea is very natural. Since we know that $\mathbb{E}(W_2^2) \sim N^{-1}\log N$ exceeds the square N of the "natural" length scale $\ell_N \sim N^{-1/2}$, we may hope to regularize just a bit the random densities $\rho \mapsto P_t\rho$, with $t = t_N = o(\frac{\log N}{N})$, so that one can apply the deterministic estimate (in "nice" domains)

$$W_2^2(P_t\rho, \rho) \le Ct = o\Big(\frac{\log N}{N}\Big).$$

Then, we can try to find an *exact* coupling between the regularized densities $P_t\rho_0$ and $P_t\rho_1$ and use the triangle inequality

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Dacorogna-Moser interpolation

Given "nice" probability densities $\rho_0,\ \rho_1$, one can find a transport map T from ρ_0 to ρ_1 as the solution at $t = 1$ of the ODE

$$\frac{d}{dt}\boldsymbol{X}(t,x) = \boldsymbol{b}_t\big(\boldsymbol{X}(t,x)\big), \qquad \boldsymbol{X}(0,x) = x,$$

where the vector field $\boldsymbol{b}_t$ is $\rho_t^{-1}\nabla\phi$ and ϕ can be found solving the elliptic PDE

$$-\mathrm{div}\big(\nabla\phi\big) = \rho_1 - \rho_0 = \frac{d}{dt}\rho_t \quad \text{(with Neumann b.c.)} \qquad (*)$$

with $\rho_t = (1-t)\rho_0 + t\rho_1$.

The reason (and the link with Benamou-Brenier) is that, since $\boldsymbol{b}_t\rho_t = -\nabla\phi$, the equation (*) above can be written in the form of continuity equation:

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One has then, with simple computations,

$$\begin{aligned} W_2^2(\rho_0,\rho_1) &\leq \int |T(x)-x|^2\rho_0(x)\,d\boldsymbol{m}(x) \leq \int_0^1 \left(\int \frac{|\nabla\phi|^2}{\rho_t}\,d\boldsymbol{m}\right)dt \\ &= \int\int_0^1 \frac{1}{(1-t)\rho_0+t\rho_1}\,dt\,|\nabla\phi|^2\,d\boldsymbol{m} = \int \frac{|\nabla\phi|^2}{M(\rho_0,\rho_1)}\,d\boldsymbol{m}. \end{aligned}$$

The quantity $M(a,b)=(a-b)/(\log a-\log b)$ above is the so-called *logarithmic mean* of a and b.

Dacorogna-Moser interpolation

One has then, with simple computations,

$$\begin{aligned} W_2^2(\rho_0,\rho_1) &\le \int |T(x)-x|^2\rho_0(x)\,d\boldsymbol{m}(x) \le \int_0^1 \left(\int \frac{|\nabla\phi|^2}{\rho_t}\,d\boldsymbol{m}\right)dt \\ &= \int\int_0^1 \frac{1}{(1-t)\rho_0+t\rho_1}\,dt\,|\nabla\phi|^2\,d\boldsymbol{m} = \int \frac{|\nabla\phi|^2}{M(\rho_0,\rho_1)}\,d\boldsymbol{m}. \end{aligned}$$

The quantity $M(a,b)=(a-b)/(\log a-\log b)$ above is the so-called *logarithmic mean* of a and b.

Ideas from the proof: upper bound

Eventually, with some computations based on semigroup techniques we find:

$$\begin{aligned}\frac{N}{\log N}\mathbb{E}(W_2^2(\rho_0,\rho_1)) &\lesssim \frac{N}{\log N}E\Big(\int \frac{|\nabla\phi|^2}{M(\rho_0,\rho_1)}\,d\boldsymbol{m}\Big)\\ &\sim \frac{N}{\log N}E\Big(\int |\nabla\phi|^2\,d\boldsymbol{m}\Big)\\ &\sim \frac{2}{\log N}\int_{1/N}^{\infty}\Big(\int p_{2t}(x,x)\,d\boldsymbol{m}(x)-1\Big)\,dt.\end{aligned}$$

The crucial quantity in this formula is $T(s) := \int p_s(x,x)\,d\boldsymbol{m}(x)$, which is related to the spectrum $\sigma(\Delta)$ of Δ by the *trace formula*

$$T(s) = \sum_{\lambda\in\sigma(\Delta)} e^{\lambda s}$$

(it is sufficient to write $p_t(x,y) = \sum_\lambda e^{\lambda t} f_\lambda(x) f_\lambda(y)$ with $y = x$ and integrate).

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It turns out that the relevant limit is

$$\lim_N \frac{2}{\log N} \int_{1/N}^{\infty} \Big(\int p_{2t}(x,x)\, d\boldsymbol{m}(x) - 1 \Big)\, dt = \lim_N \frac{2}{\log N} \int_{1/N}^{\infty} \sum_{\lambda \in \sigma(\Delta)\setminus\{0\}} e^{2\lambda t}\, dt.$$

One can then use the asymptotic formula (McKean, Brown)

$$T(s) = \frac{1}{4\pi s}\Big(\boldsymbol{m}(D) - \frac{\sqrt{\pi s}}{2} \mathscr{H}^1(\partial D) + o(\sqrt{s}) \Big) \quad \text{as } s \to 0$$

to compute the limit (we assume $\boldsymbol{m}(D) = 1$) to get

$$\limsup_{N\to\infty} \frac{N}{\log N} \mathbb{E}\Big(W_2^2 \big(\sum_{i=1}^N \frac{1}{N} \delta_{X_i}, \boldsymbol{m} \big) \Big) \le \frac{1}{4\pi}$$

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In the proof of the lower bound we use that D has no boundary, and let's assume that one of the densities, say ρ_1, is 1, we set $\rho_0 = \rho$.

For the lower bound it is natural to use Kantorovich duality: for any map ϕ one has

$$\frac{1}{2}W_2^2(\rho, 1) \geq -\int \phi\rho\, dm + \int Q_1\phi\, dm,$$

where $Q_t\phi$ is given by the Hopf-Lax formula

$$Q_t\phi(y) := \inf_{x\in D} \phi(x) + \frac{1}{2t}d^2(x,y) \quad \text{solving} \quad \frac{d}{dt}Q_t\phi + \frac{1}{2}|\nabla Q_t\phi|^2 = 0.$$

If we choose ϕ with the ansatz, namely $-\Delta\phi = 1 - \rho$, let us try to estimate the lower bound from below, getting the term we had in the upper bound:

$$\begin{aligned} -\int \phi\rho\, dm + \int Q_1\phi\, dm &= \int \phi(1-\rho)\, dm + \int (Q_1\phi - \phi)\, dm \\ &= \int |\nabla\phi|^2\, dm - \frac{1}{2}\int_0^1 \int |\nabla Q_s\phi|^2\, dm\, ds. \end{aligned}$$

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where the last step is justified by the estimate

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\int |\nabla Q_s\phi|^2\, d\boldsymbol{m} \le (1 + O(\|\Delta\phi\|_\infty)) \int |\nabla\phi|^2\, d\boldsymbol{m}.
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For instance, if D has nonnegative Ricci curvature, it comes from

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Recalling that ϕ solves the random PDE

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we need to show that $1 - \rho$ is small in L^∞ with high probability.

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The actual proof is a bit different, because $Q_t\phi$ is not so smooth. Hence, to prove the apriori estimates above on $\int |\nabla Q_s\phi|^2$ we use the regularized HJ equation

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whose solution is explicitly given by the Hopf-Cole transform

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and let $\sigma \to 0^+$ (here we need that D has no boundary).

Finally we achieve the case $D = (0,1)^2$ using the fact that the distance on the torus is smaller than the the distance on $(0,1)^2$, and that the proof of the upper bound works also for domains with boundary. Therefore a lower bound for $\mathbb{T}^2$ and an upper bound for $(0,1)^2$ provide the result for both.

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The bipartite case

In the case of bipartite matching (N blue points, N red points) we expect

$$\mathbb{E}\Big(W_2^2\big(\frac{1}{N}\sum_i \delta_{X_i}, \frac{1}{N}\sum_i \delta_{Y_i}\big)\Big) \sim 2\mathbb{E}\Big(W_2^2\big(\frac{1}{N}\sum_i \delta_{X_i}, \boldsymbol{m}\big)\Big).$$

The heuristic argument is that on small scales $\mathscr{P}_2(D)$ is Hilbertian, so that

$$|a+b|^2 \sim |a|^2 + |b|^2 + 2|a||b|\cos\theta$$

and, since the "vectors" a and b pointing from $\boldsymbol{m}$ to the random measures $\frac{1}{N}\sum_i \delta_{X_i}$, $\frac{1}{N}\sum_i \delta_{Y_i}$ are independent, on average the cosine term should give a null contribution.

We have been able to turn this heuristic argument into a proof (the inequality $\gtrsim$ is the hardest one).

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Open problems: the case $p = 1$

This is the problem raised in Talagrand's book. If we want to attack even this one by PDE methods, we should go back to the PDE formulation of optimal transport (Evans-Gangbo)

$$\begin{cases} -\mathrm{div}(a\nabla u) = \rho_1 - \rho_0 \\ |\nabla u| \le 1,\ a(1 - |\nabla u|) = 0 \end{cases}$$

where $a \ge 0$ is the transport density, and to its q-Laplacian approximation, $q \to \infty$:

$$\begin{cases} -\mathrm{div}(|\nabla u|^{q-2}\nabla u) = \rho_1 - \rho_0 \\ \dfrac{\partial u}{\partial n} = 0. \end{cases}$$

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More open problems

Even in the case $p = 2$, $D = \mathbb{T}^d$, there many more open (at least for mathematicians) questions, with formal proofs and computations in the physics literature:

- For $D = \mathbb{T}^2$ prove

$$\lim_{n\to\infty} \left(\frac{n}{\log n} \mathbb{E}\left[W_2^2(\mu^n, \nu^n) \right] - \frac{1}{2\pi} \right) \log n \in \mathbb{R}.$$

- For $d > 2$, prove with this method existence of the limit

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In this case we lose the extra room granted in 2-d by the logarithmic correction. We know from Barthe-Bordenave that the limit exists for $d \geq 5$.

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Thank you for the attention!

Slides available upon request