

# From Brenier to Knothe and from Knothe to Brenier: convergence, PDE and numerical ideas

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Modelisation with optimal transport

## 1 Monotone transports

- The 1D monotone transport
- The Brenier map, gradient of a convex potential
- The Knothe-Rosenblatt map

## 2 Convergence as $t \rightarrow 0$ for the cost $|x_1 - y_1|^2 + t|x_2 - y_2|^2$

- A conjecture by Y. Brenier
- A proof in the spirit of  $\Gamma$ -developments
- Assumptions and counter-examples
- Atoms in the disintegrated measures

## 3 Dynamics as $t$ moves in the semi-discrete case

- An ODE for the potential
- Evolution of cells

## 4 Dynamics in the continuous case

- The PDE for the potential
- The initial condition
- Well-posedness
- Numerical solution

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# Monotone transports

## 1D, Brenier, Knothe

# Very briefly, something you all know about the optimal transport problem

**Monge Problem** :  $\min \int c(x, T(x))\mu(dx) : T_{\#}\mu = \nu$   
 proposed by G. Monge in 1781, for  $c(x, y) = |x - y|$ .

**Kantorovich Problem** : (1942)  $\min \int c(x, y)d\gamma : \gamma \in \Pi(\mu, \nu)$   
 where  $\Pi(\mu, \nu) := \{\gamma : (\pi_x)_{\#}\gamma = \mu, (\pi_y)_{\#}\gamma = \nu\}$ .  
 This gives again Monge's framework when  $\gamma = (id \times T)_{\#}\mu$ .

Advantages of Kantorovich's formulation

- it's a convex problem
- it always has a solution (if  $c$  is l.s.c.)
- it has a dual formulation :

$$\min \int c d\gamma = \sup \int \phi d\mu + \int \psi d\nu : \phi(x) + \psi(y) \leq c(x, y).$$

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# The monotone transport in 1D

Given  $\mu, \nu \in \mathcal{P}(\mathbb{R})$ , if  $\mu$  has no atoms, there exists unique an increasing map  $T : \mathbb{R} \rightarrow \mathbb{R}$  such that  $T_{\#}\mu = \nu$ .

If  $F$  and  $G$  are the cumulative distribution functions of  $\mu$  and  $\nu$ , respectively, and if  $G$  is strictly increasing on  $\text{spt } \nu$  (i.e. if  $\text{spt } \nu$  is an interval), we can compute it through  $T = G^{-1} \circ F$  (if  $\nu$  has not full support a generalized inverse of  $G$  should be used).

This map turns out to be optimal for all the costs of the form  $c(x, y) = h(x - y)$  with  $h$  convex (and it is the unique optimizer if  $h$  is strictly convex). In particular, this covers the quadratic case  $c(x, y) = |x - y|^2$ .

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## The quadratic cost in $\mathbb{R}^d$

If  $d > 1$  and  $\mu, \nu$  are measures on  $\Omega \subset \mathbb{R}^d$  the situation is trickier but Brenier proved the following : if  $\mu$  is nice (for instance  $\mu \ll \mathcal{L}^d$ ), then there exists unique an optimal map, and it given by  $T = \nabla\phi$ , with  $\phi$  convex.

It has some monotonicity property (for instance,  $DT$  is a symmetric and positive definite matrix). But it is trickier to compute. The change-of-variable-formula, if  $\mu = f(x)dx$  and  $\nu = g(y)dy$ , gives the Jacobian condition  $\det DT = \frac{f}{g \circ T}$ , which reads here

$$\det(D^2\phi) = \frac{f}{g \circ \nabla\phi}, \quad \text{with } \phi \text{ convex,}$$

(Monge-Ampère equation). Its “boundary” condition is given by  $\nabla\phi(x) \in \Omega$  for all  $x \in \Omega$ . This PDE is nonlinear and difficult to solve, both numerically and theoretically.

Some regularity theorems exist giving  $\phi \in C^{k+2,\alpha}$  if  $f, g$  are bounded from below and belong to  $C^{k,\alpha}$  and  $\text{spt } \nu$  is convex.. In this case  $T$  is  $C^{k+1,\alpha}$ .

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## The Knothe-Rosenblatt rearrangement

Here is another reasonable transport (increasing for the lexicographic order) : there exists unique a map  $T_K$  of the form

$$T_K(x_1, x_2, \dots, x_d) := (T^1(x_1), T^2(x_1, x_2), \dots, T^d(x_1, x_2, \dots, x_d))$$

where all the  $T^i(x_1, x_2, \dots, x_{i-1}, \cdot)$  are increasing, sending  $\mu$  onto  $\nu$ .

**Recursive construction** : If  $d = 1$  just take the monotone map. If  $d > 1$ , let  $\mu_1$  and  $\nu_1$  be the projections on of  $\mu$  and  $\nu$  on the first variable and  $T^1$  be the monotone map between them. Then, disintegrate  $\mu$  and  $\nu$  according to the first variable, and define  $(T^2, T^3, \dots, T^d)(x_1, \cdot, \dots, \cdot)$  as the Knothe transport in dimension  $(d - 1)$  between  $\mu_{x_1}$  and  $\nu_{T^1(x_1)}$ .

$T_K$  is much easier to compute than the Brenier map. Yet, it is not optimal, and its definition is anisotropic.

**Regularity** :  $T_K$  has the same regularity of the densities, not more. Its Jacobian  $DT_K$  is triangular, with positive coefficients on the diagonal.

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## Convergence of quadratic costs to Knothe

The cost  $|x_1 - y_1|^2 + t|x_2 - y_2|^2$  as  $t \rightarrow 0$

## A reasonable conjecture

Let us consider the weighted quadratic cost

$$c_t(x, y) := \sum_{i=1}^d t^{i-1} |x_i - y_i|^2.$$

If  $\mu \ll \mathcal{L}^d$ , the corresponding optimal transportation problem admits a unique solution  $T_t$ . According to a **conjecture by Y. Brenier**, it is natural to expect the convergence of  $T_t$  to the Knothe transport  $T_K$ .

**Why?** because as  $t \rightarrow 0$  the main criterion becomes the minimization of the cost  $|x_1 - y_1|^2$ . This selects  $T^1$  but gives nothing on the other variables. We pass to the second most important criterion : minimizing  $|x_2 - y_2|^2$ , and this provides  $T^2$ . And we go on.

This is **in the same spirit of a  $\Gamma$ -convergence development**  $c_t = c^1 + tc^2 + t^2c^3 + \dots$ . If  $c^1$  has not a unique minimizer, we select the one that also minimizes  $c^2$  among minimizers of  $c^1$ . And if it has not uniqueness neither, we look at  $c^3 \dots$

## An example

Let's see a case where explicit solutions are available. Take  $d = 2$ , and  $\mu$  and  $\nu$  two Gaussian measures where

$$\mu = N(0, \text{Id}) \quad \text{and} \quad \nu = N\left(0, \begin{pmatrix} a & b \\ b & c \end{pmatrix}\right)$$

(with  $ac > b^2$ ,  $a > 0$ ). We can check that  $T_t$  is linear with matrix

$$T_t = \frac{1}{\sqrt{a + ct^2 + 2t\sqrt{ac - b^2}}} \begin{pmatrix} a + t\sqrt{ac - b^2} & bt \\ b & ct + \sqrt{ac - b^2} \end{pmatrix}$$

which converges as  $t \rightarrow 0$  to

$$\begin{pmatrix} \sqrt{a} & 0 \\ b/\sqrt{a} & \sqrt{c - b^2/a} \end{pmatrix}$$

which is precisely the matrix of the Knothe transport from  $\mu$  to  $\nu$ .

## A theorem

**Assumption (H-source)** : the measure  $\mu^1$ , as well as  $\mu^1$ —almost all the measures  $\mu_{x_1}^2$ , and the measures  $\mu_{x_1, x_2}^3 \dots$  up to almost all the measures  $\mu_{x_1, x_2, \dots, x_{d-1}}^d$ , which are all measures on the real line, have no atoms.

**Assumption (H-target)** : the measure  $\nu^1$ , as well as  $\nu^1$ —almost all the measures  $\nu_{x_1}^2$ , and the measures  $\nu_{x_1, x_2}^3 \dots$  up to almost all the measures  $\nu_{x_1, x_2, \dots, x_{d-2}}^{d-1}$ , have no atoms neither.

### Theorem

Let  $\mu$  and  $\nu$  satisfy (H-source) and (H-target),  $\gamma_t$  be an optimal plan for the costs  $c_t(x, y)$ ,  $T_K$  the Knothe-Rosenblatt map between  $\mu$  and  $\nu$  and  $\gamma_K$  the associated transport plan. Then  $\gamma_t \rightarrow \gamma_K$  as  $t \rightarrow 0$ .  
 Moreover, should the plans  $\gamma_t$  be induced by transport maps  $T_t$ , then these maps would converge to  $T_K$  in  $L^2(\mu)$  as  $t \rightarrow 0$ .

G. CARLIER, A. GALICHON, F. SANTAMBROGIO, From Knothe's transport to Brenier's map and a continuation method for optimal transport, *SIAM J. Math. An.*, 2010

# Atoms

**Counter-example.** Surprisingly, the absence of atoms in  $\nu$  is really necessary. Look at this example in  $[-1, 1] \times [-1, 1] \subset \mathbb{R}^2$  where

$$\mu = \frac{1}{2} \mathbf{1}_{\{x_1 x_2 < 0\}} dx \quad \text{and} \quad \nu = \frac{1}{2} \mathcal{H}^1|_S \quad \text{with} \quad S = \{0\} \times [-1, 1].$$

The Knothe-Rosenblatt map is  $T_K(x) := (0, 2x_1 + \text{sgn}(x_2))$ . The optimal transport for each cost  $c_t$  is  $T_t(x) := (0, x_1)$  (no transport may do better than this one, which projects on the support of  $\nu$ ). The reason for the lack of convergence is the atom in the measure  $\nu^1 = \delta_0$ .

**Don't despair!** This means that we cannot apply the result if  $\nu$  itself is purely atomic...yet, looking at the proof we can also deal with the following case. Keep (*H-source*) on  $\mu$  but suppose that  $\nu$  is concentrated on a set  $S$  with the property

$$y, z \in S, \quad y \neq z \Rightarrow y_1 \neq z_1.$$

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## Semi-discrete evolution

### An ODE for the potential

## From Knothe to Brenier

The Knothe transport  $T_K$  is easy to compute because it is essentially 1D; the Brenier map is the optimal map for  $c_1$ ; the optimal maps for  $c_t$  converge to  $T_K$  as  $t \rightarrow 0$ .

**Idea** : can we start from  $T_K$  and let  $t$  improve from 0 to 1 in order to compute  $T_1$ ?

Let us start from the semidiscrete case, i.e.  $\mu$  is a smooth density on  $\Omega$  and  $\nu$  is a finite atomic measure with  $N$  atoms, say  $\mu$  uniform on some convex polyhedron  $\Omega \subset \mathbb{R}^2$  and  $\nu = \frac{1}{N} \sum_{i=1}^N \delta_{y_i}$  (where all the points  $y_i$  have a different first coordinate  $y_i^{(2)}$ ).

The transport map, piecewise constant on some unknown Voronoi-type cells, can be computed from the **potential in the dual problem**.

The dual problem reads

$$\sup_p \Phi(p, t) := \frac{1}{N} \sum_{i=1}^N p_i + \int_{\Omega} p_t^*(x) dx,$$

where  $p_t^*(x) = \min_i \{c_t(x, y_i) - p_i\}$  and we set  $p_1 = 0$ . For each  $t$ , there is a unique maximizer  $p(t)$ . It belongs to  $\mathbb{R}^N$  and we look for its evolution.



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# The ODE

For each  $(p, t)$ , set  $C(p, t)_i = \{x \in \Omega : \inf_j c_t(x, y_j) - p_j = c_t(x, y_i) - p_i\}$ .  
 The function  $\Phi(\cdot, t)$  is concave differentiable and its gradient is given by

$$\frac{\partial \Phi_t}{\partial p_i}(p, t) = \frac{1}{N} - |C(p, t)_i|.$$

By concavity, the maximizer  $p(t)$  is characterized by  $\nabla \Phi_t(p(t), t) = 0$ .

Differentiating, we obtain a differential equation for the evolution of  $p(t)$  :

$$\frac{\partial}{\partial t} \nabla_p \Phi(p(t), t) + D_{p,p}^2 \Phi(p(t), t) \cdot \frac{dp}{dt}(t) = 0.$$

All the quantities we are interested in depend on the position of the vertices of the cells  $C(p, t)_i$ , which are all polygons.

**Result** : The positions of these vertices depend in a Lipschitz way on  $p$  and  $t$ ; the matrix  $D_{p,p}^2 \Phi(p(t), t)$  is invertible in a suitable domain; we can apply Cauchy-Lipschitz theorem to the ODE

$$\frac{dp}{dt}(t) = -D_{p,p}^2 \Phi(p(t), t)^{-1} \left( \frac{\partial}{\partial t} \nabla_p \Phi(p(t), t) \right)$$

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$$\frac{\partial \Phi_t}{\partial p_i}(p, t) = \frac{1}{N} - |C(p, t)_i|.$$

By concavity, the maximizer  $p(t)$  is characterized by  $\nabla \Phi_t(p(t), t) = 0$ .  
 Differentiating, we obtain a differential equation for the evolution of  $p(t)$  :

$$\frac{\partial}{\partial t} \nabla_p \Phi(p(t), t) + D_{p,p}^2 \Phi(p(t), t) \cdot \frac{dp}{dt}(t) = 0.$$

All the quantities we are interested in depend on the position of the vertices of the cells  $C(p, t)_i$ , which are all polygons.

**Result** : The positions of these vertices depend in a Lipschitz way on  $p$  and  $t$ ; the matrix  $D_{p,p}^2 \Phi(p(t), t)$  is invertible in a suitable domain; we can apply Cauchy-Lipschitz theorem to the ODE

$$\frac{dp}{dt}(t) = -D_{p,p}^2 \Phi(p(t), t)^{-1} \left( \frac{\partial}{\partial t} \nabla_p \Phi(p(t), t) \right)$$

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# Cells evolution

Different shapes of the cells in a simple semi-discrete case for  $t \in [0, +\infty[$ .

## Continuous evolution

### A PDE for the potential

# Monge-Ampère equation

In  $\mathbb{R}^d$ , take the matrix

$$A_t = \begin{pmatrix} 1 & 0 \\ 0 & t \end{pmatrix}$$

and the cost  $c_t(x, y) = \frac{1}{2} A_t(x - y) \cdot (x - y)$ . The optimal transport is given by  $T_t(x) = x - A_t^{-1} \nabla \phi_t$ . The MA equation gives

$$\det(\text{Id} - A_t^{-1} D^2 \phi_t) = \frac{f}{g(x - A_t^{-1} \nabla \phi_t(x))}.$$

Let us take the easiest case, i.e.  $g = 1$  and let's differentiate w.r.t.  $t$ :

$$\text{trace} [(A_t - D^2 \phi_t)^{-1} D^2 \phi_t'] = -\text{trace} \left[ (\text{Id} - A_t^{-1} D^2 \phi_t)^{-1} \left( \frac{d}{dt} (A_t)^{-1} \right) D^2 \phi_t \right].$$

The equation is therefore

$$\frac{\partial \phi_t}{\partial t} = \chi \quad \text{with} \quad \text{trace} [(\text{Id} - A_t^{-1} D^2 \phi_t)^{-1} D^2 \chi] = h(t, D^2 \phi_t).$$



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# Initial condition

What about  $\lim_{t \rightarrow 0} \phi_t$ ? Unfortunately, the limit potential is that associated to the cost  $\frac{1}{2}|x_1 - y_1|^2$ , i.e. it only depends on the measures  $\mu_1$  and  $\nu_1$ . In particular, there is no hope for a uniqueness result.

**Good idea** Write  $\phi_t = u_t(x_1) + tv_t(x_1, x_2)$  (in higher dimension we put  $+t^2w_t(x_1, x_2, x_3) \dots$ ). This allows to

- give initial conditions :  $u_0$  is the potential between  $\mu_1$  and  $\nu_1$  and, for each  $x_1$ , the function  $v_0(x_1, \cdot)$  is the potential between  $\mu_{x_1}$  and  $\nu_{y_1}$  with  $y_1 = T^1(x_1)$ ;
- de-singularize the equation, since

$$A_t^{-1}D^2\phi = \begin{pmatrix} 1 & 0 \\ 0 & t^{-1} \end{pmatrix} \cdot \begin{pmatrix} \partial_{11}u + t\partial_{11}v & t\partial_{12}v \\ t\partial_{11}v & t\partial_{22}v \end{pmatrix} = \begin{pmatrix} \partial_{11}u + t\partial_{11}v & t\partial_{12}v \\ \partial_{11}v & \partial_{22}v \end{pmatrix}$$

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# Well-posedness

For  $t > 0$ , an implicit function theorem in the space  $\mathbb{R} \times C^{2,\alpha}(x_1) \times C^{2,\alpha}(x_1, x_2)$  applied to the function  $(t, u, v) \mapsto \det(I - A_t^{-1} D^2(u + tv))$  allows to prove well-posedness of the equation.

Problem : for  $t = 0$  there is a **loss of regularity** :  $u_t, v_t$  have two extra derivatives w.r.t.  $f$ , while  $v_0$  has the same regularity in  $x_1$  as  $f$ . No space  $C^{k\alpha}$  is suitable for this IFT.

**Solution** : we must choose the space  $C^\infty$  and use the IFT by **Nash-Moser**. Nicolas worked hard on that, and proved (on the torus, to avoid boundary issues) that it works!

Notice that, besides the theoretical speculations, the equation is not so bad, and suggests that an explicit method can be used to solve it.

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# Some numerical pictures – Knothe

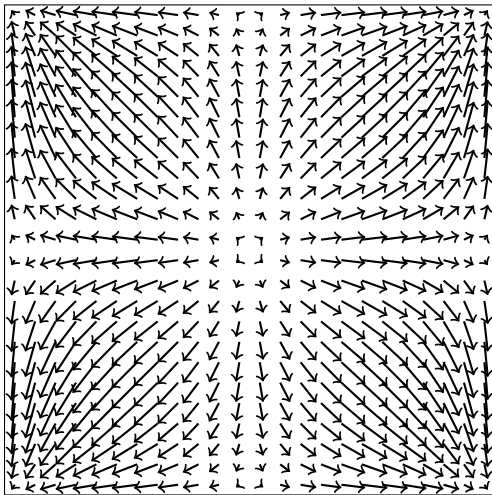
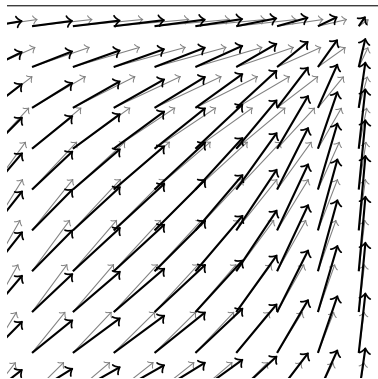


FIGURE: The Knothe–Rosenblatt rearrangement.

## Some numerical pictures – Knothe 2



**FIGURE:** The black arrows represent the Knothe–Rosenblatt rearrangement, and the gray ones its symmetric. The discrepancy comes from the fact that the rearrangement’ is anisotropic.

# Some numerical pictures – computation of the optimal map

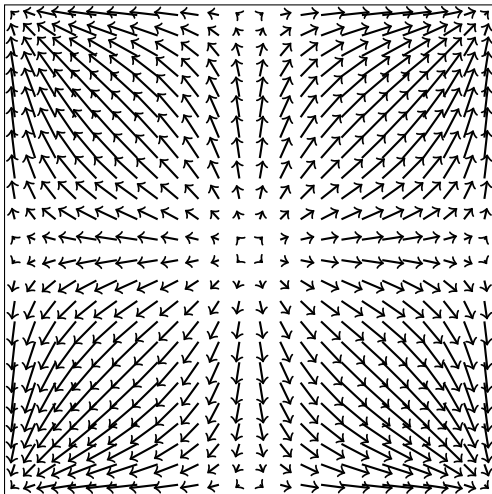
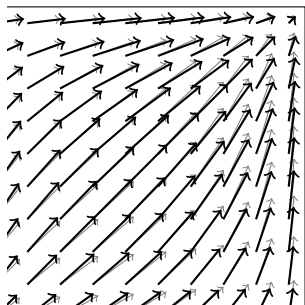


FIGURE: Computation of Brenier's optimal map by the evolution  $u_t + tv_t$ .

# Some numerical pictures – comparison Knothe-Brenier



**FIGURE:** The black arrows represent Brenier's optimal transport map, and the gray ones the Knothe–Rosenblatt rearrangement.

Here it is,

Thanks for your attention