Mathématiques - Informatique

Ecole Jeunes Chercheurs GDR IM
Géométrie Numérique

Partie I: Transport Optimal (Lundi) *B. Lévy*
Partie II: Résolution de systèmes linéaires (Jeudi) *N. Ray*

Bruno Lévy
ALICE Géométrie & Lumière
CENTRE INRIA Nancy Grand-Est

OVERVIEW

Part. 1. Goals and Motivations

Part. 2. Introduction to Optimal Transport

Part. 3. Semi-Discrete Optimal Transport

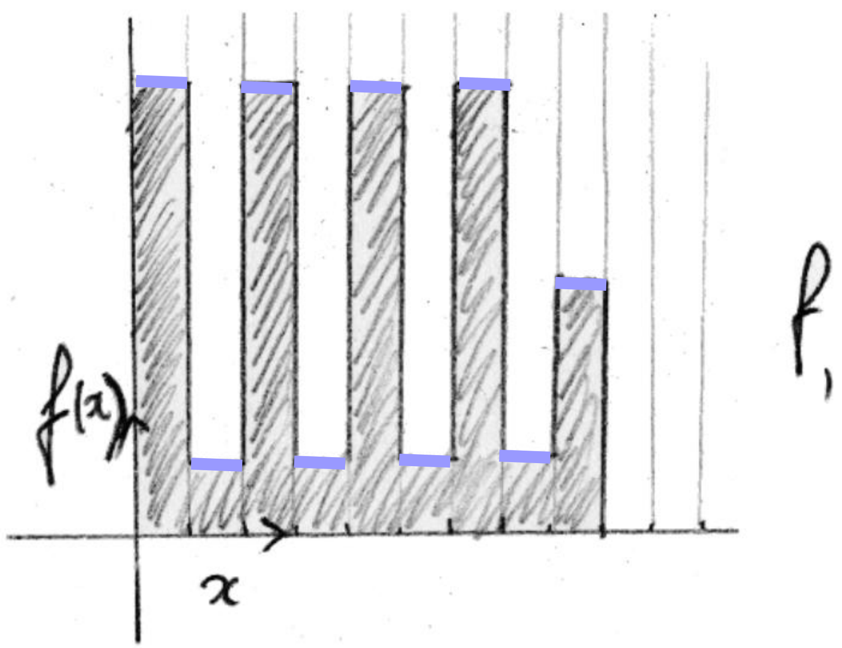
Part. 4. Applications in Computational Physics

1

Goals and Motivations

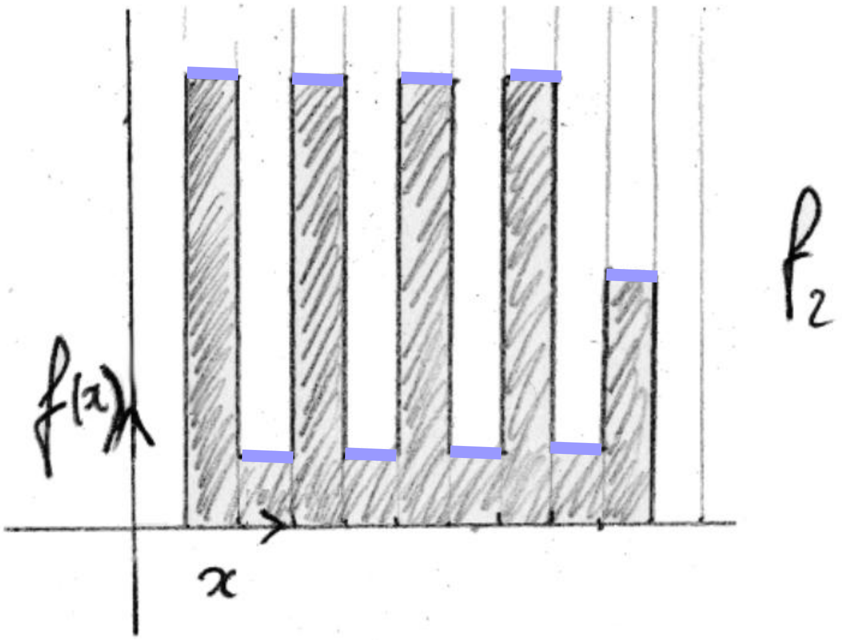
Part. 1 Optimal Transport

Measuring distances between functions



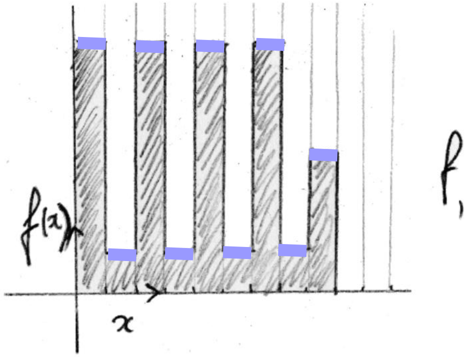
Part. 1 Optimal Transport

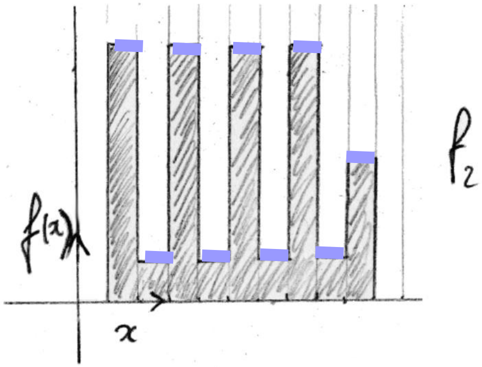
Measuring distances between functions



Part. 1 Optimal Transport

Measuring distances between functions

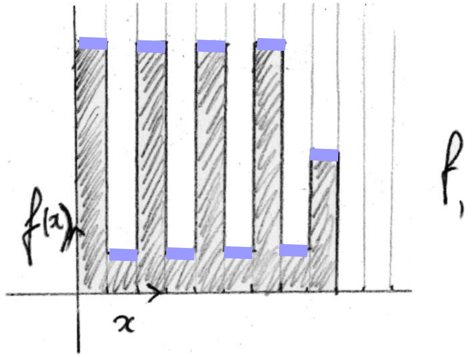


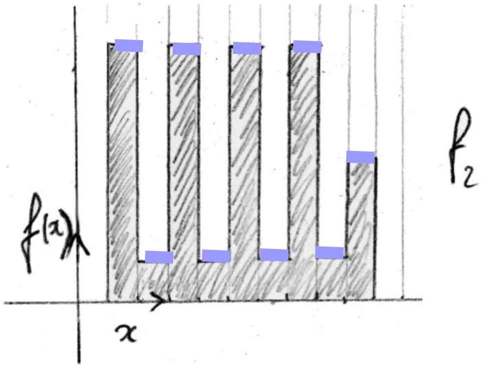


$$d_{L_2}(f_1, f_2) = \int (f_1(x) - f_2(x))^2 \, dx$$

Part. 1 Optimal Transport

Measuring distances between function





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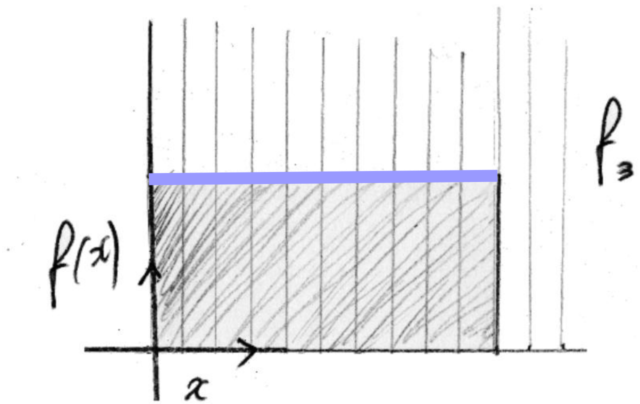
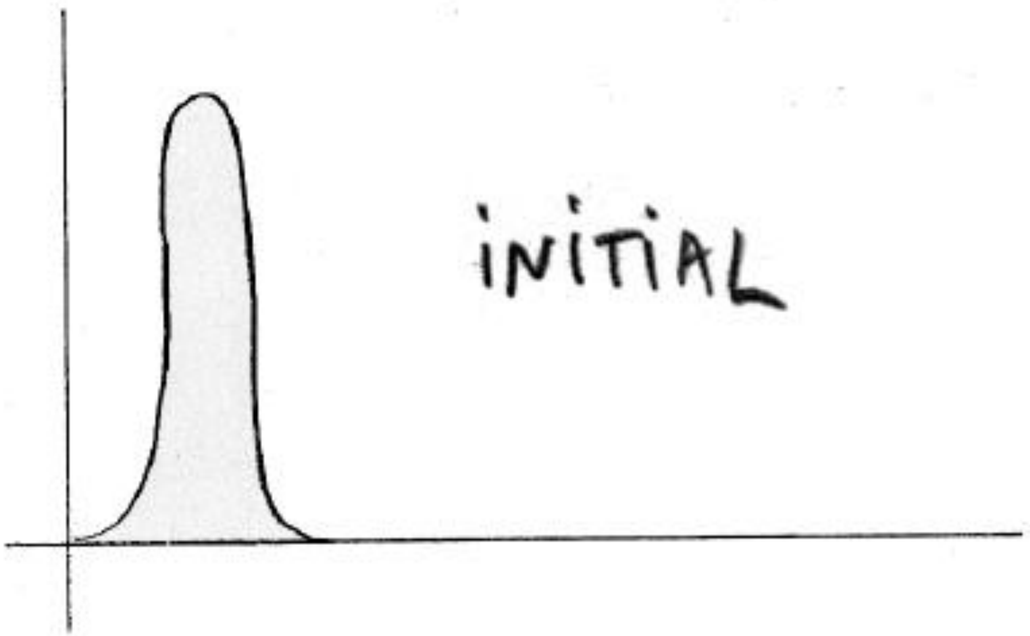


Part. 1 Optimal Transport
Interpolating functions



Part. 1 Optimal Transport

Interpolating functions

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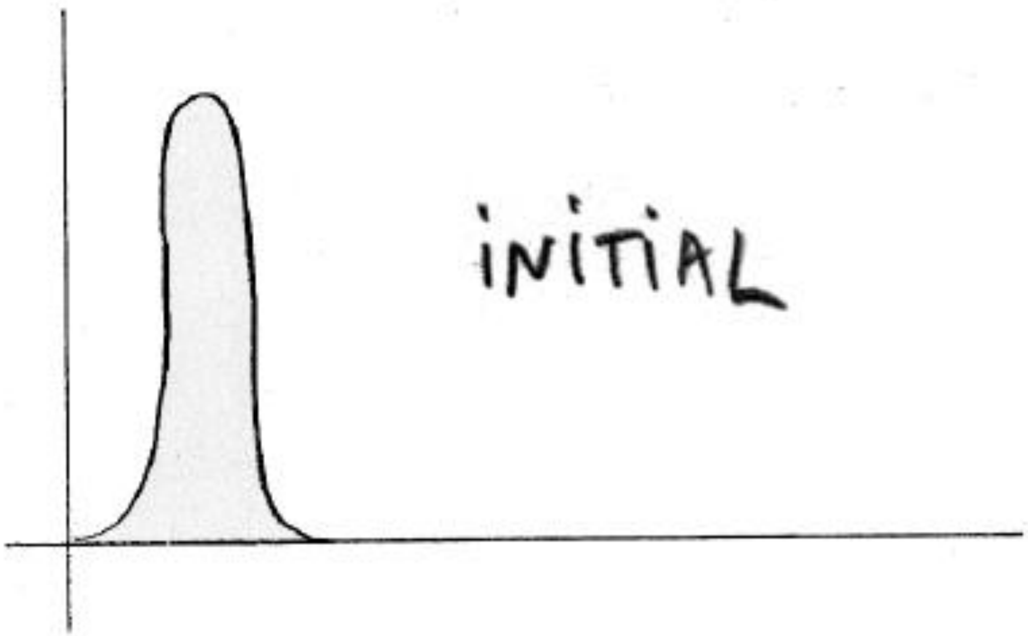
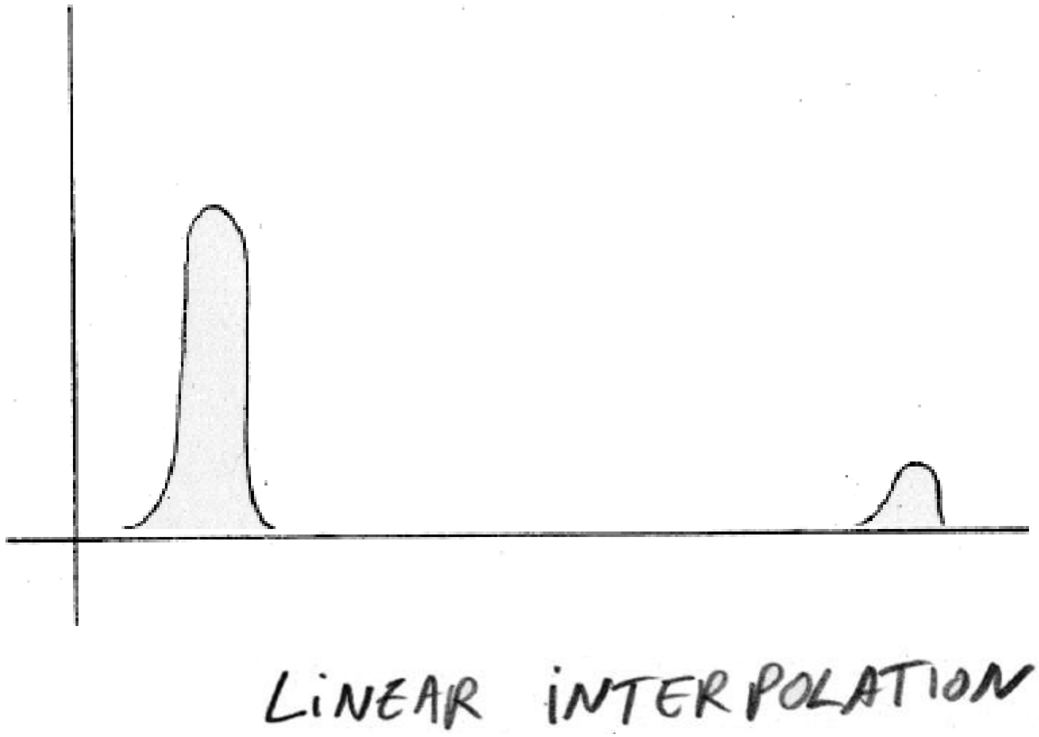


LiNEAR iNTERPOLATiON

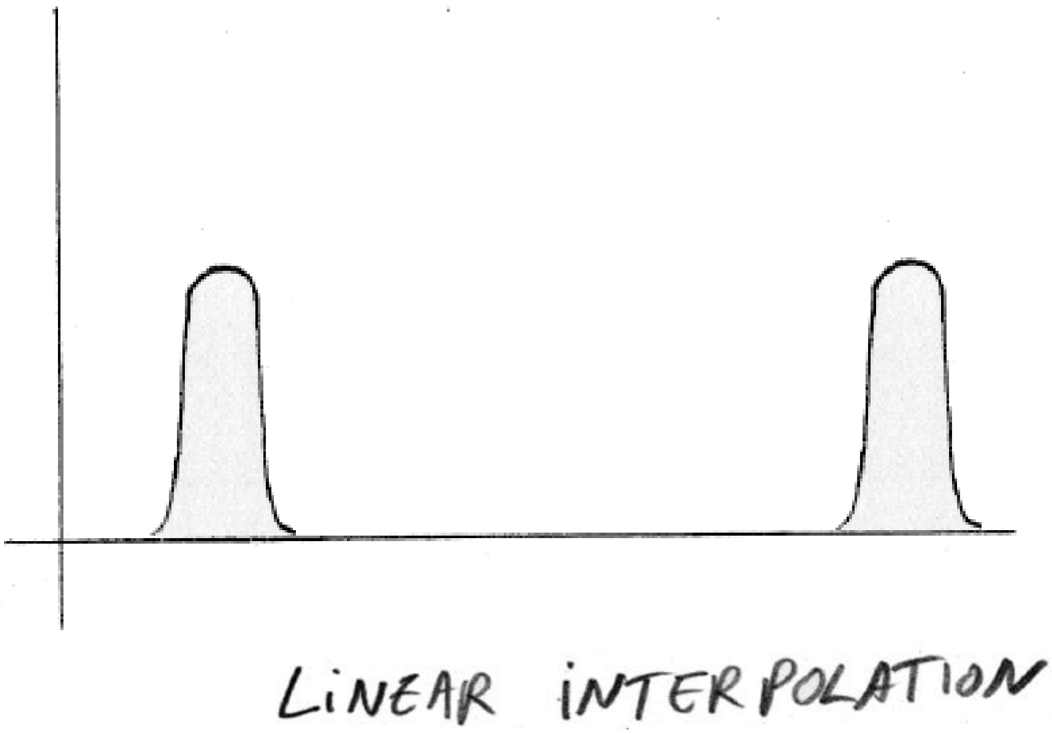
Part. 1 Optimal Transport

Interpolating functions



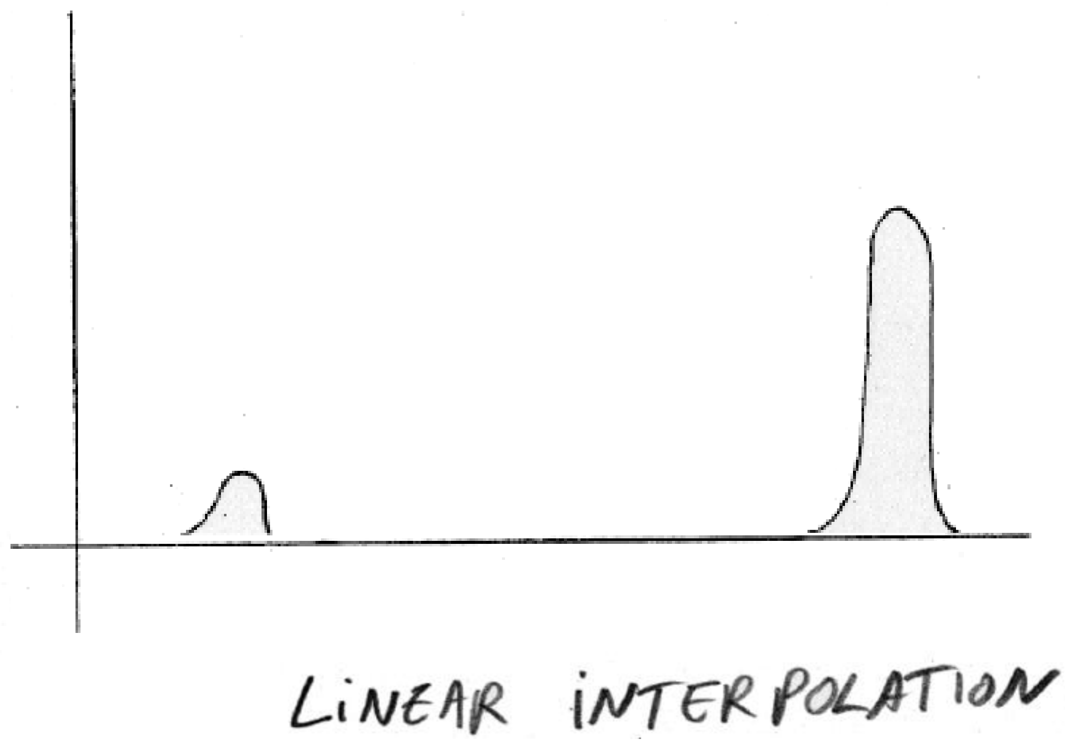
Part. 1 Optimal Transport

Interpolating functions



Part. 1 Optimal Transport

Interpolating functions

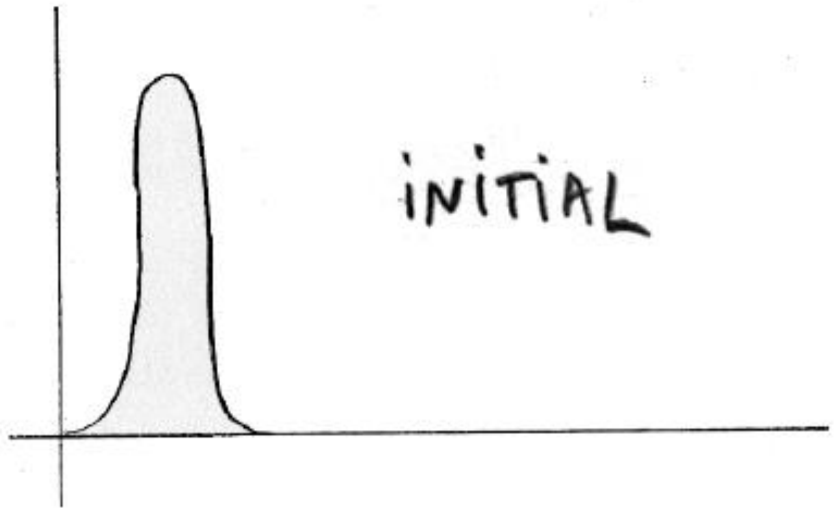


Interpolating functions

LINEAR INTERPOLATION

Part. 1 Optimal Transport

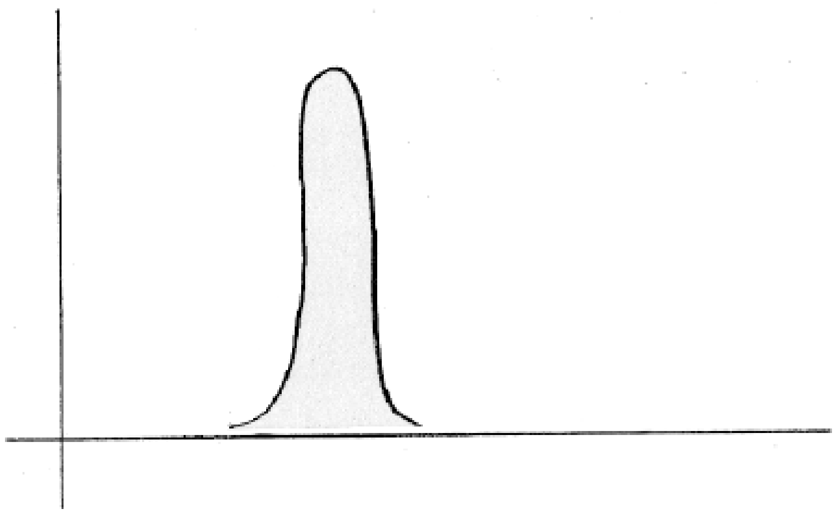
Interpolating functions



DISPLACEMENT INTERPOLATION

Part. 1 Optimal Transport

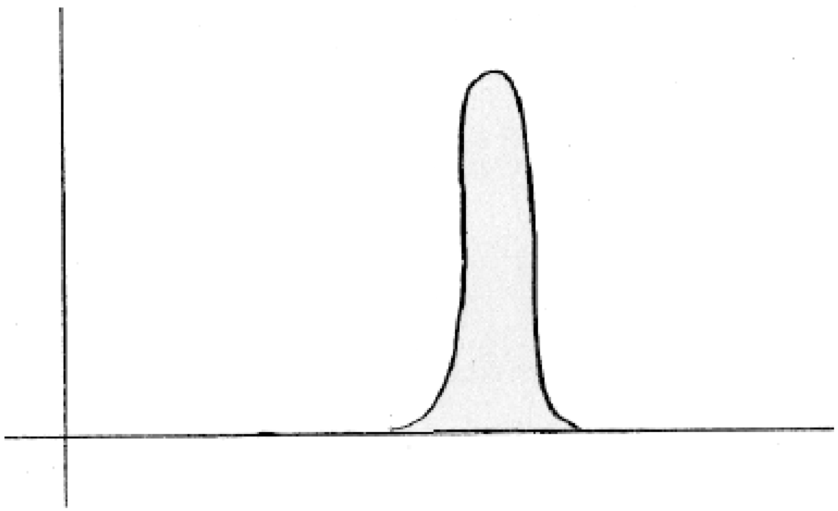
Interpolating functions



DISPLACEMENT INTERPOLATION

Part. 1 Optimal Transport

Interpolating functions



DISPLACEMENT INTERPOLATION

Part. 1 Optimal Transport

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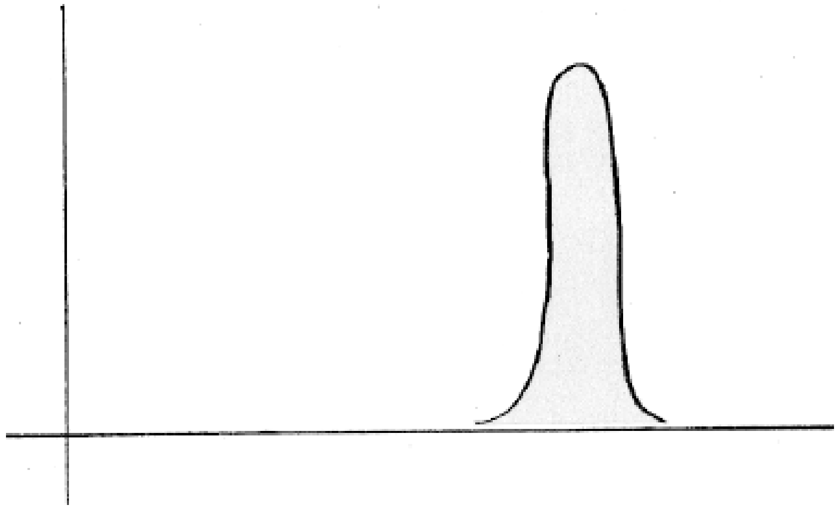


DISPLACEMENT INTERPOLATION

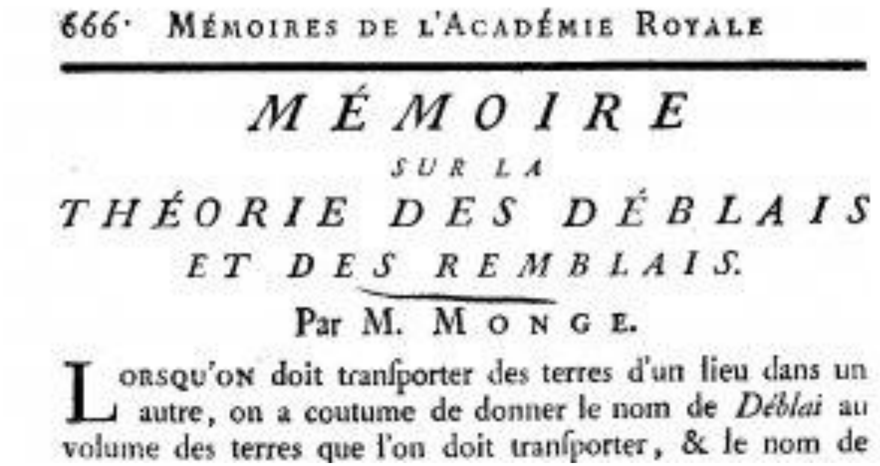
Part. 1 Optimal Transport

Interpolating functions

DISPLACEMENT INTERPOLATION

Part. 1 Optimal Transport

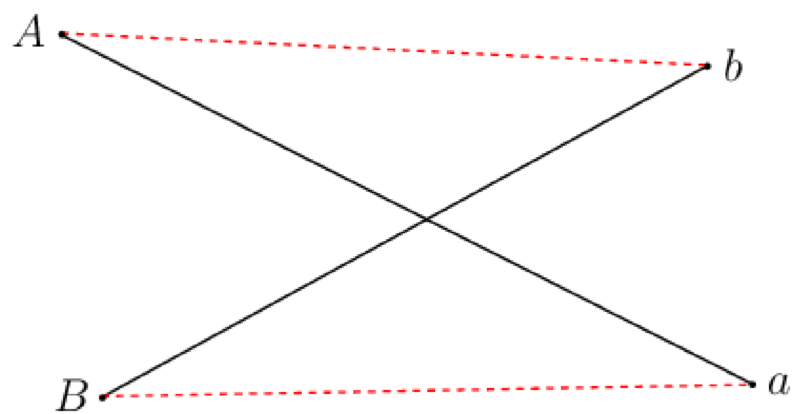
Gaspard Monge - 1784


666· MÉMOIRES DE L'ACADÉMIE ROYALE

MÉMOIRE SUR LA THÉORIE DES DÉBLAIS ET DES REMBLAIS.

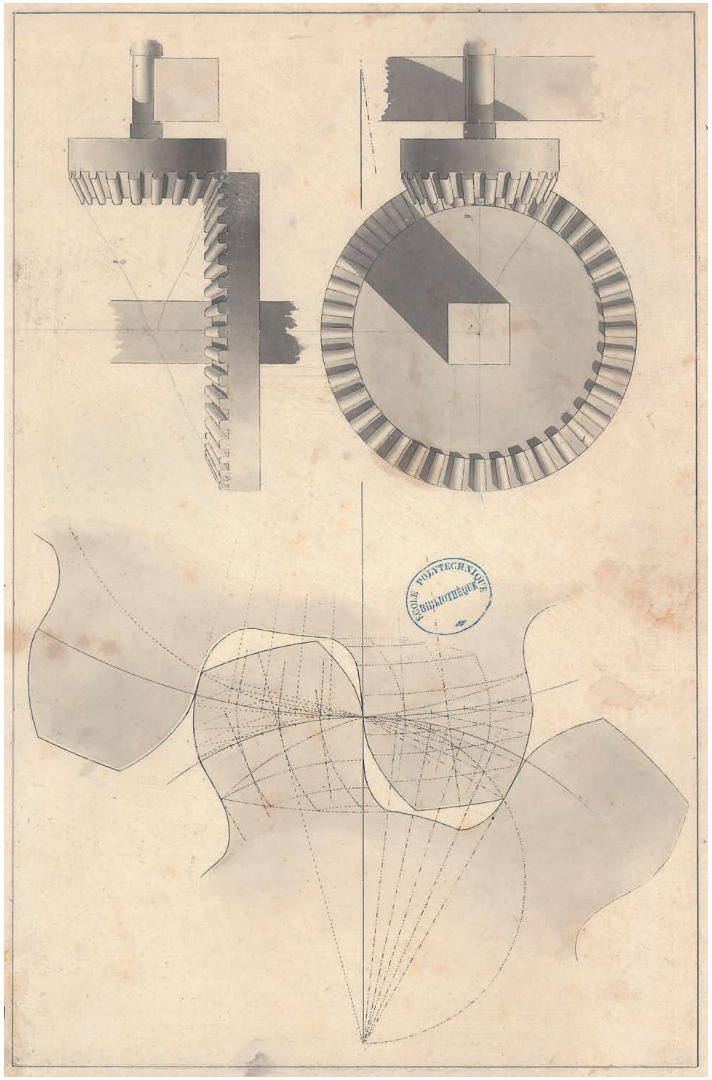
Par M. MONGE.

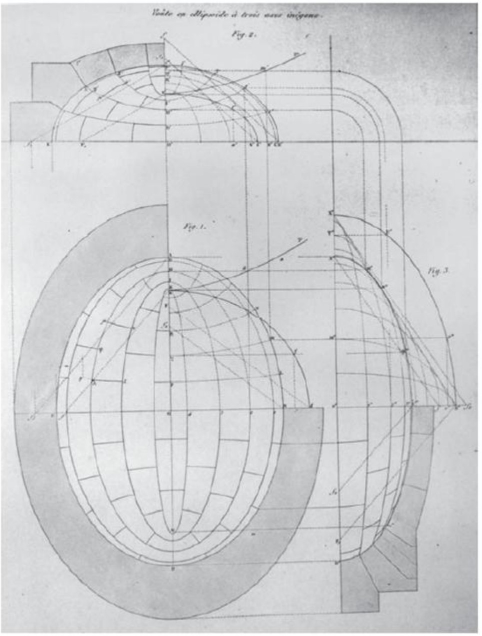
Lorsqu'on doit tranſporter des terres d'un lieu dans un autre, on a coutume de donner le nom de *Déblai* au volume des terres que l'on doit tranſporter, & le nom de



Part. 1 Optimal Transport

Gaspard Monge – geometry and light





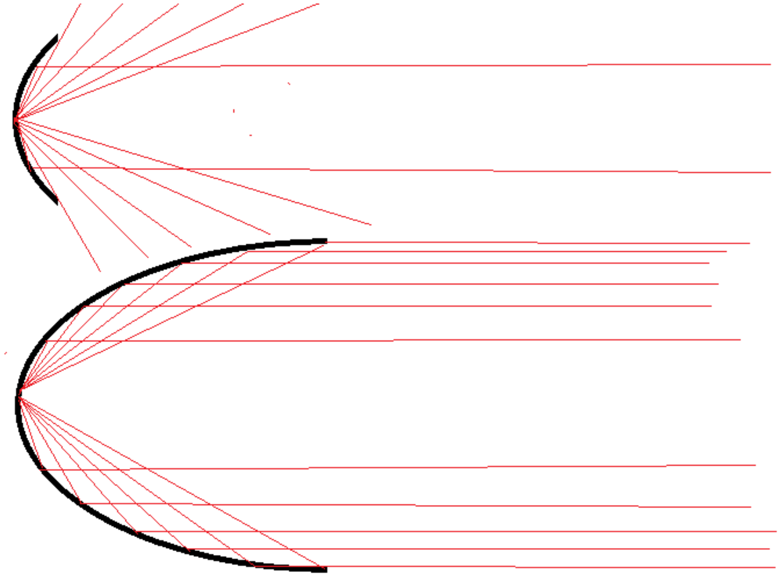
Part. 1 Optimal Transport

Monge-Brenier-Villani, the french connection

Cédric Villani
Optimal Transport Old & New
Topics on Optimal Transport

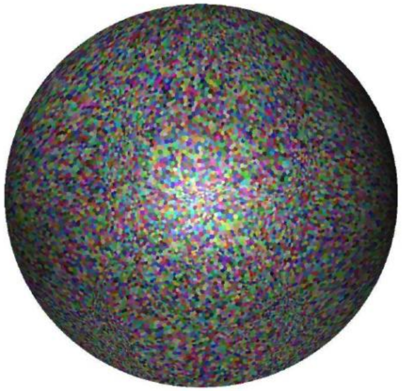
Yann Brenier
The polar factorization theorem
(Brenier Transport)

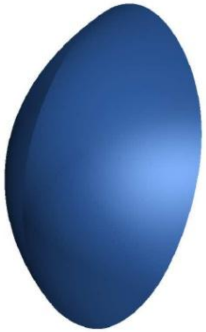
Part. 1 Optimal Transport



Optimal transport
geometry and light

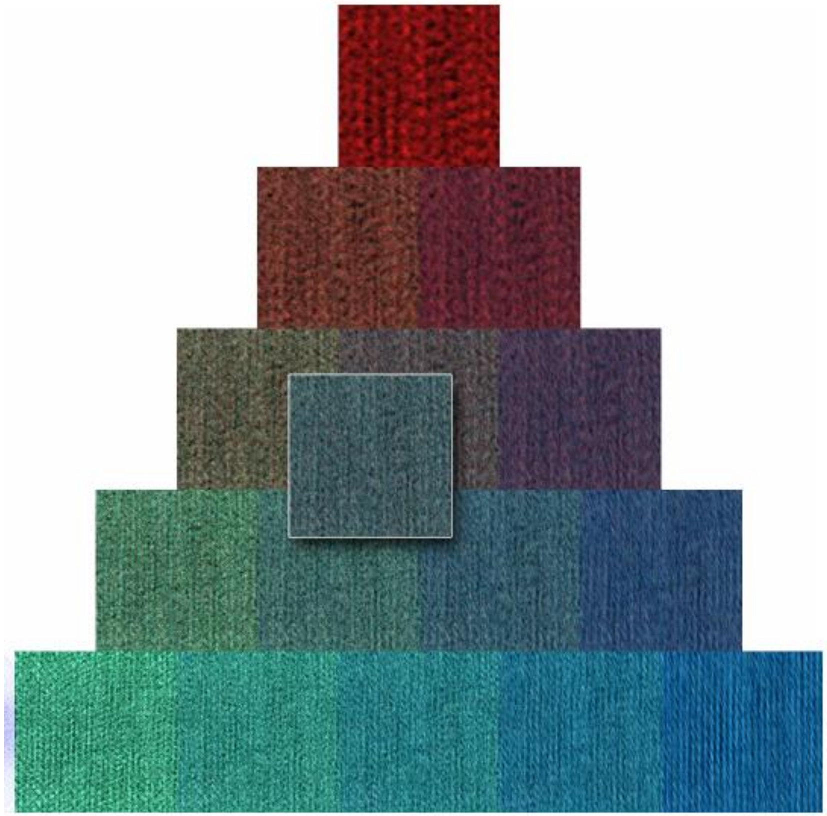
[Caffarelli, Kochengin, and Oliker 1999]





[Castro, Merigot, Thibert 2014]

Part. 1 Optimal Transport – Image Processing



Barycenters / mixing textures

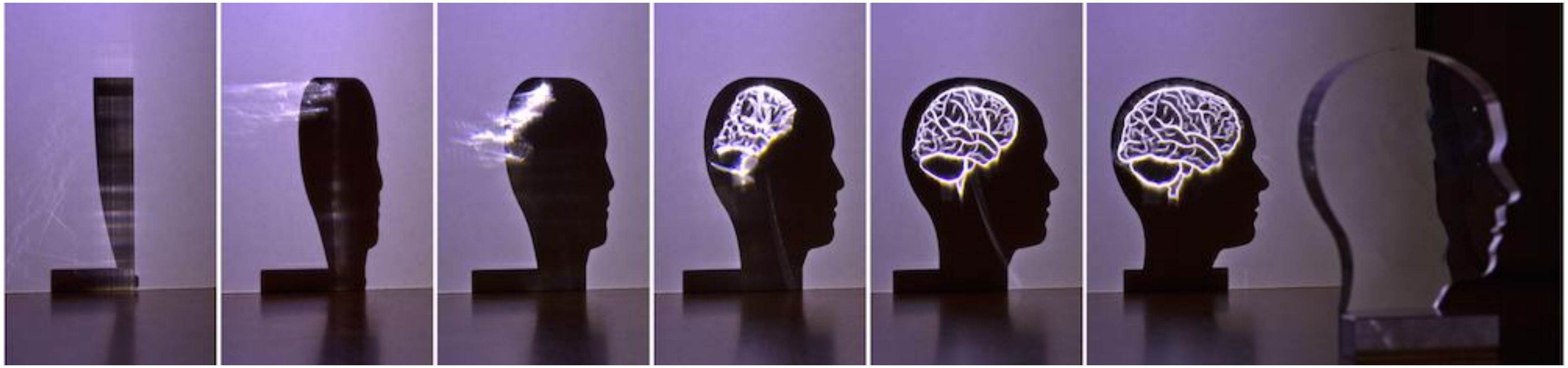
[Nicolas Bonneel, Julien Rabin, Gabriel Peyré, Hanspeter Pfister]

Video-style transfer,
A.I., "data sciences"

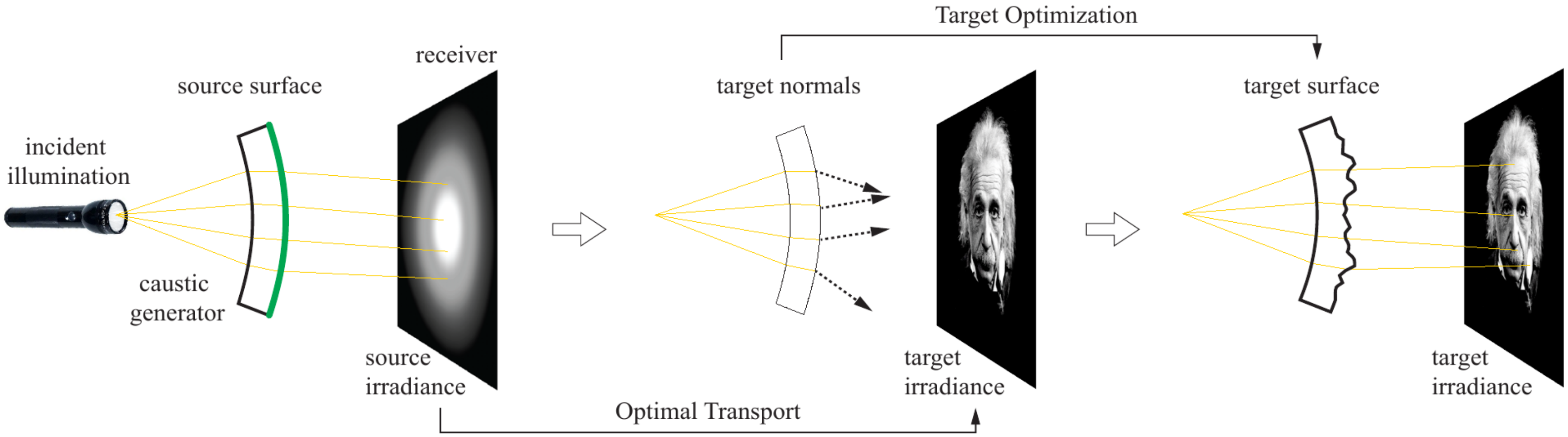
[Nicolas Bonneel, Kalyan Sunkavalli, Sylvain Paris, Hanspeter Pfister]
[Marco Cuturi, Gabriel Peyré]

Part. 1 Optimal Transport

Optimal transport - geometry and light



[Chwartzburg, Testuz, Tagliasacchi, Pauly, SIGGRAPH 2014]

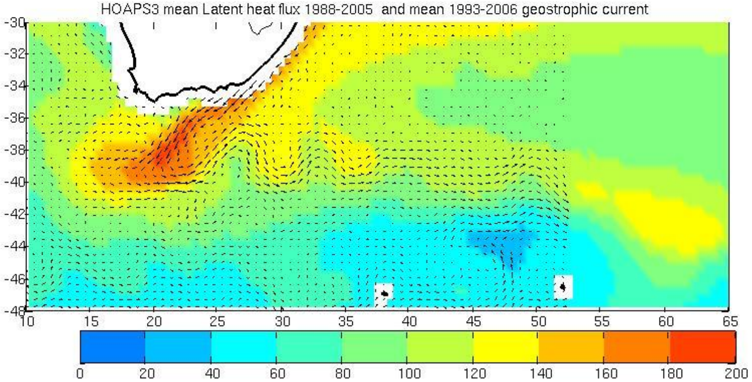


Part. 1. Motivations

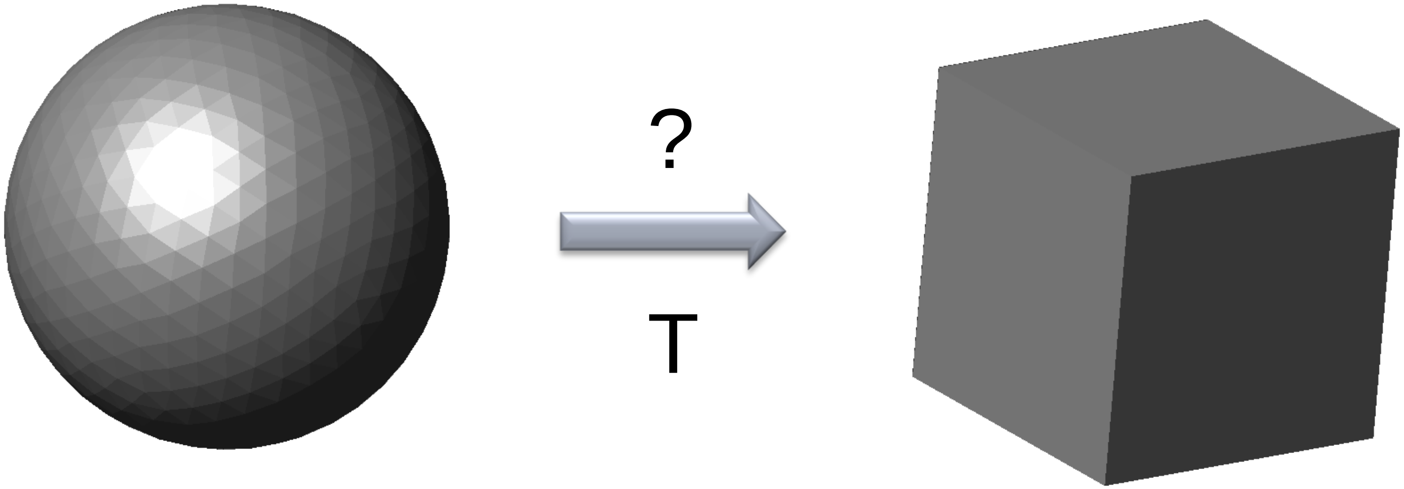
Discretization of functionals involving the Monge-Ampère operator,
Benamou, Carlier, Mérigot, Oudet
arXiv:1408.4536

The variational formulation of the Fokker-Planck equation
Jordan, Kinderlehrer and Otto
SIAM J. on Mathematical Analysis

Geostrophic current

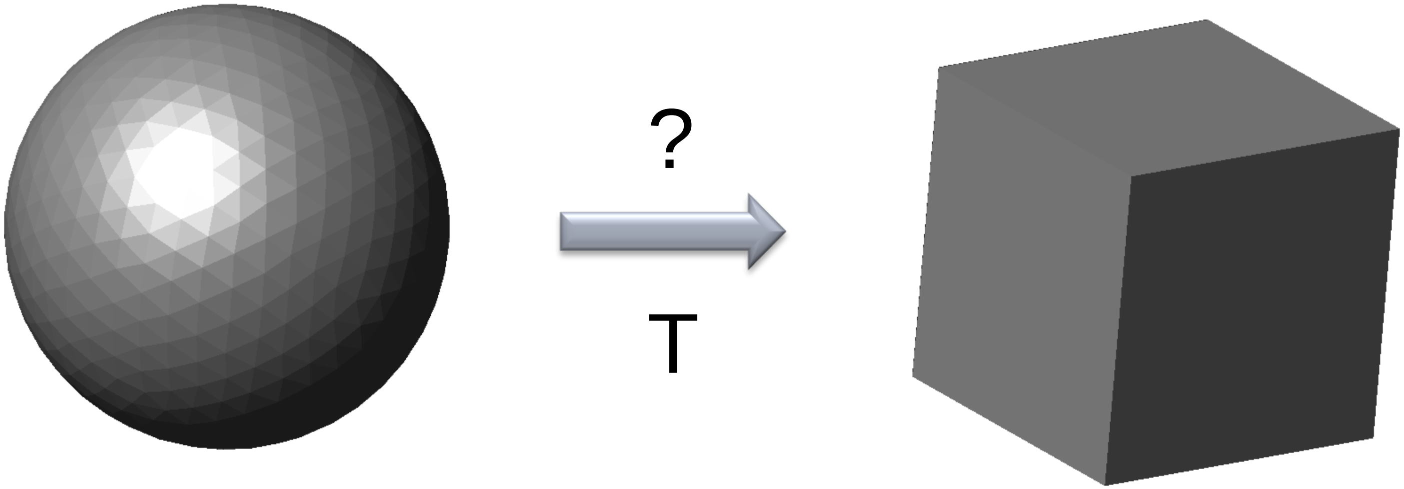


Part. 1 Optimal Transport



How to "morph" a shape into another one of same mass while minimizing the "effort" ?

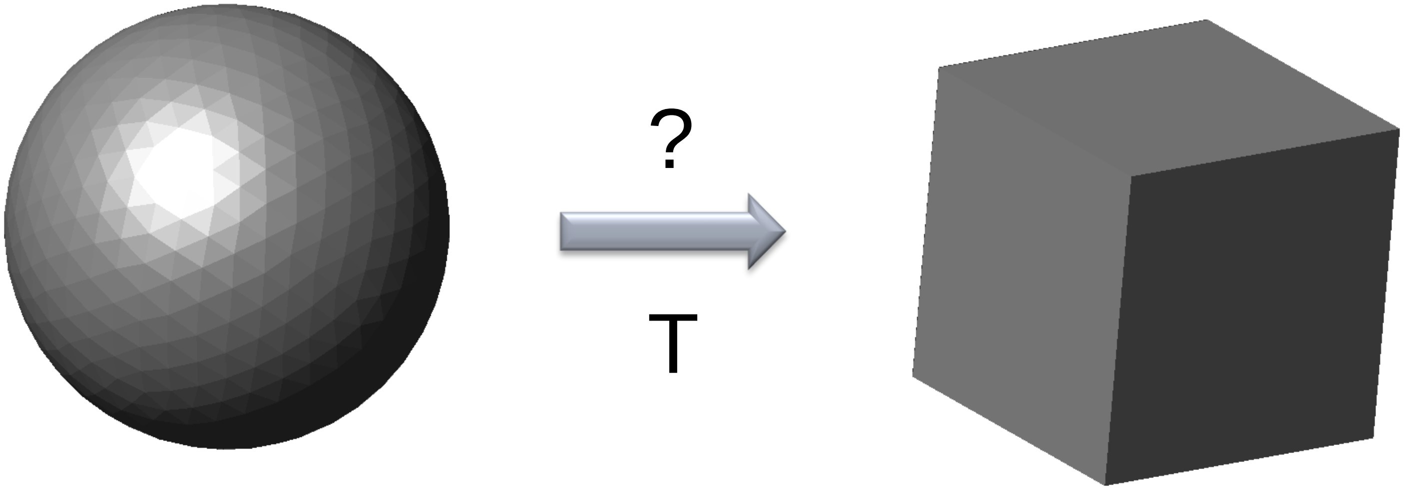
Part. 1 Optimal Transport



How to “morph” a shape into another one of same mass while minimizing the “effort” ?

The “effort” of the best T defines a **distance** between the shapes

Part. 1 Optimal Transport



How to "morph" a shape into another one
while preserving mass and minimizing the effort ?

Part. 1 Optimal Transport

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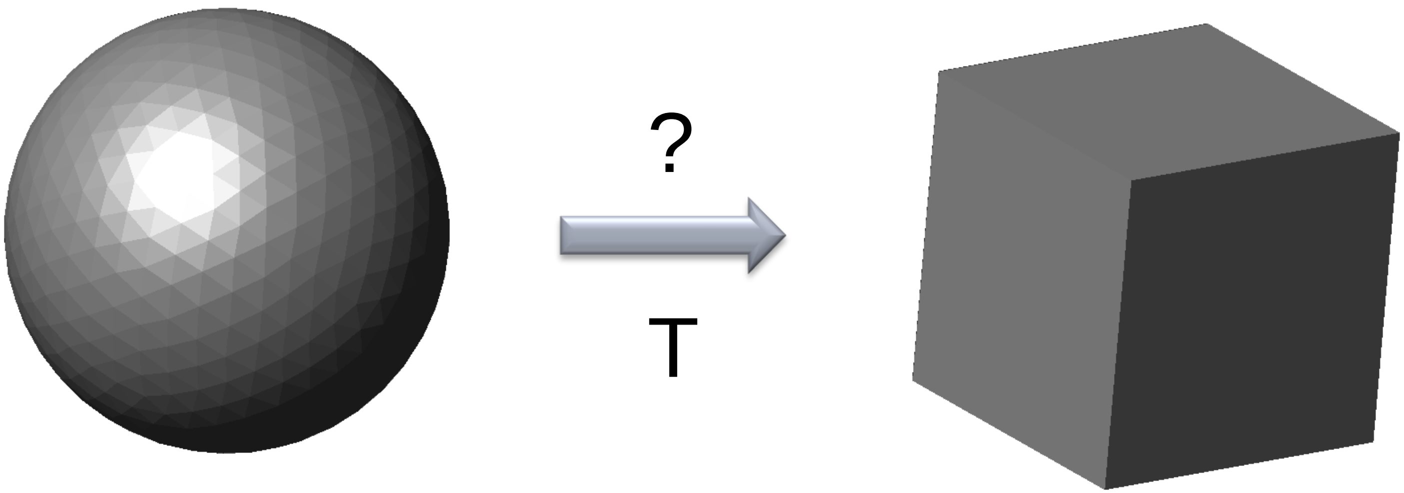
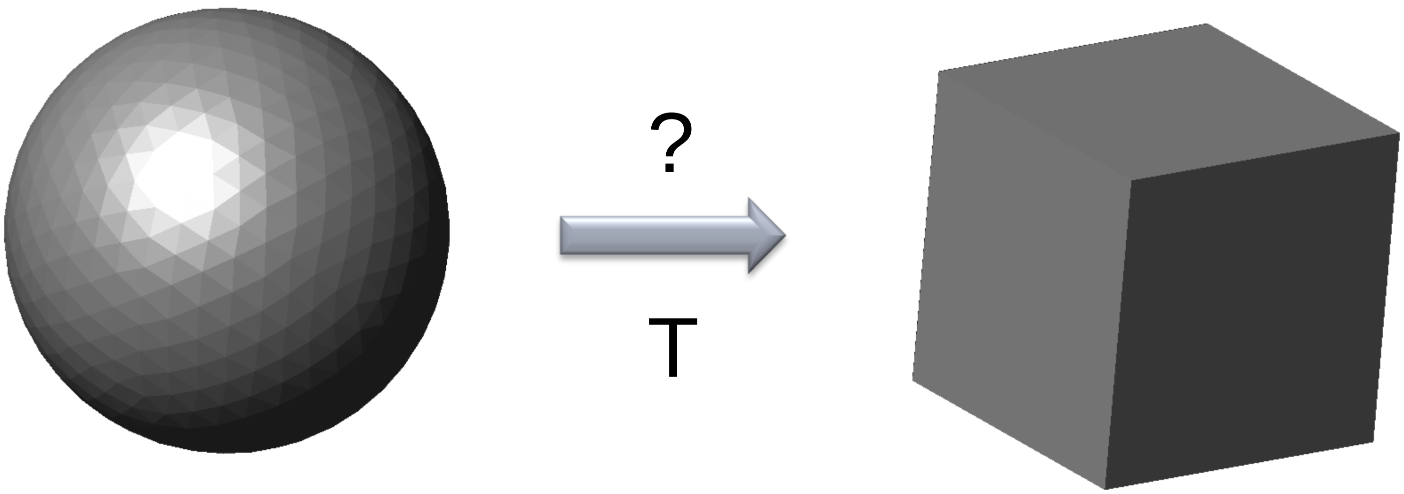


How to "morph" a shape into another one
while preserving mass and **minimizing the effort** ?

"minimum action principle"

Part. 1 Optimal Transport



How to “morph” a shape into another one
while **preserving mass** and **minimizing the effort** ?

“conservation law”

“minimum action principle”

Part. 1 Optimal Transport

OT=

“minimum action principle subject to conservation law”

Yann Brenier:

“Each time the Laplace operator is used in a PDE,
it can be replaced with the Monge-Ampère operator”

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New ways of simulating physics with a computer

Part. 1 Optimal Transport

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"minimum action principle subject to conservation law"

Yann Brenier:

"Each time the <u>Laplace operator</u> is used in a PDE,
it can be replaced with the Monge-Ampère operator"

<u>Fast Fourier Transform</u>

New ways of simulating physics with a computer

Part. 1 Optimal Transport

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"minimum action principle subject to conservation law"

Yann Brenier:

"Each time the Laplace operator is used in a PDE,
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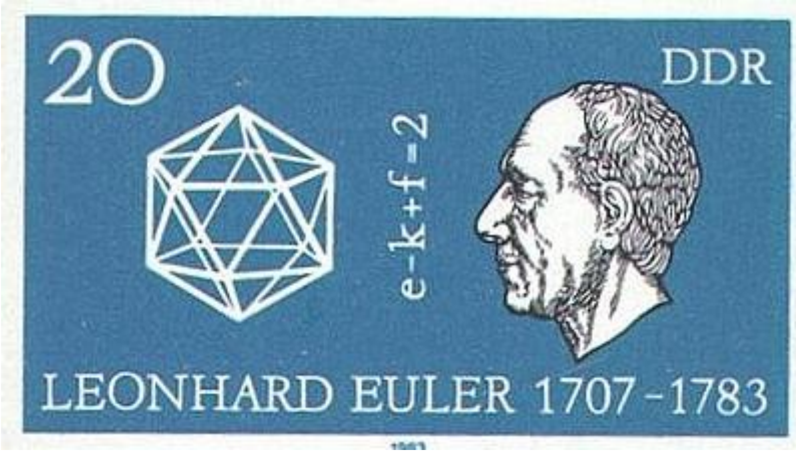
Fast Fourier Transform

Fast OT algo. ???

New ways of simulating physics with a computer



Euler

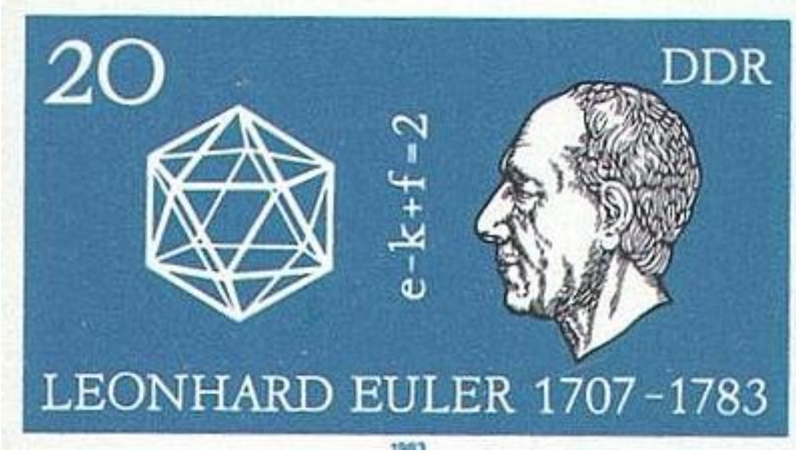
Hamilton,
Legendre,
Maupertuis

Lagrange

The Least Action Principle

Axiom 1: There exists a function $L(x,\dot{x},t)$ that describes the state of a physical system

Short summary of the 1st chapter of Landau,Lifshitz Course of Theoretical Physics



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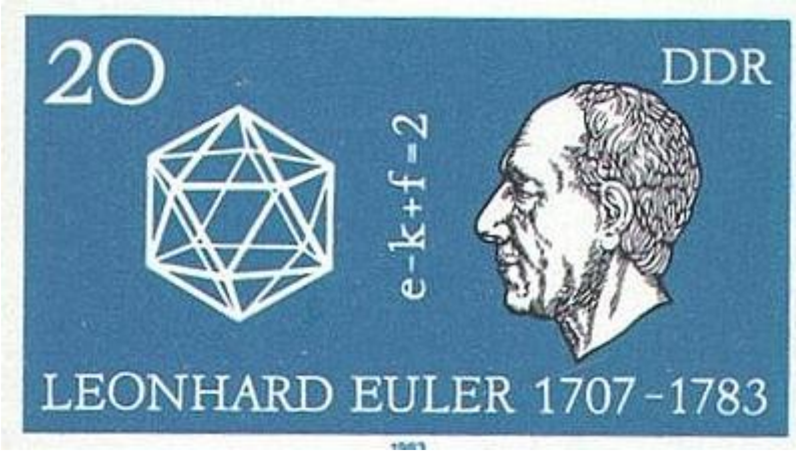
position



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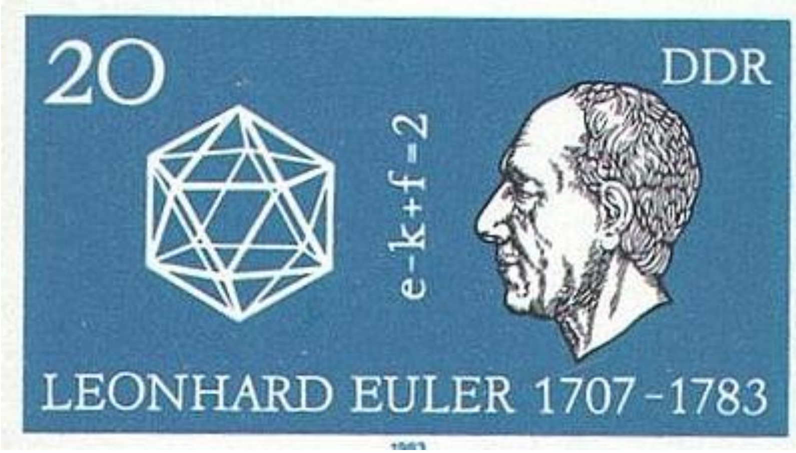
position

speed



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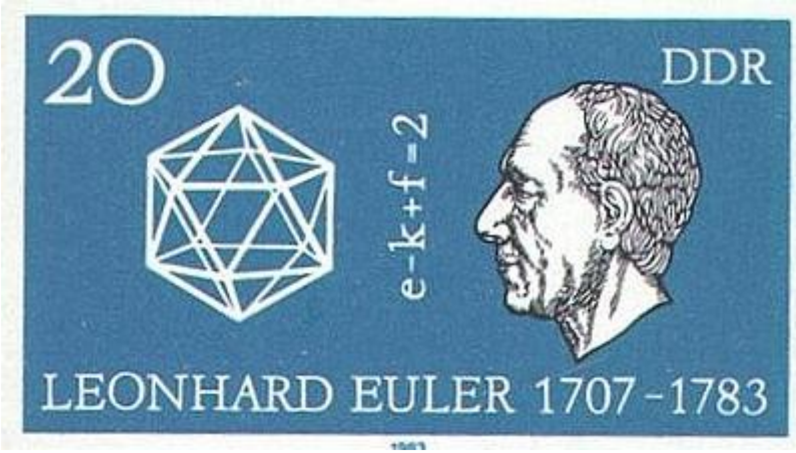
- x: position
- $\dot{x}$: speed
- t: time



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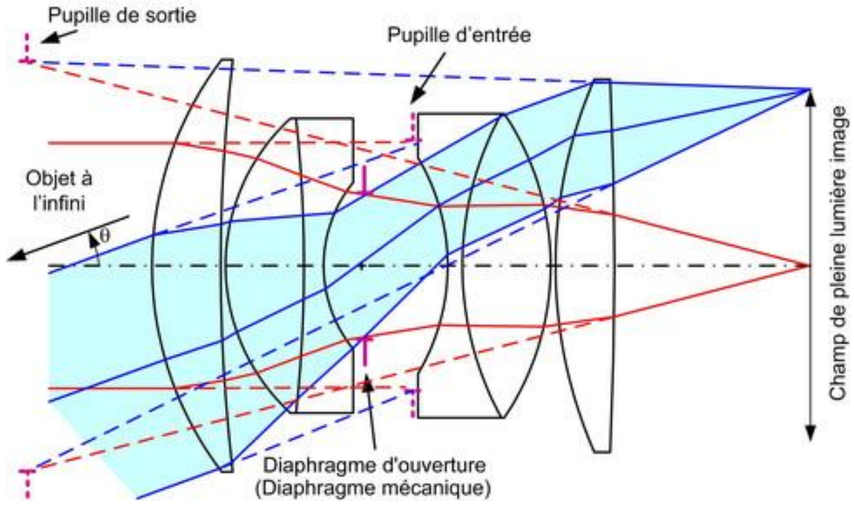
The Least Action Principle

Axiom 1: There exists a function $L(x,\dot{x},t)$ that describes the state of a physical system

Axiom 2: The movement (time evolution) of the physical system minimizes the following integral

$$\int_{t_1}^{t_2} L(x,\dot{x},t)\, dt$$



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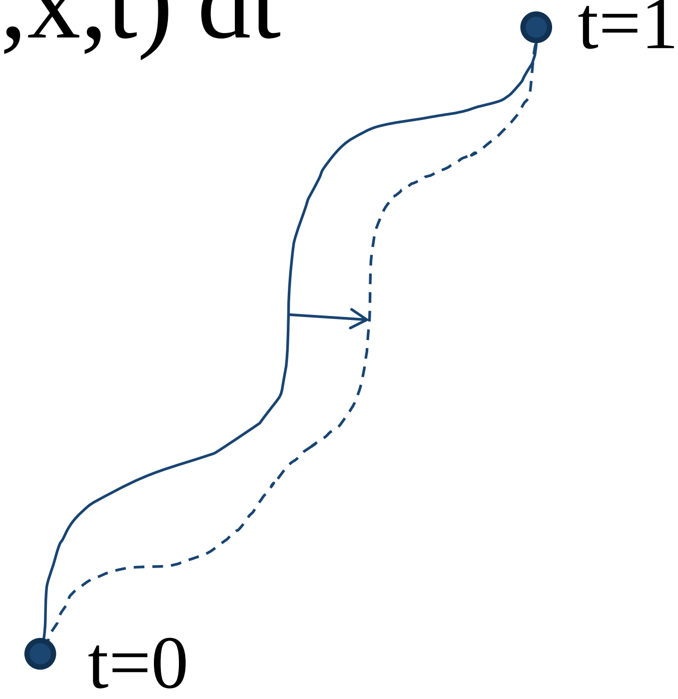

Theorem 1: (Lagrange equation):

$$\frac{\partial L}{\partial x} = \frac{d}{dt}\frac{\partial L}{\partial \dot{x}}$$

The Least Action Principle

Axiom 1: There exists L
Axiom 2: The movement minimizes

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Axiom 3:
Invariance w.r.t. change of Gallileo frame + hom. + isotrop. :

$$\begin{matrix} x' \\ t' \end{matrix} = \begin{matrix} x+vt \\ t \end{matrix}$$

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Theorem 2:

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Homogeneity of time → Preservation of **energy**

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Homogeneity of space → Preservation of **momentum**

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Homogeneity of time →
Preservation of **energy**

Homogeneity of space →
Preservation of **momentum**

Isotropy of space →
Preservation of **angular momentum**

The Least Action Principle

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Preserved quantities
"Integrals of Motion"
Noether's theorem

Theorem 1: (Lagrange equation):

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Homogeneity of space → Preservation of **momentum**

Isotropy of space → Preservation of **angular momentum**

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Homogeneity of time →
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Homogeneity of space →
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Isotropy of space →
Preservation of **angular momentum**

<u>Free particle:</u>

Theorem 3: v = cte ***(Newton's law I)***

The Least Action Principle

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Theorem 1: (Lagrange equation):

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Free particle:

Theorem 3: v = cte *(Newton's law I)*

Expression of the Lagrangian:

$$L = ½\, m\, v^2$$

Axiom 3:
Invariance w.r.t. change of Gallileo frame + hom. + isotrop. :

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Theorem 2:

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Homogeneity of time → Preservation of **energy**

Homogeneity of space → Preservation of **momentum**

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Homogeneity of space → Preservation of **momentum**

Isotropy of space → Preservation of **angular momentum**

Free particle:

Theorem 3: $v = cte$ ***(Newton's law I)***

Expression of the Lagrangian:

$$L = \tfrac{1}{2}\, m\, v^2$$

Expression of the Energy:

$$E = \tfrac{1}{2}\, m\, v^2$$

The Least Action Principle

Axiom 1: There exists L

Axiom 2: The movement minimizes $\int L$

Theorem 1: (Lagrange equation):

$$\frac{\partial L}{\partial x} = \frac{d}{dt}\frac{\partial L}{\partial \dot{x}}$$

Axiom 3:
Invariance w.r.t. change of Gallileo frame + hom. + isotrop. :

$$\begin{matrix} x' \\ t' \end{matrix} = \begin{matrix} x+vt \\ t \end{matrix}$$

Free particle:

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Particle in a field:

Expression of the Lagrangian:

$$L = \tfrac{1}{2}\, m\, v^2 - U(x)$$

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$$E = \frac{1}{2} m v^2 + U(x)$$

Theorem 4:

$$m\ddot{x} = -\nabla U$$ *(Newton's law II)*

The Least Action Principle
(relativistic setting – just for fun…)

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Axiom 2: The movement minimizes $\int L$

Theorem 1: (Lagrange equation):

$$\frac{\partial L}{\partial x} = \frac{d}{dt} \frac{\partial L}{\partial \dot{x}}$$

Axiom 3:
Invariance w.r.t. Lorentz change of frame

$$\begin{pmatrix} x' \\ t' \end{pmatrix} = \begin{pmatrix} (x-vt) \times \gamma \\ (t - vx/c^2) \times \gamma \end{pmatrix}$$

$$\gamma = 1 / \sqrt{(1 - v^2 / c^2)}$$

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$$\gamma = 1 / \sqrt{(1 - v^2 / c^2)}$$

Theorem 5:

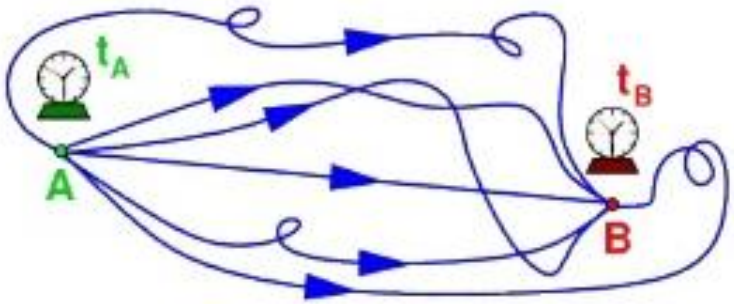
$$E = \tfrac{1}{2} \gamma m v^2 + mc^2$$

The Least Action Principle

(quantum physics setting – just for fun…)

In quantum mechanics non just the extreme path contributes to the probability amplitude

$$P(B,A)=|K(2,1)|^2$$



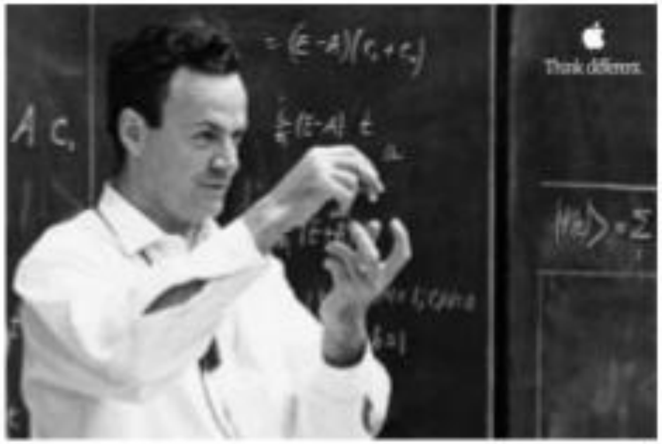
$$K(B,A)=\sum_{over\,all\,possible\,paths}\phi[x(t)]$$

where

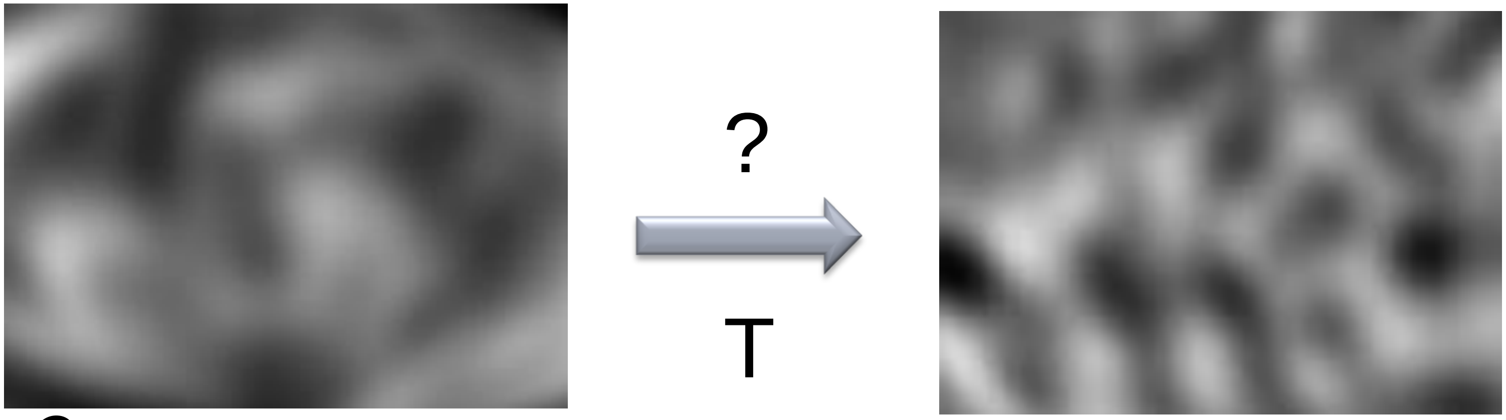
$$\phi[x(t)]=A\exp\left\{\frac{i}{\hbar}S[x(t)]\right\}$$

Feynman's path integral formula

$$K(B,A)=\int_A^B\exp\left(\frac{i}{\hbar}S[B,A]Dx(t)\right)$$

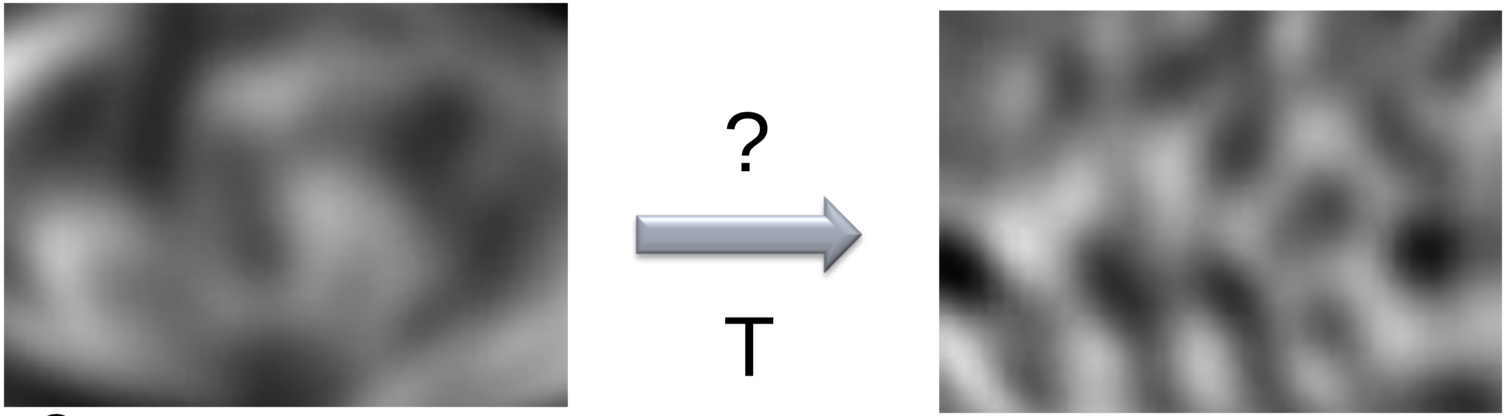


Fluids – Benamou Brenier



ρ_1 ρ_2

Fluids – Benamou Brenier



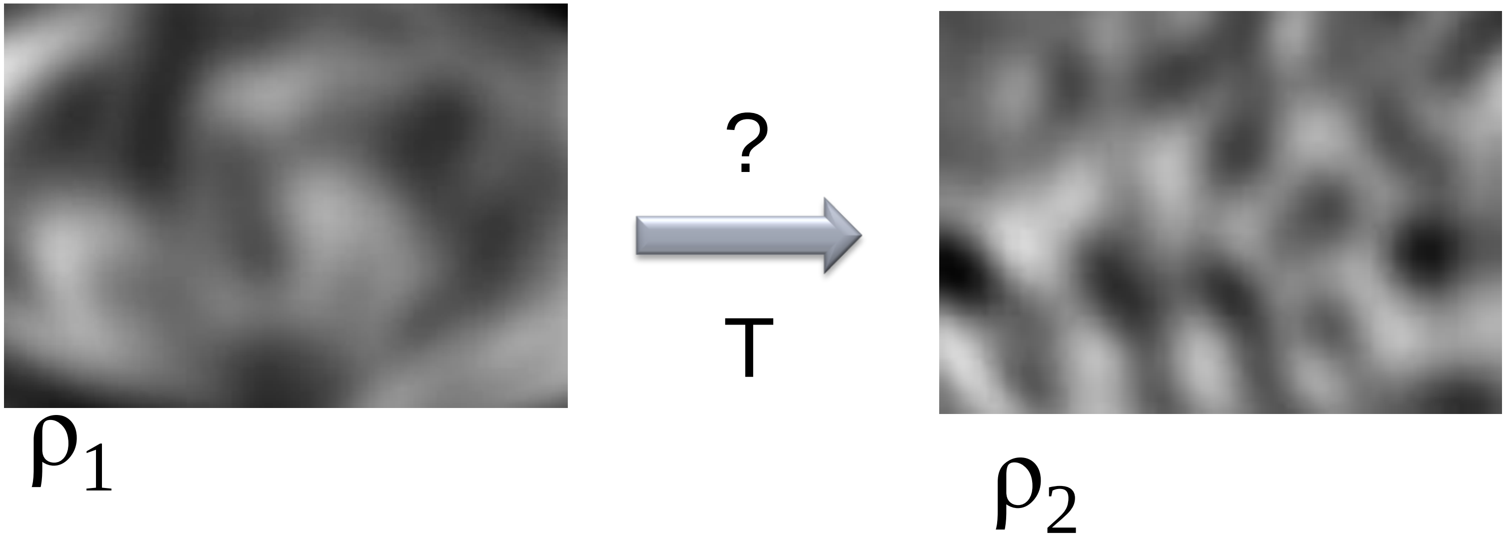
ρ_1 ρ_2

Minimize

$$A(\rho,v) = (t_2-t_1) \int_{t_1}^{t_2} \int_{\Omega} \rho(x,t)\, \|v(t,x)\|^2 dx dt$$

s.t. $\rho(t_1,.) = \rho_1$; $\rho(t_2,.) = \rho_2$; $\frac{d\rho}{dt} = -\operatorname{div}(\rho v)$

Fluids – Benamou Brenier



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s.t. $\rho(t_1,.) = \rho_1$; $\rho(t_2,.) = \rho_2$; $\frac{d\rho}{dt} = -\operatorname{div}(\rho v)$

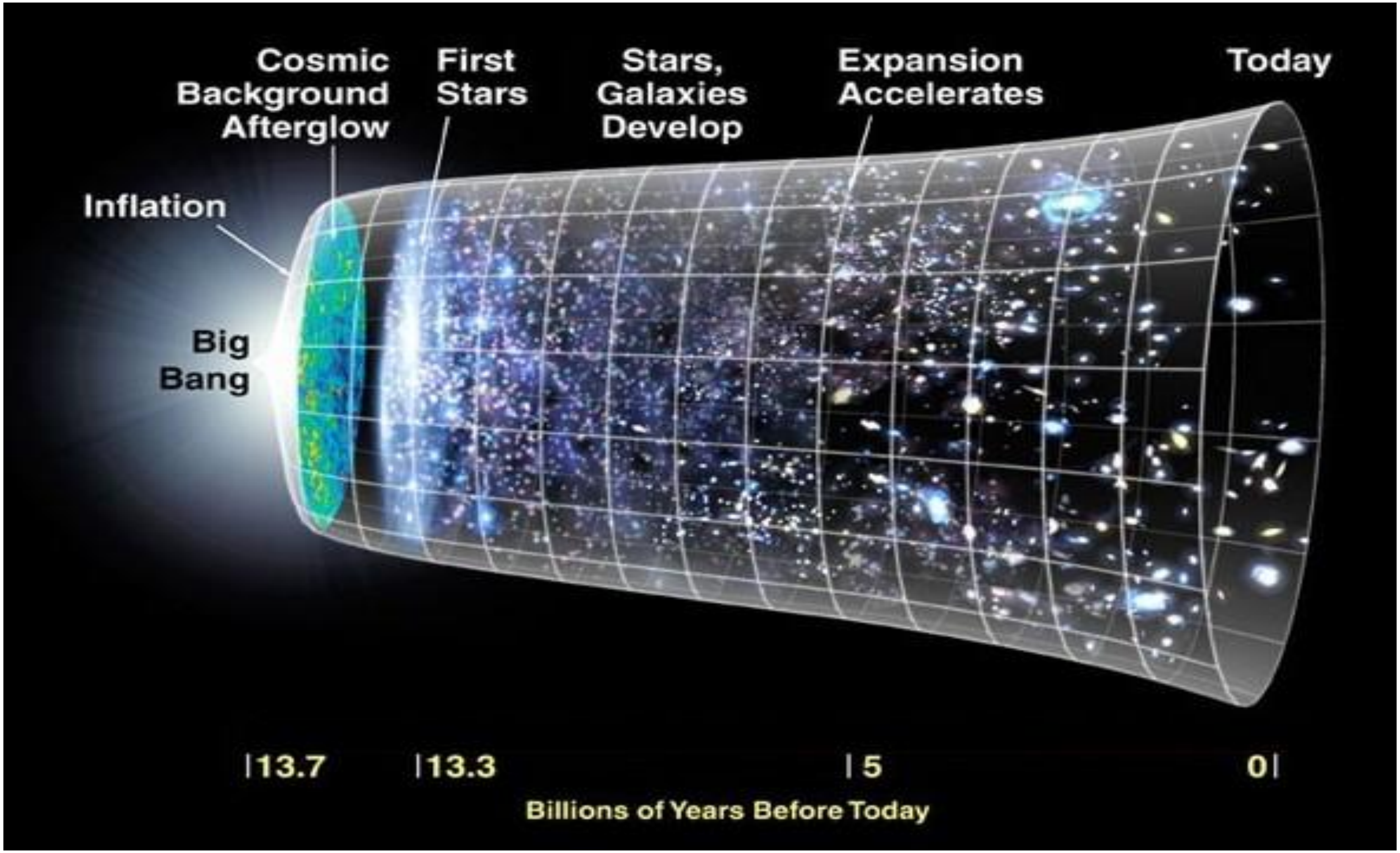
⟷

Minimize C(T) =

$$\int_{\Omega} \rho_1(x) \| \; x - T(x) \; \| 2 \; dx$$

s.t. T is measure-preserving

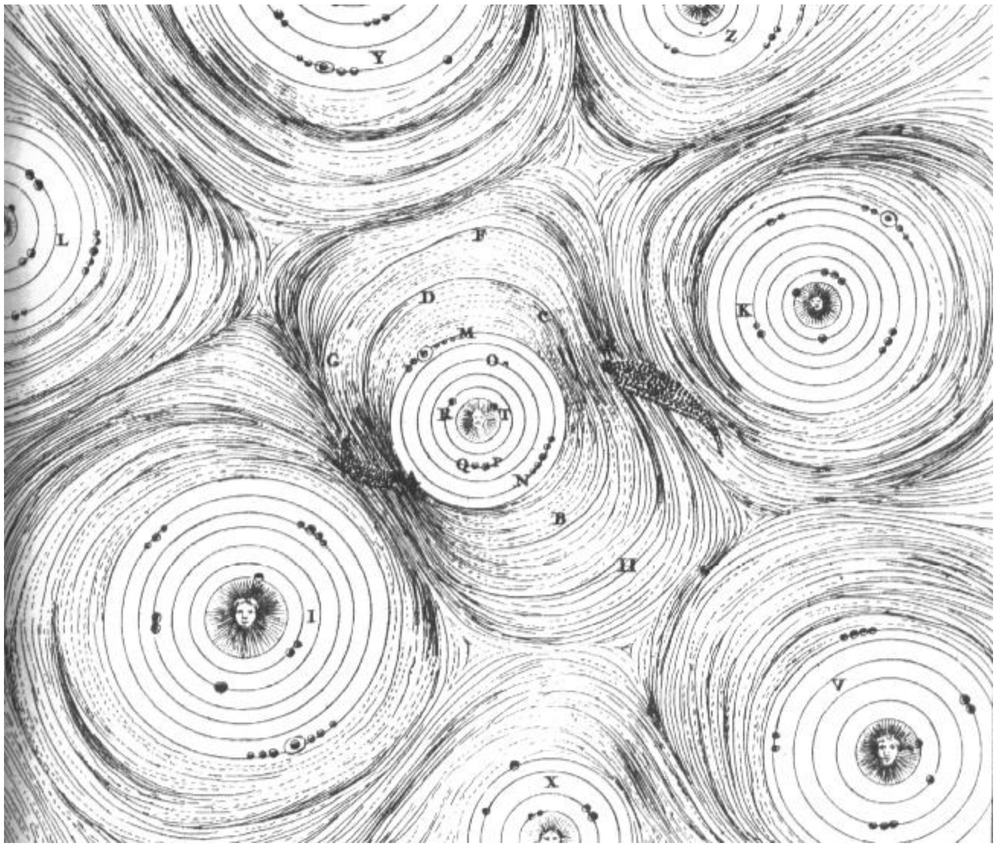
Simuler tout l'univers dans un ordinateur…

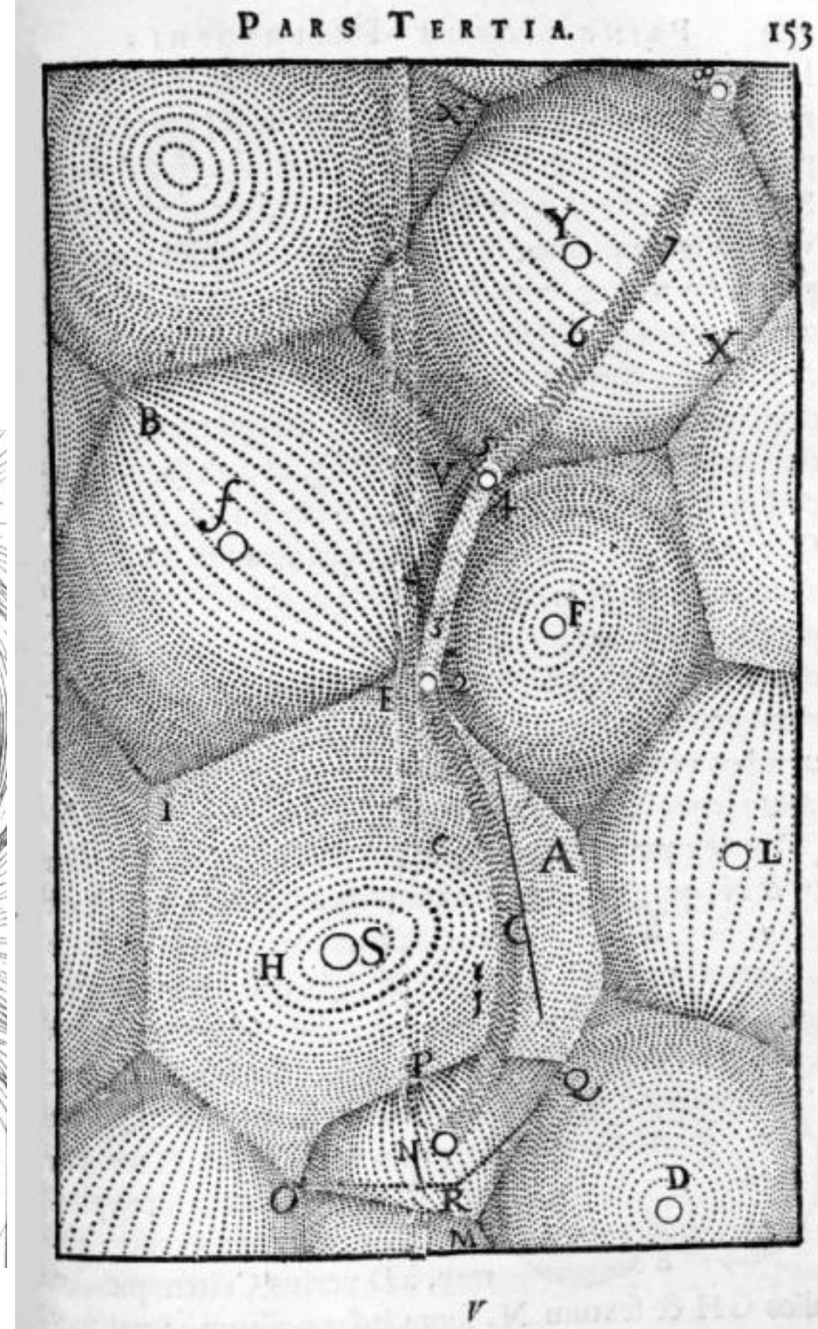


Part. 1 Optimal Transport

Des tourbillons dans l'éther ?

René Descartes - 1663



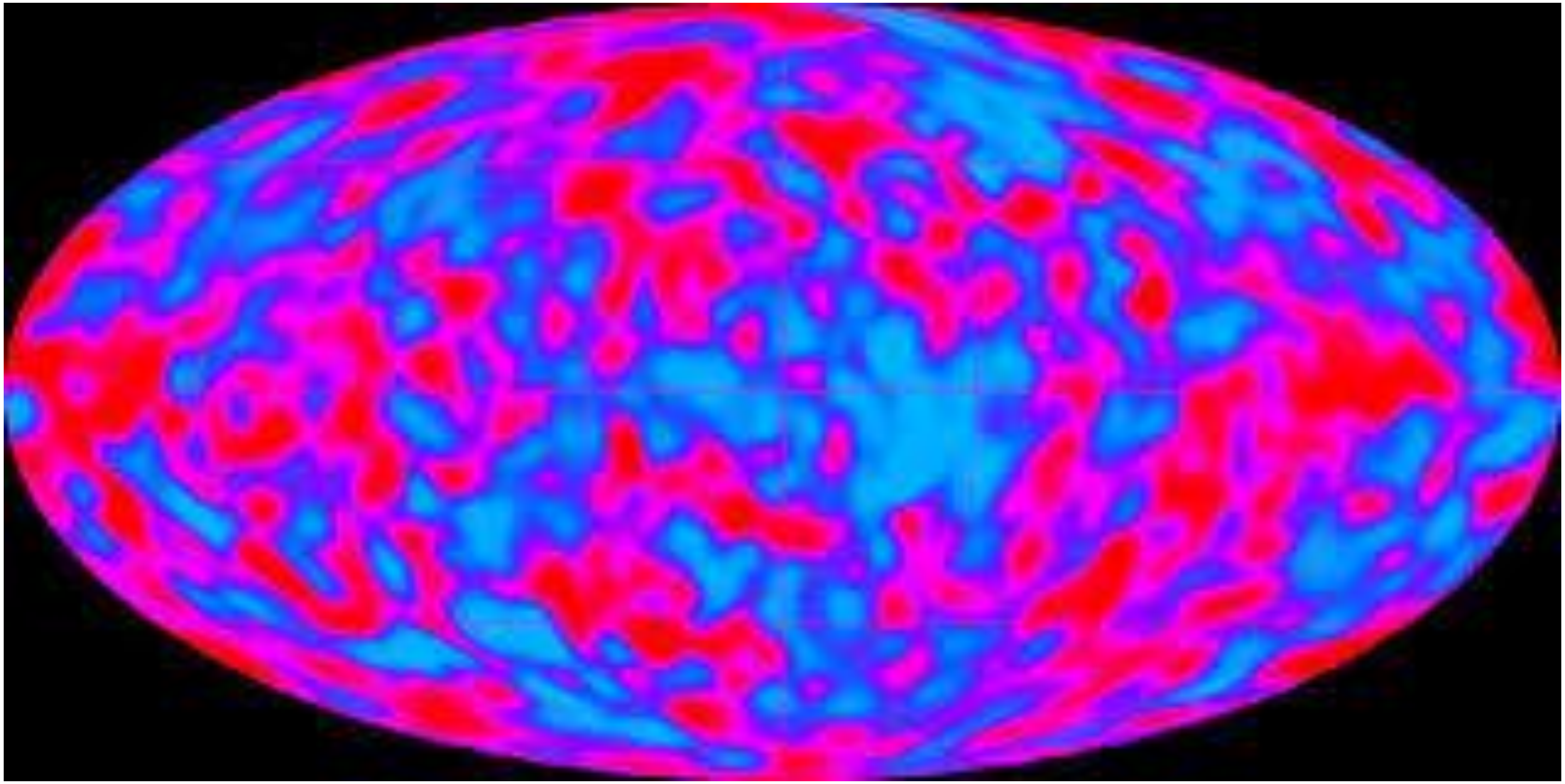


Vers l'infini et au delà …

COBE 1992

Reconstruction de l univers primordial

Les données – Fond de rayonnement cosmologique



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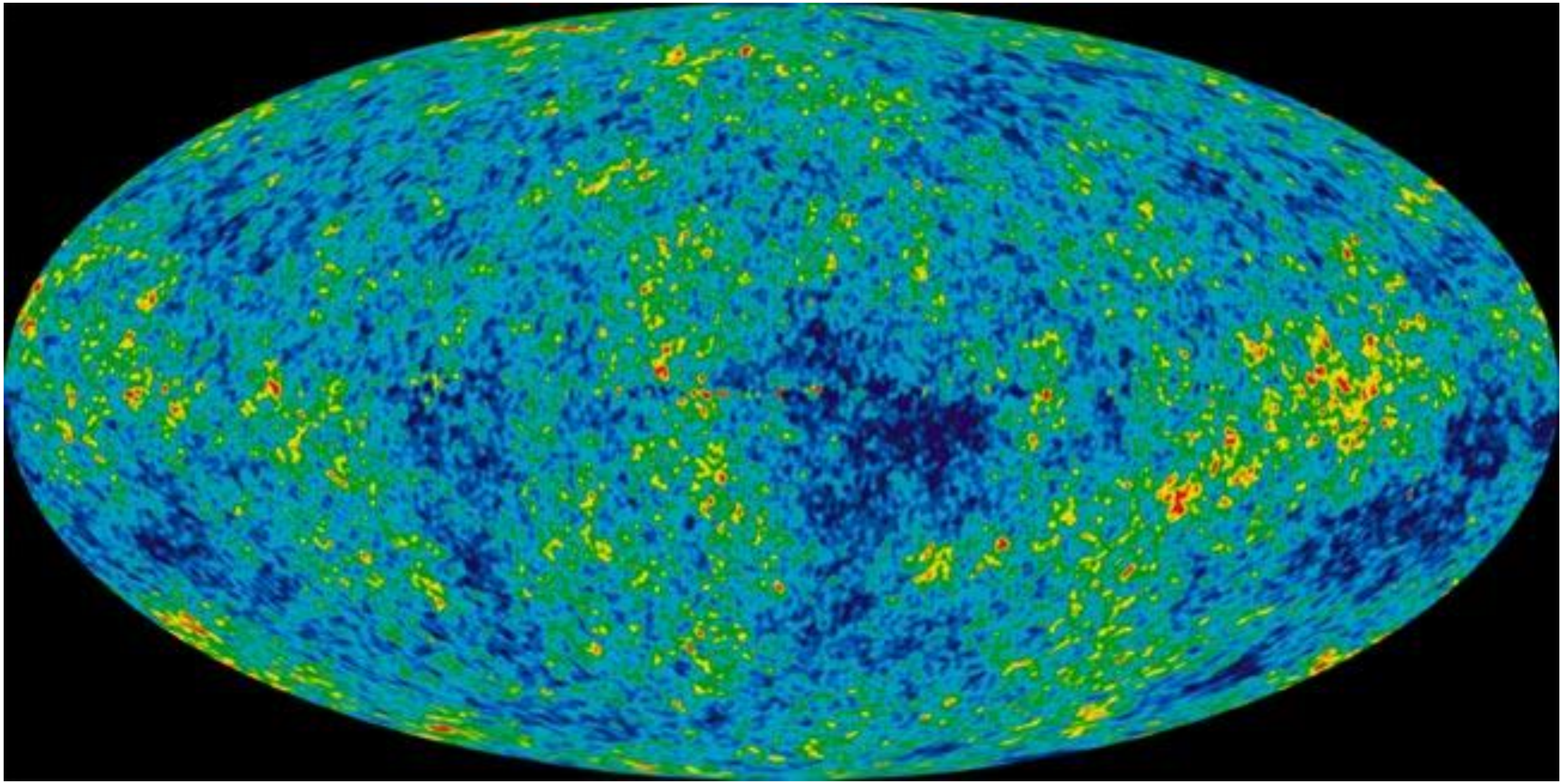
Les données – Fond de rayonnement cosmologique

WMAP 2003
2006
2008
2010



Vers l'infini et au delà …

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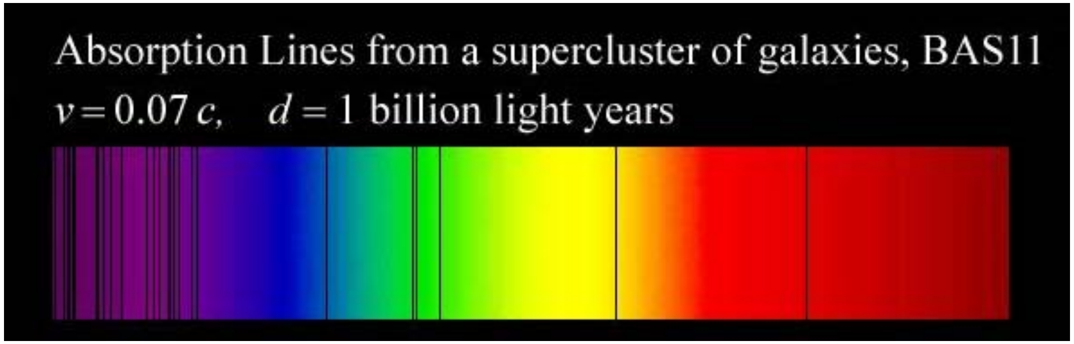
Les données – campagnes d’acquisition red-shift



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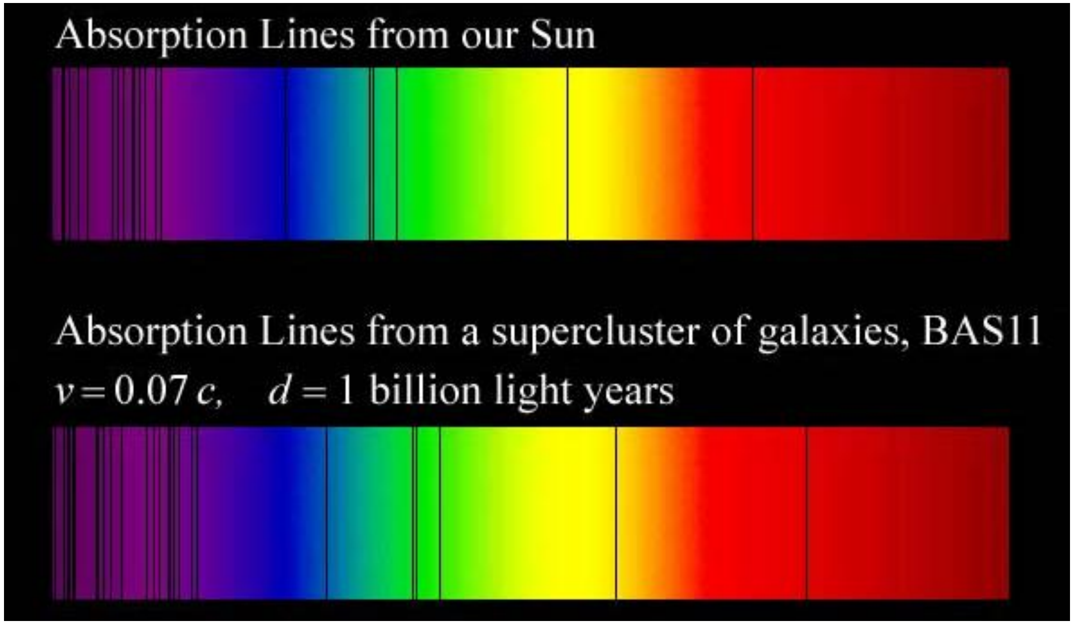

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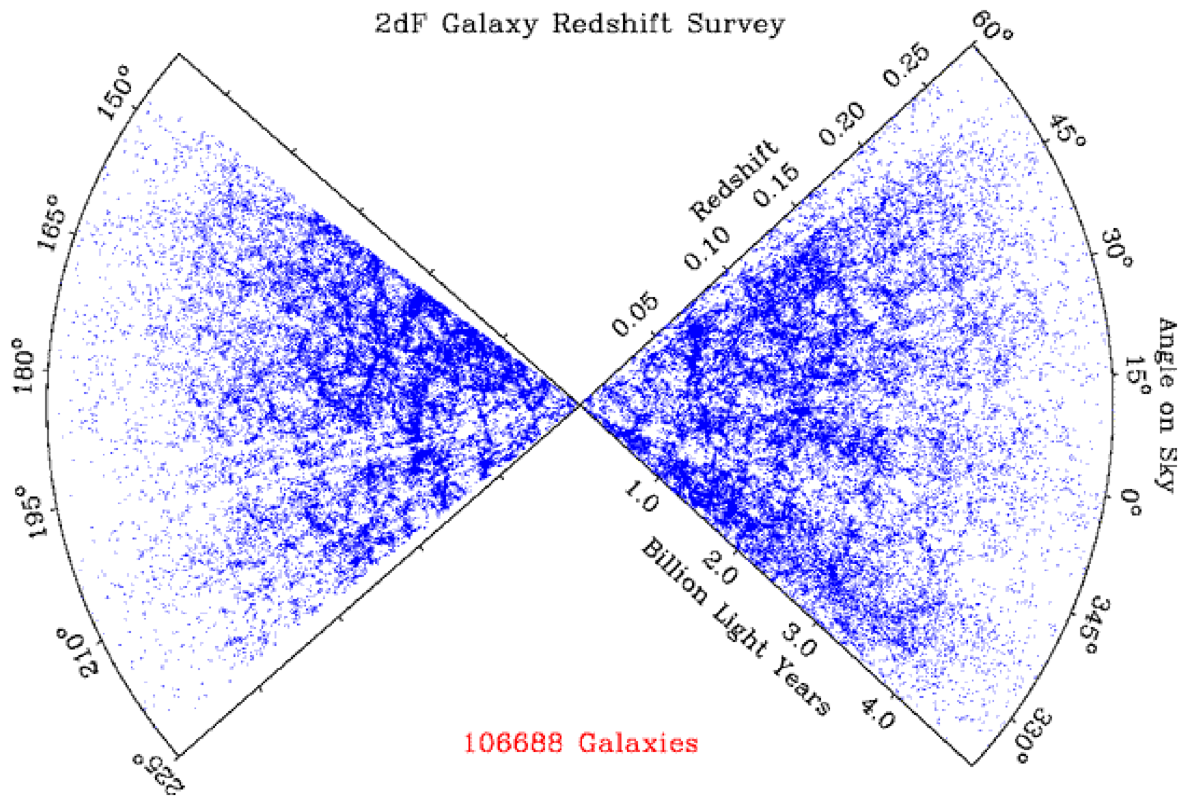
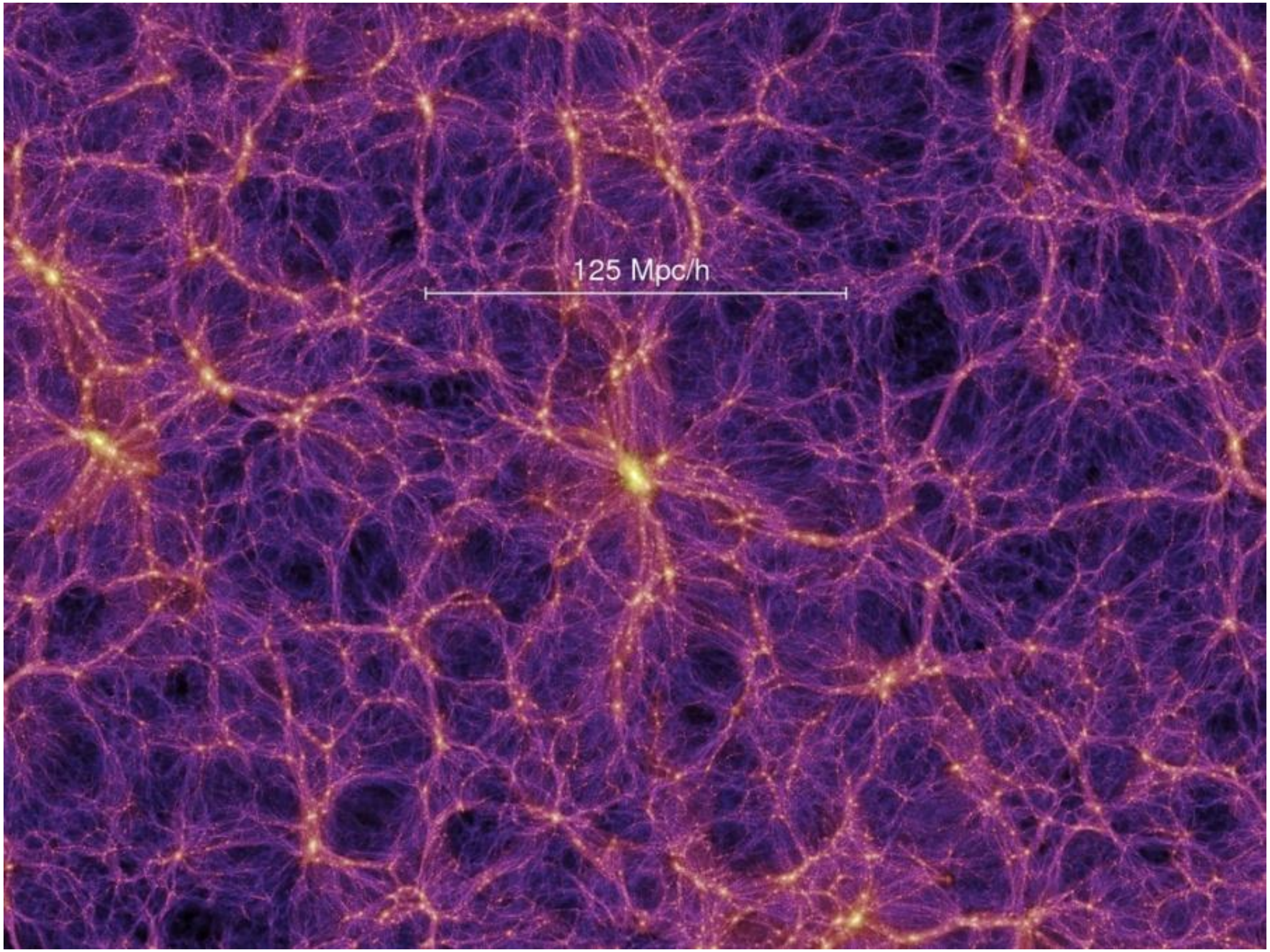


Vers l'infini et au delà …

pc/h : parsec (= 3.2 années lumières)

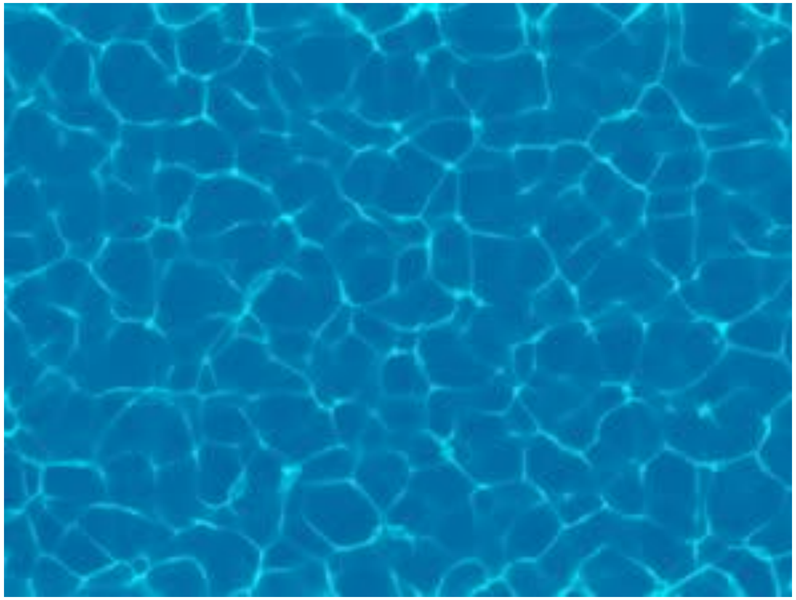


The millenium simulation project, Max Planck Institute fur Astrophysik

Vers l'infini et au delà …

Reconstruction de l état primordial de l univers

La piscine universelle



Vers l'infini et au delà …

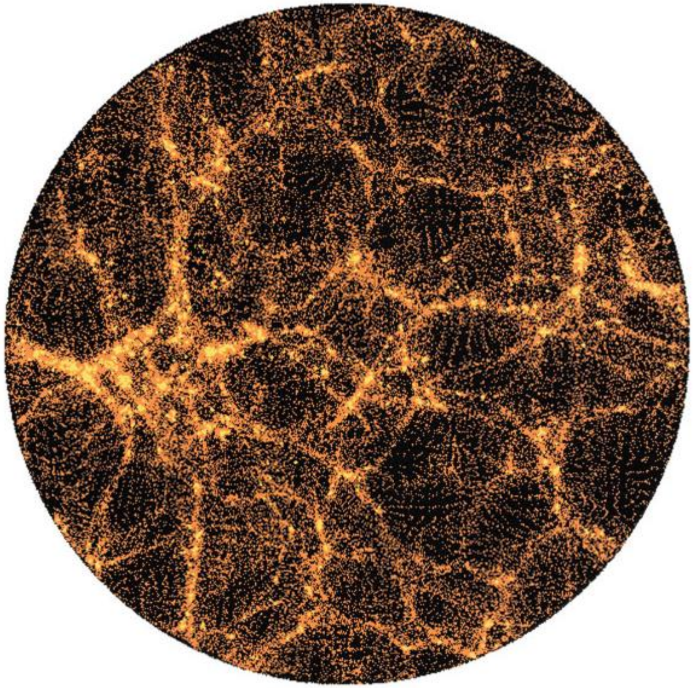
Inverser les équations de Newton / Einstein pour remonter le temps de 14 milliards d années

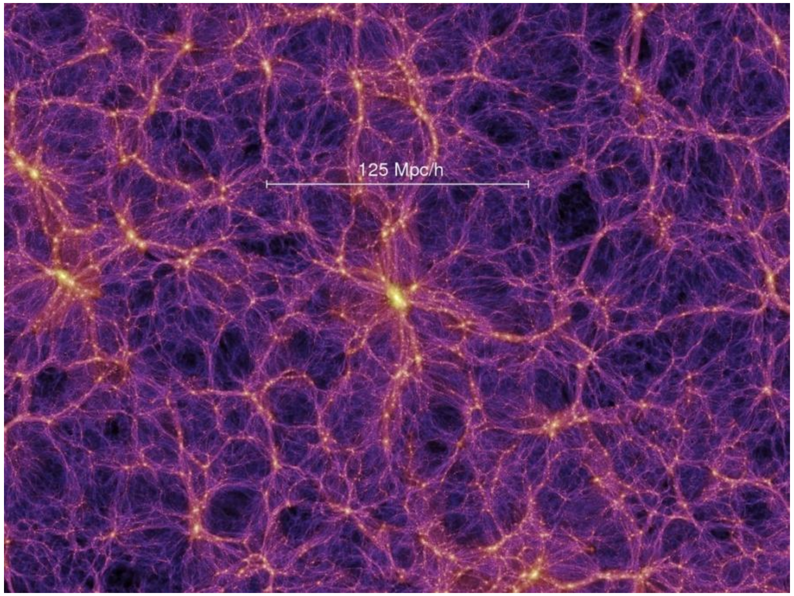
RECONSTRUCTION OF THE EARLY UNIVERSE, ZELDOVICH APPROXIMATION AND MONGE-AMPÈRE GRAVITATION

YANN BRENIER

U. Frisch, S. Matarrese, R. Mohayaee, A. Sobolevski, *A reconstruction of the initial conditions of the Universe by optimal mass transportation*, Nature 417 (2002) 260-262.

pc/h : parsec (= 3.2 light years)





The millenium simulation project,
Max Planck Institute fur Astrophysik

Vers l'infini et au delà ...

En 2002: 5 heures de calcul
sur un super-ordinateur / **5000** points

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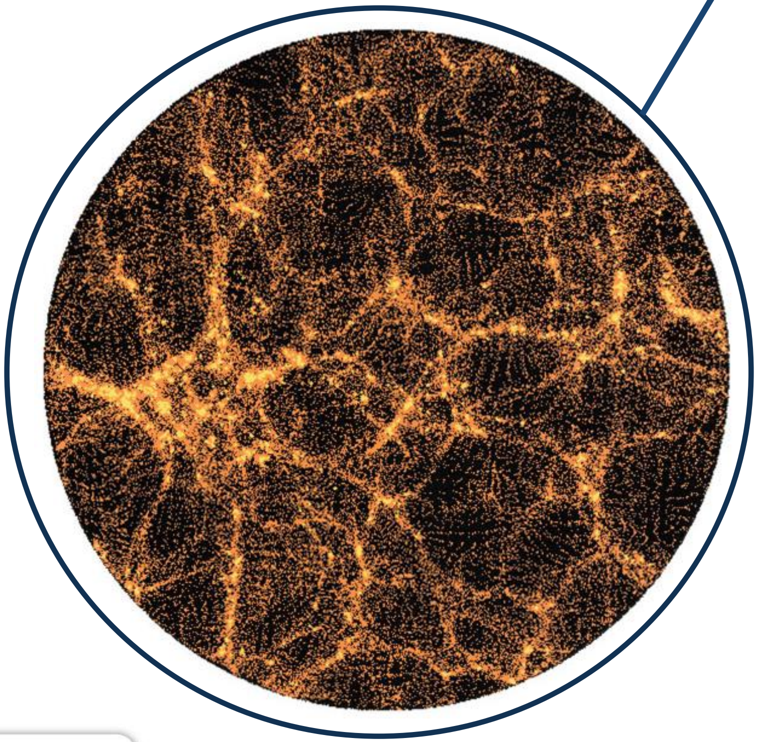

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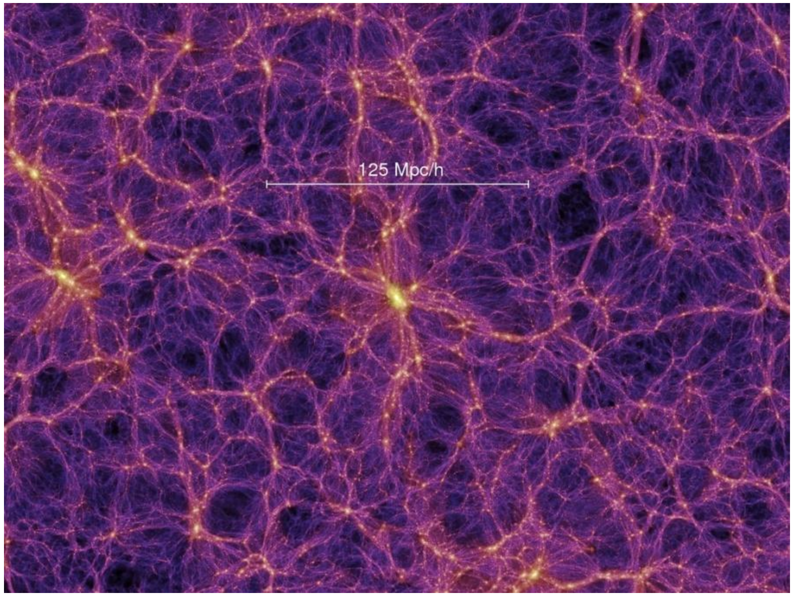

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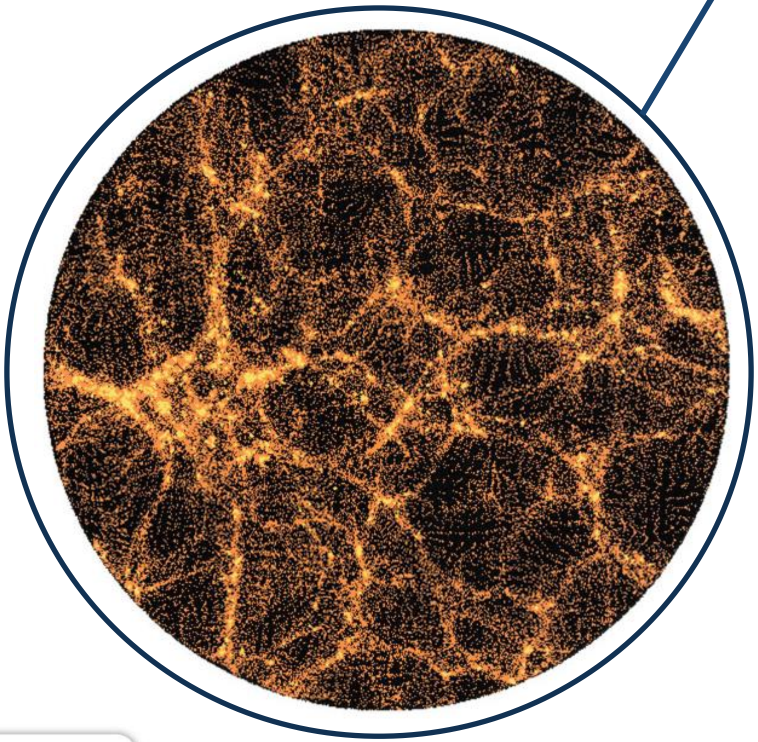

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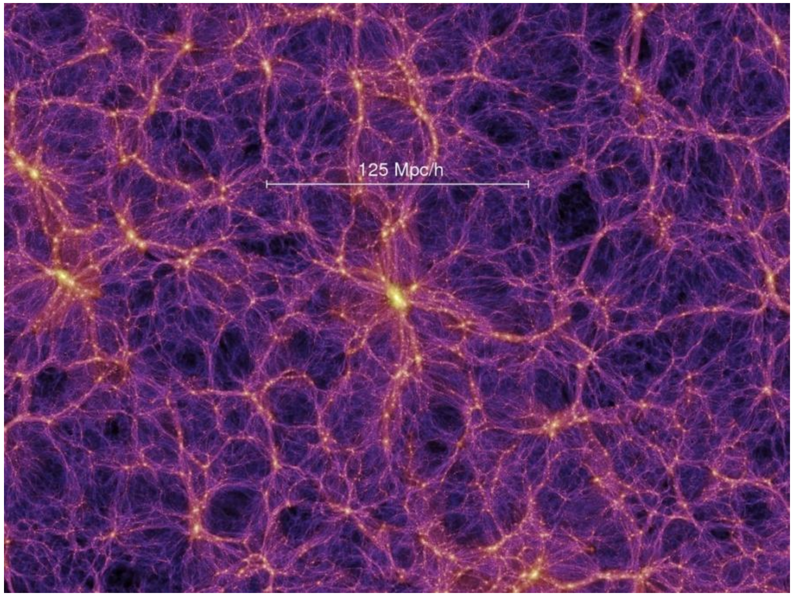

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Peut-on faire le calcul avec **1 000 000** points ?

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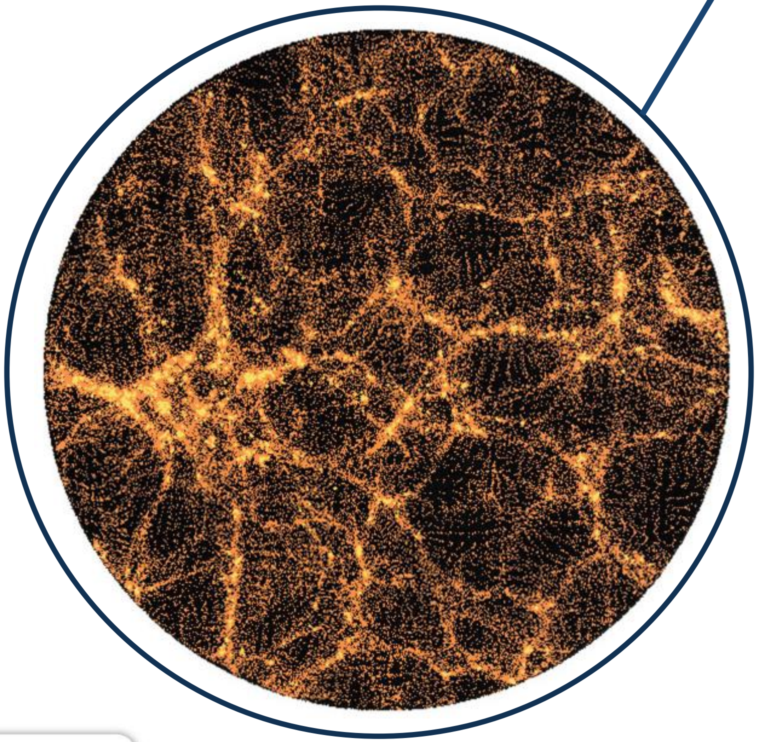

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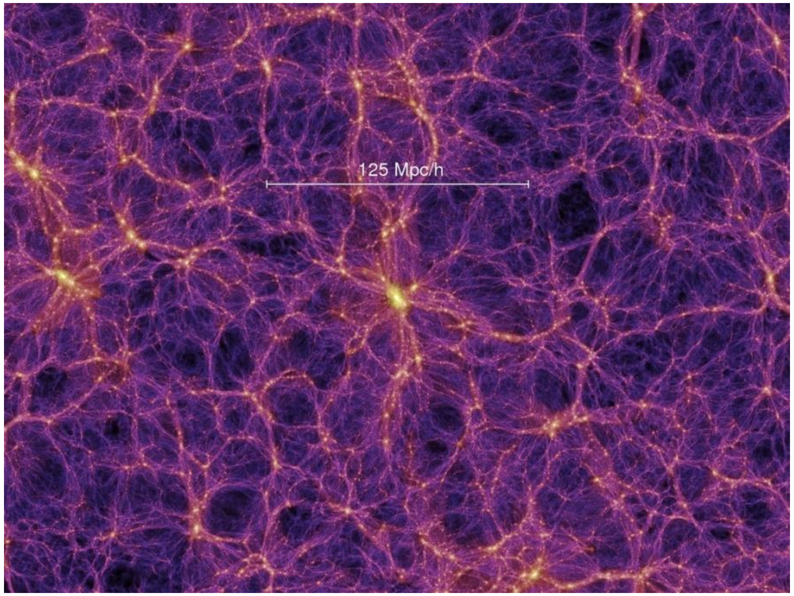

The millenium simulation project,
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Peut-on faire le calcul avec
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Oui si on attend (4500 ans !!)

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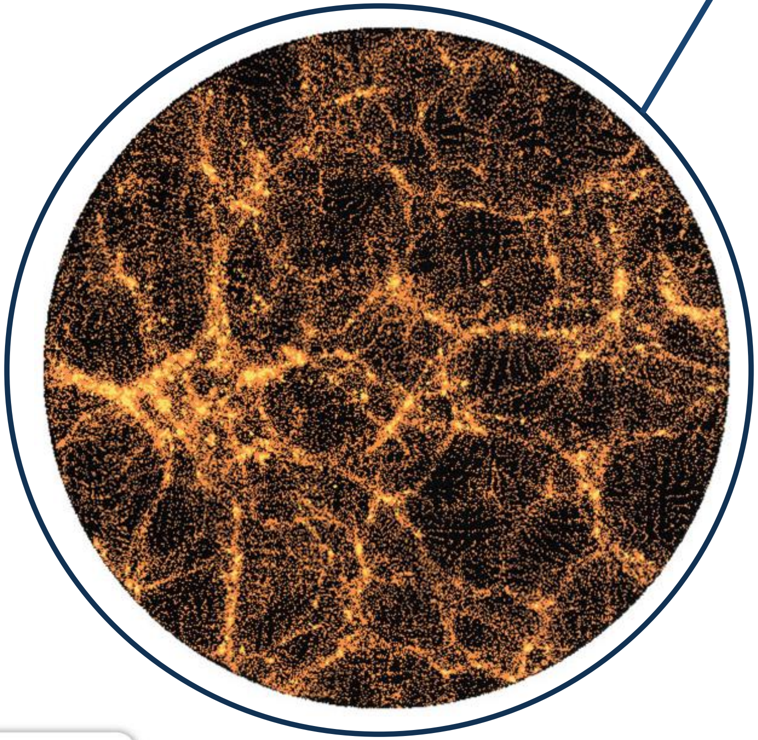

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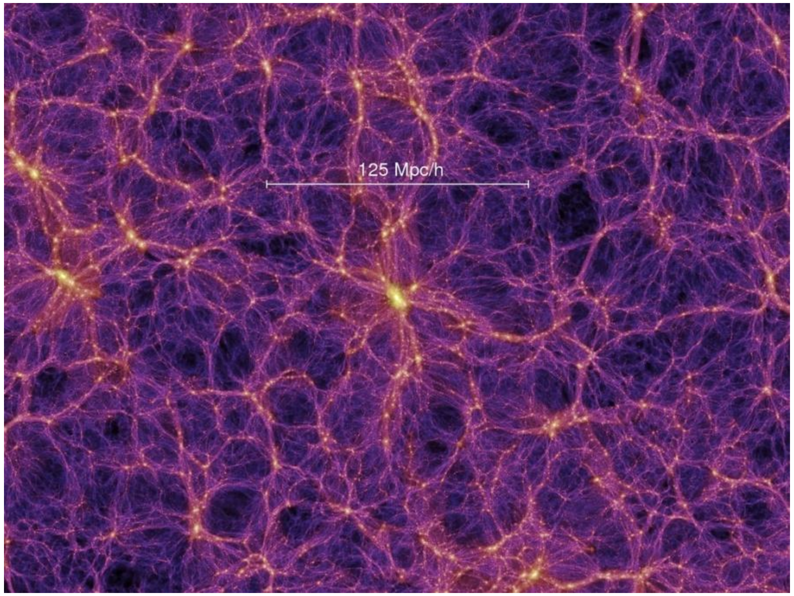

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Transport and Physics

- Euler fluids – geodesics [Galouet, Mirebeau, Mérigot]
- Euler fluids – Cauchy problem
- Gradient flows – Jordan Kinderlehrer Otto

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Iterative schemes, need to solve multiple OT problems

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Iterative schemes, need to solve multiple OT problems

Need for an efficient solver
(there is no “FFT for OT”, what can we do instead ?)

2

Optimal Transport

an elementary introduction

Part. 2 Optimal Transport – Monge's problem

(X;μ)

(Y;v)

Two measures μ, v such that $\int_X d\mu(x) = \int_Y dv(x)$

Part. 2 Optimal Transport – Monge's problem

(X;μ)

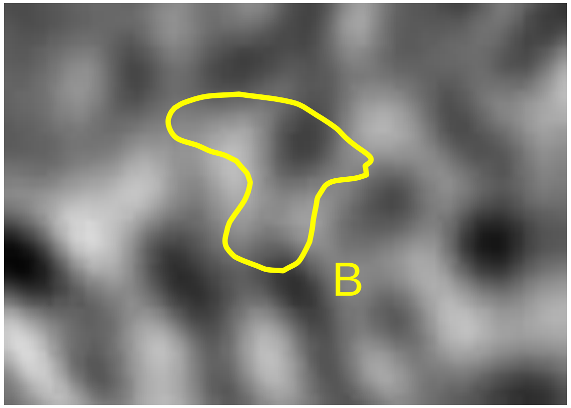
(Y;ν)

A map T is a ***transport map*** between μ and ν if

$\mu(T^{-1}(B)) = \nu(B)$ for any Borel subset B of Y

Part. 2 Optimal Transport – Monge's problem

(X;μ)



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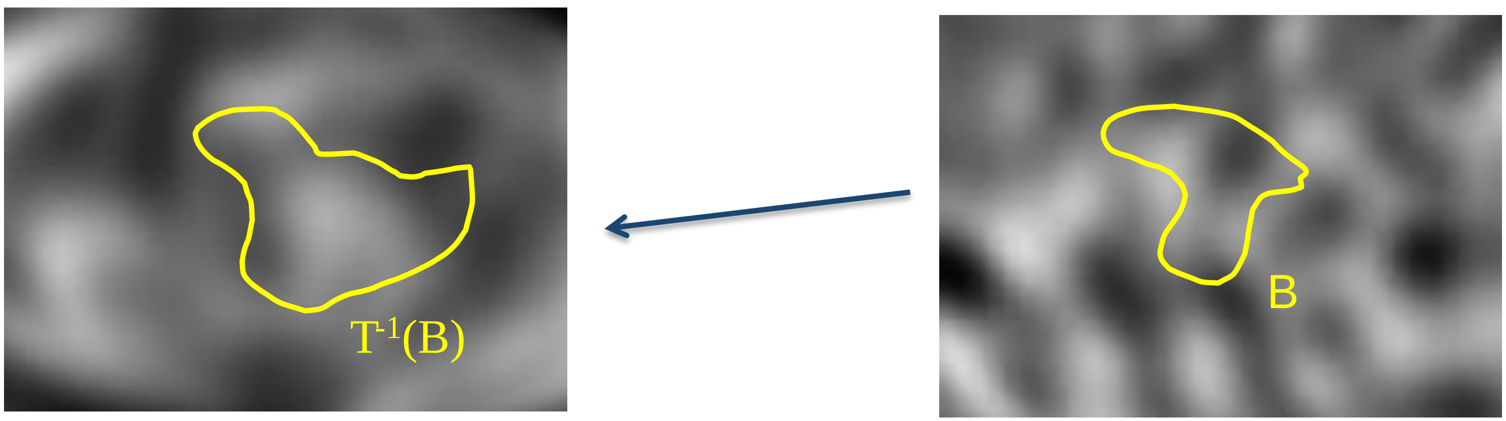

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(X;μ)

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(or $\nu = T\#\mu$ the ***pushforward*** of μ)

Part. 2 Optimal Transport – Monge's problem

(X;μ)

(Y;ν)

Monge's problem:

Find a transport map T that minimizes $C(T) = \int_X \| x - T(x) \|^2 \, d\mu(x)$

Part. 2 Optimal Transport – Monge's problem

Monge's problem:

Find a transport map T that minimizes $C(T) = \int_X \| x - T(x) \|^2 \, d\mu(x)$

- Difficult to study
- If μ has an atom (isolated Dirac),
  it can only be mapped to another Dirac
  (T needs to be a map)

Part. 2 Optimal Transport – Monge's problem

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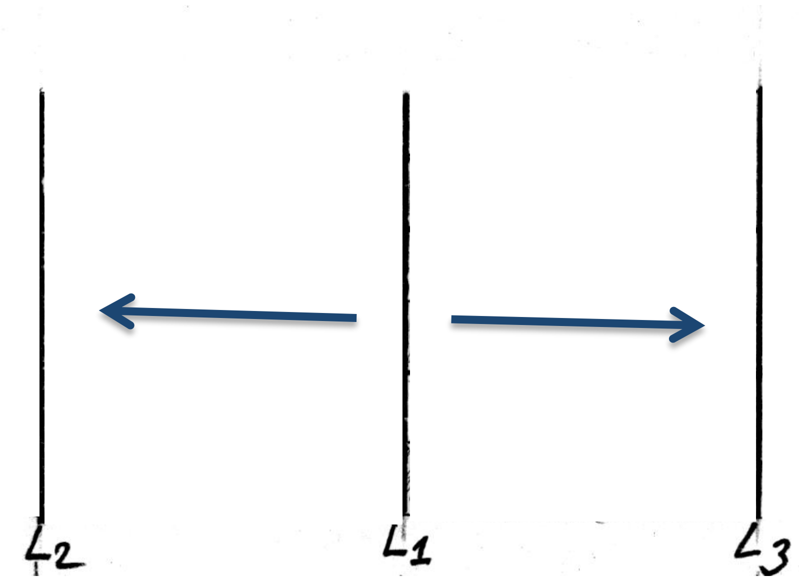
Find a transport map T that minimizes $C(T) = \int_X || x - T(x) ||^2 d\mu(x)$



Transport from a measure concentrated on L_1 onto another one concentrated on L_2 and L_3

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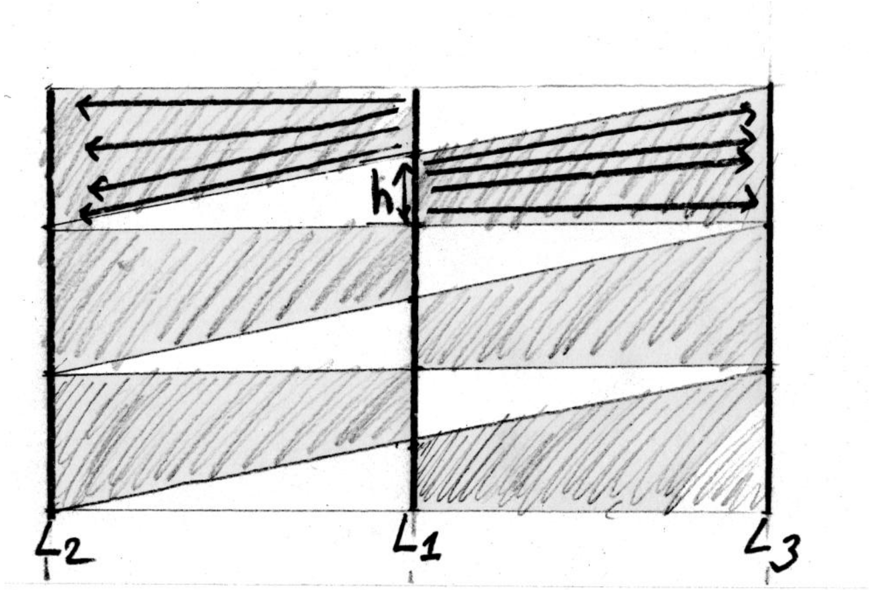

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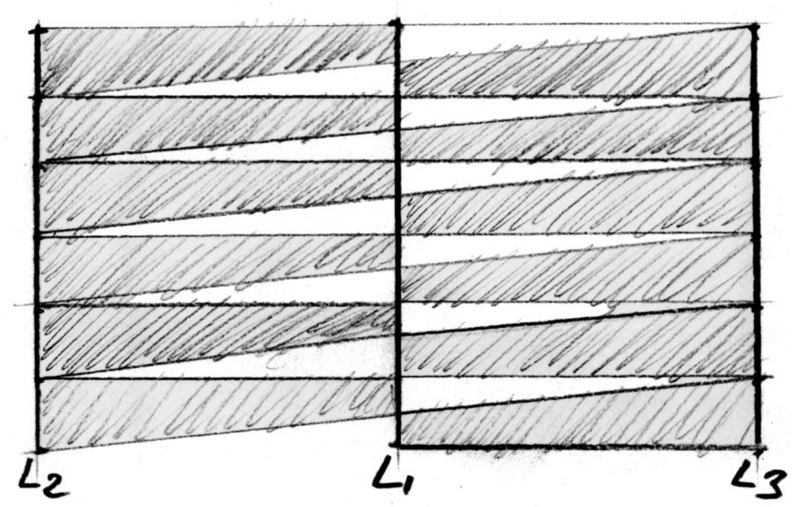

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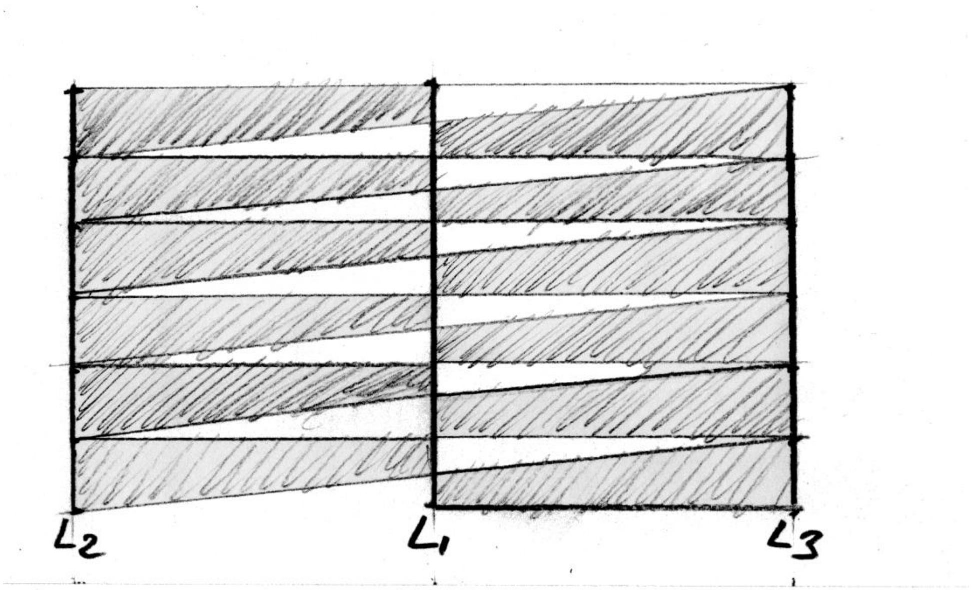

Transport from a measure concentrated on L_1 onto another one concentrated on L_2 and L_3

The infimum is never realized by a map, need for a relaxation

Part. 2 Optimal Transport – Kantorovich

Monge's problem:

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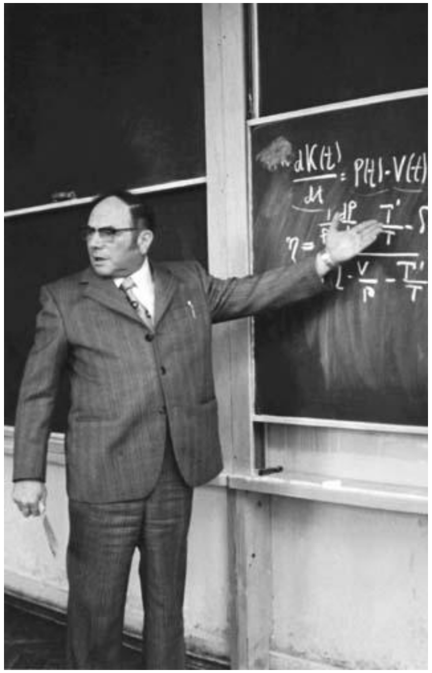
***Kantorovich's problem* (1942):**



Find a measure γ defined on $X \times Y$

such that $\int_{x \text{ in } X} d\gamma(x,y) = d\nu(y)$

and $\int_{y \text{ in } Y} d\gamma(x,y) = d\mu(x)$

that minimizes $\iint_{X \times Y} \| x - y \|^2 \, d\gamma(x,y)$

Part. 2 Optimal Transport – Kantorovich

<u>Monge's problem:</u>

Find a transport map T that minimizes $C(T) = \int_X \| x - T(x) \|^2 \, d\mu(x)$

<u>Kantorovich's problem:</u>

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that minimizes $\iint_{X \times Y} \| x - y \|^2 \, d\gamma(x,y)$

"$\gamma(x,y)$" :
How much sand goes from x to y

Part. 2 Optimal Transport – Kantorovich

Monge's problem:

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Everything that is transported **from x** sums to "μ(x)"

that minimizes $\iint_{X \times Y} \| x - y \|^2 \, d\gamma(x,y)$

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Find a measure γ defined on X x Y

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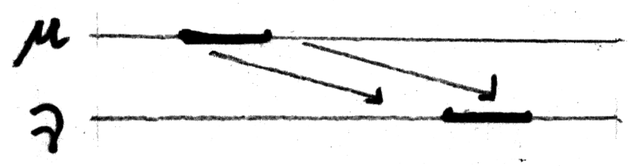
and $\int_{y \text{ in } Y} d\gamma(x,y) = d\mu(x)$

Everything that is transported **to y** sums to "ν(y)"

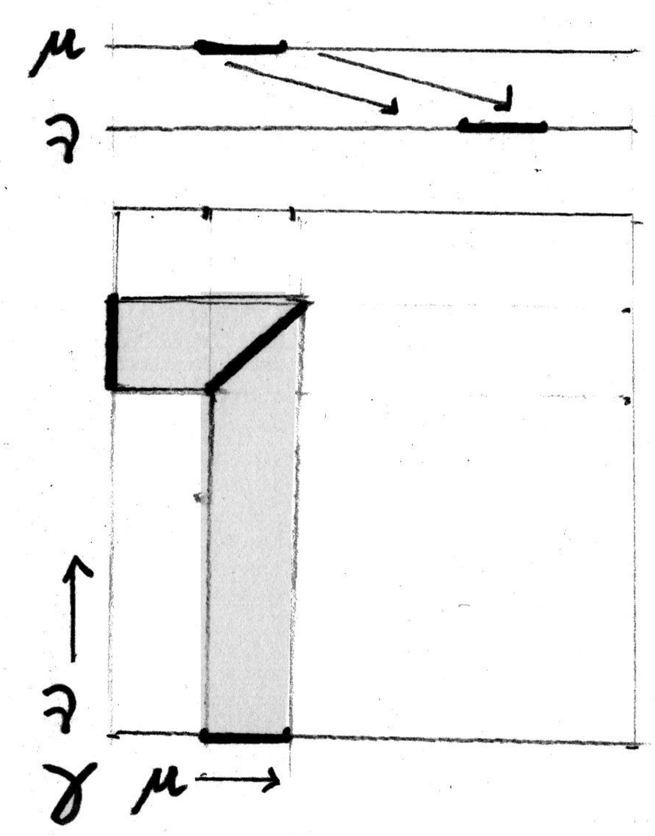
that minimizes $\iint_{X \times Y} \| x - y \|^2 \, d\gamma(x,y)$

Part. 2 Optimal Transport – Kantorovich



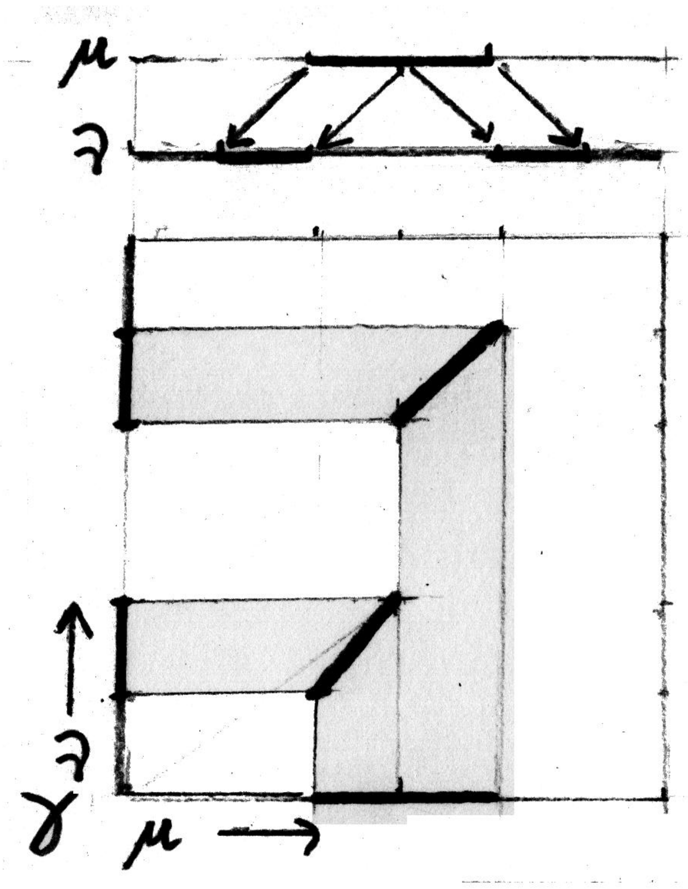
Transport plan – example 1/4 : translation of a segment

Part. 2 Optimal Transport – Kantorovich



Transport plan – example 1/4 : translation of a segment

Part. 2 Optimal Transport – Kantorovich



Transport plan – example 2/4 : spitting a segment

Part. 2 Optimal Transport – Kantorovich

Observation 1. *If* $(Id \times T)\sharp\mu \in \pi(\mu, \nu)$, *then* T *pushes* μ *to* ν.

Part. 2 Optimal Transport – Kantorovich

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Proof. $(Id{\times}T)\sharp\mu$ belongs to $\pi(\mu,\nu)$, therefore $(P_2)\sharp(Id{\times}T)\sharp\mu = \nu$, or $((P_2) \circ (Id \times T))\,\sharp\mu = \nu$, thus $T\sharp\mu = \nu$ $\square$

Part. 2 Optimal Transport – Kantorovich

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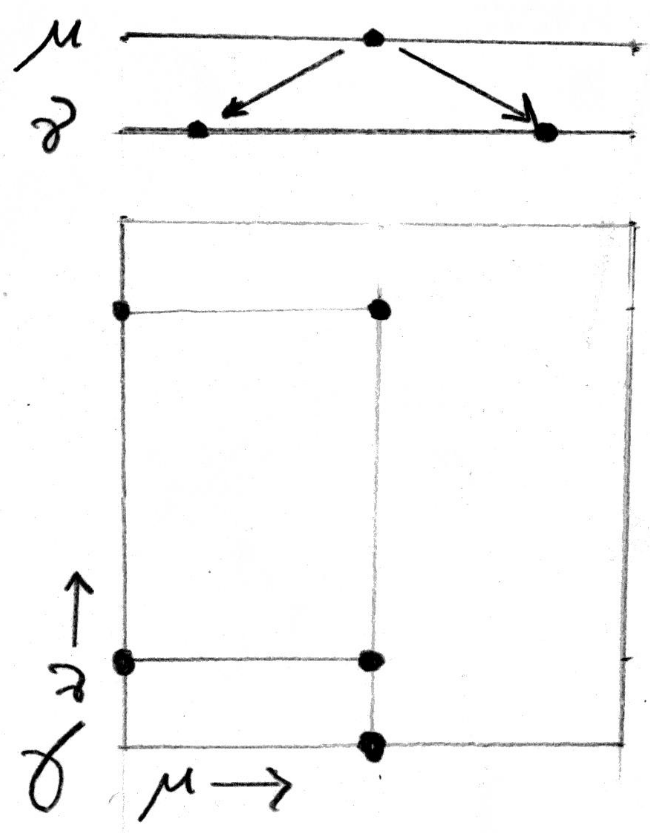
With this observation, for transport plans of the form $\gamma = (Id \times T)\sharp\mu$, (K) becomes

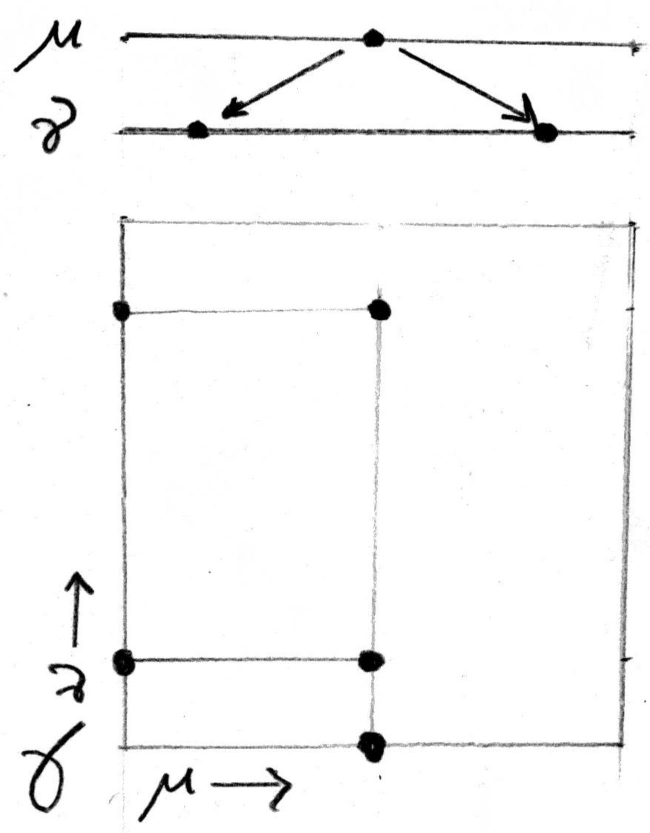
$$\min\left\{\int_{\Omega\times\Omega} c(x,y)d\left((Id \times T)\sharp\mu\right)\right\} \quad = \quad \min\left\{\int_{\Omega} c(x,T(x))d\mu\right)$$

Part. 2 Optimal Transport – Kantorovich



Transport plan – example 3/4 : splitting a Dirac into two Diracs

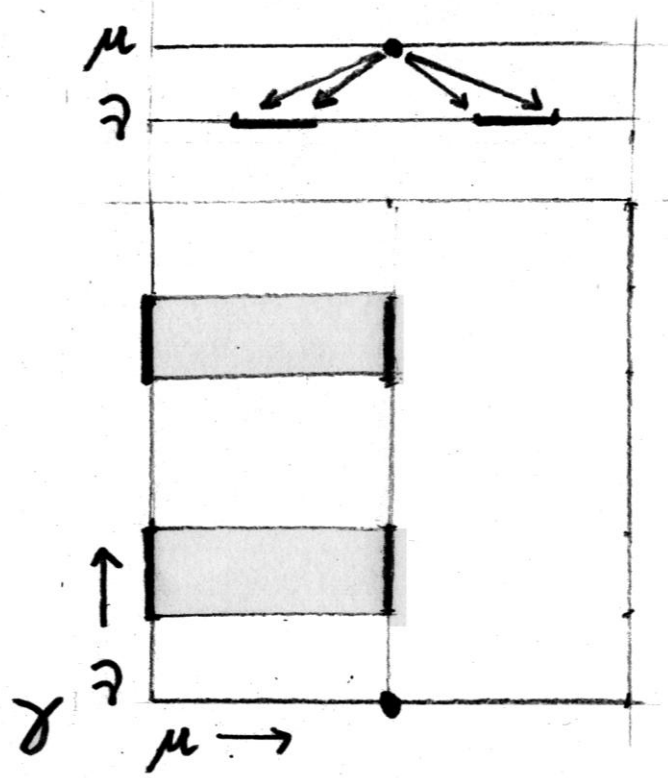
Part. 2 Optimal Transport – Kantorovich



Transport plan – example 3/4 : splitting a Dirac into two Diracs

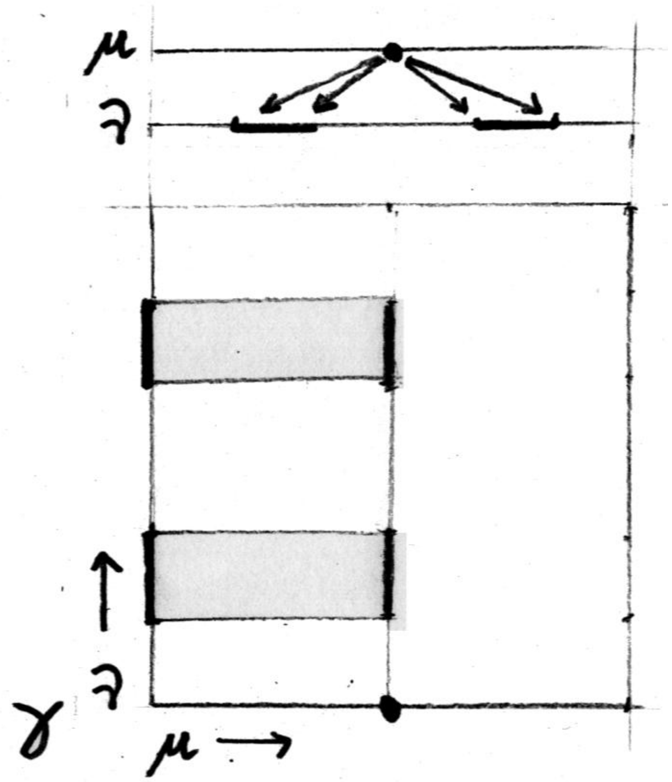
(No transport map)

Part. 2 Optimal Transport – Kantorovich



Transport plan – example 4/4 : splitting a Dirac into two segments

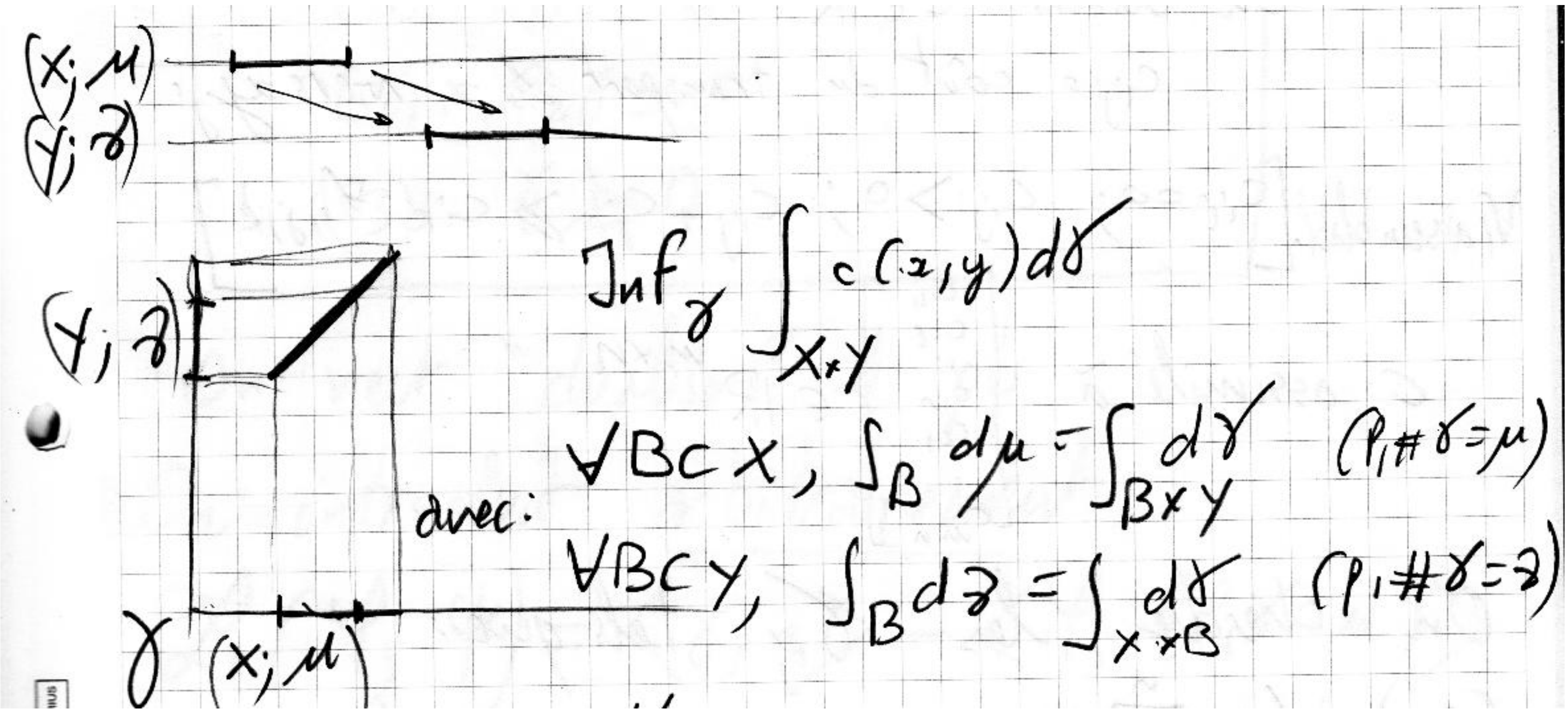
Part. 2 Optimal Transport – Kantorovich



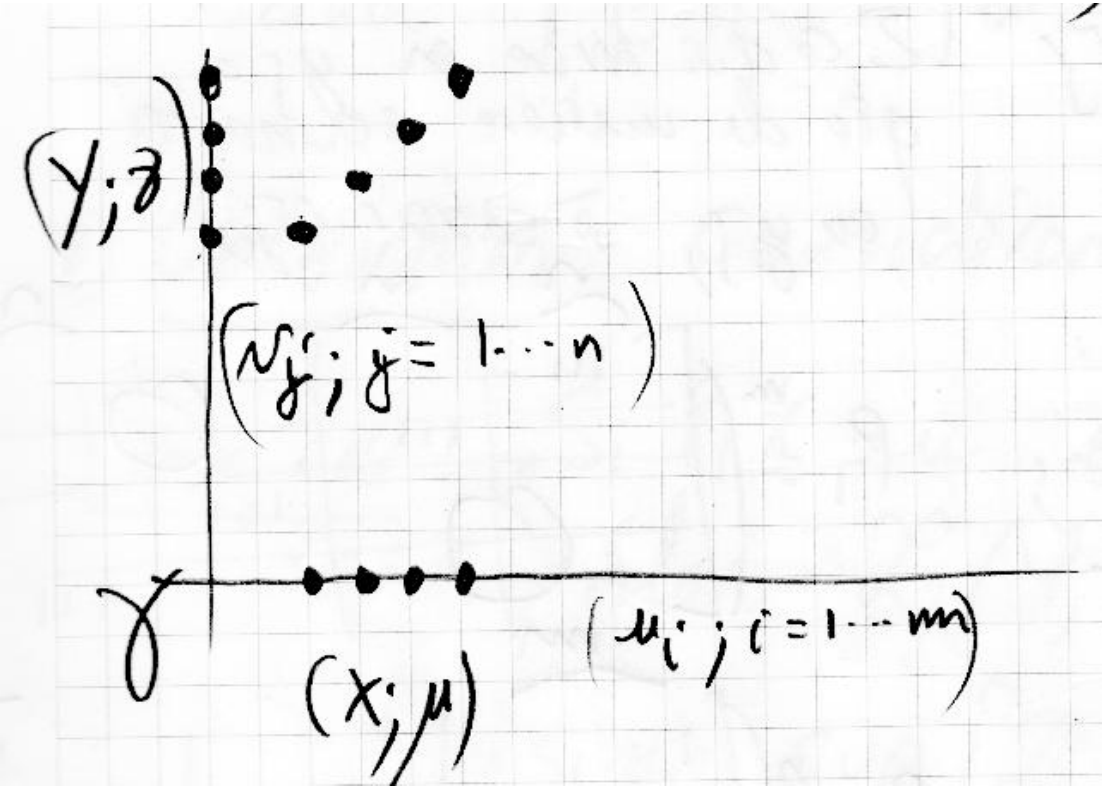
Transport plan – example 4/4 : splitting a Dirac into two segments

(No transport map)

Part. 2 Optimal Transport – Duality

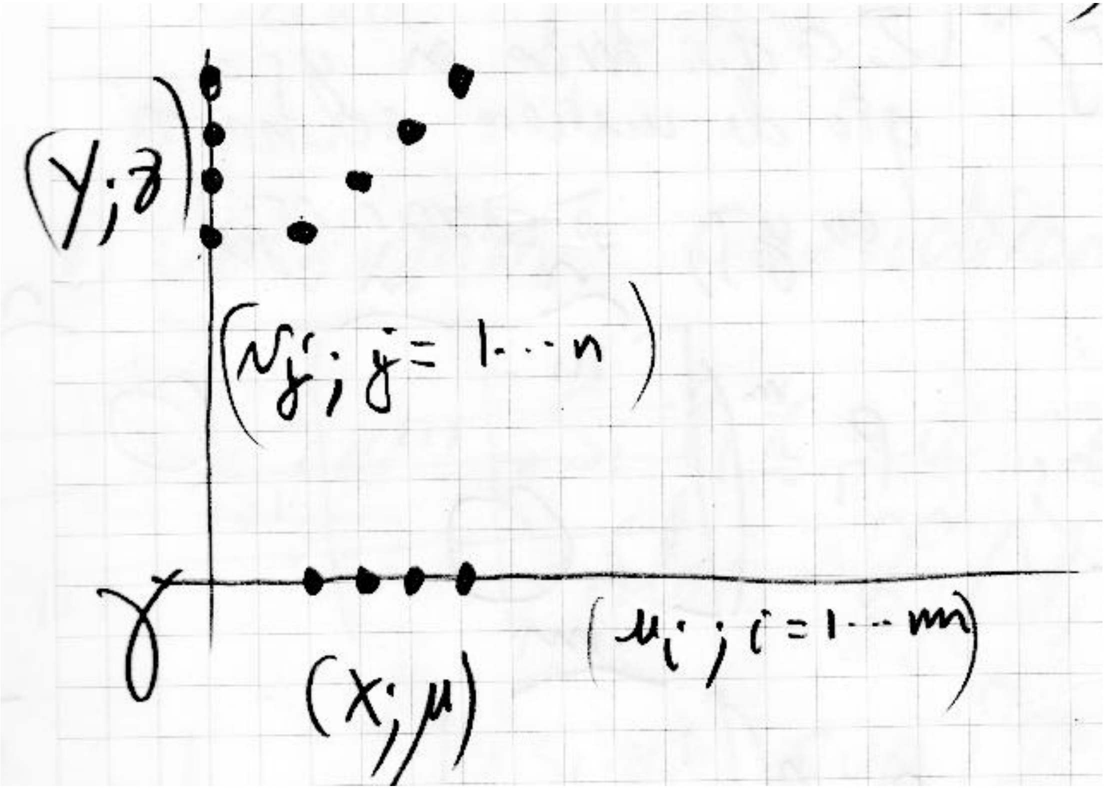


Part. 2 Optimal Transport – Duality



Duality is easier to understand with a discrete version
Then we'll go back to the continuous setting.

Part. 2 Optimal Transport – Duality

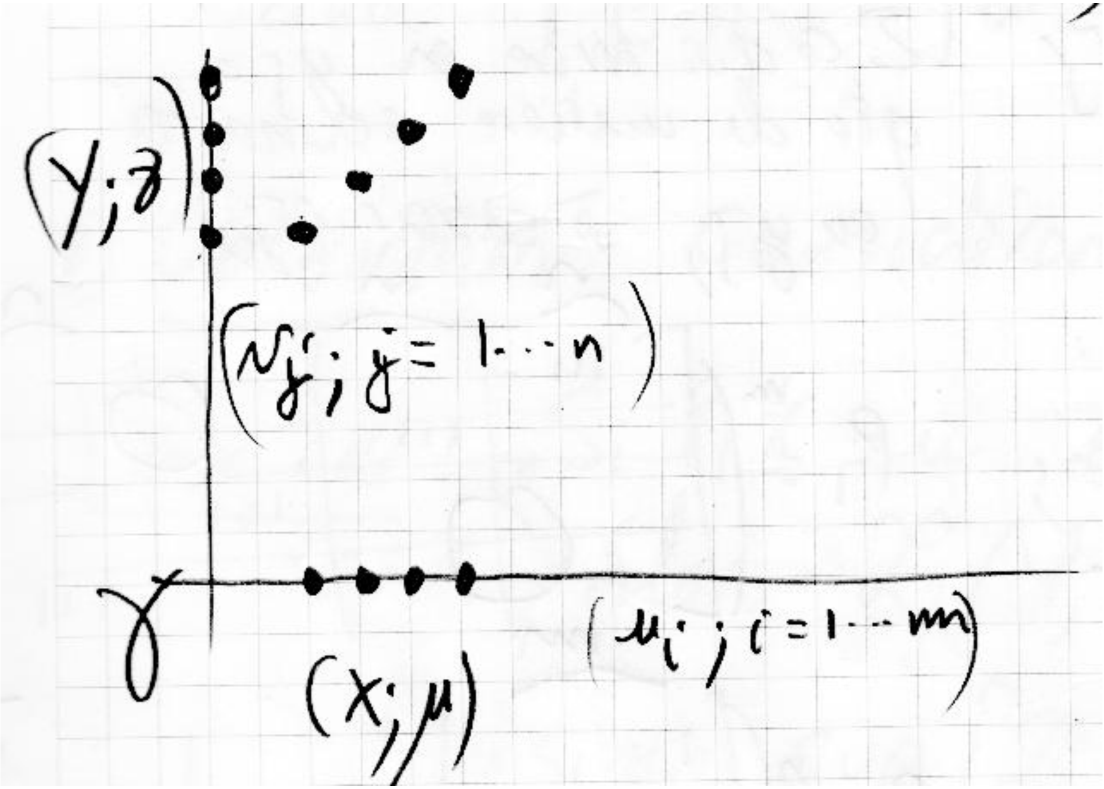


(DMK):

$$\text{Min} \quad \langle c, \gamma \rangle$$

$$s.t. \quad \begin{cases} P_1 \gamma = u \\ P_2 \gamma = v \\ \gamma \geq 0 \end{cases}$$

Part. 2 Optimal Transport – Duality



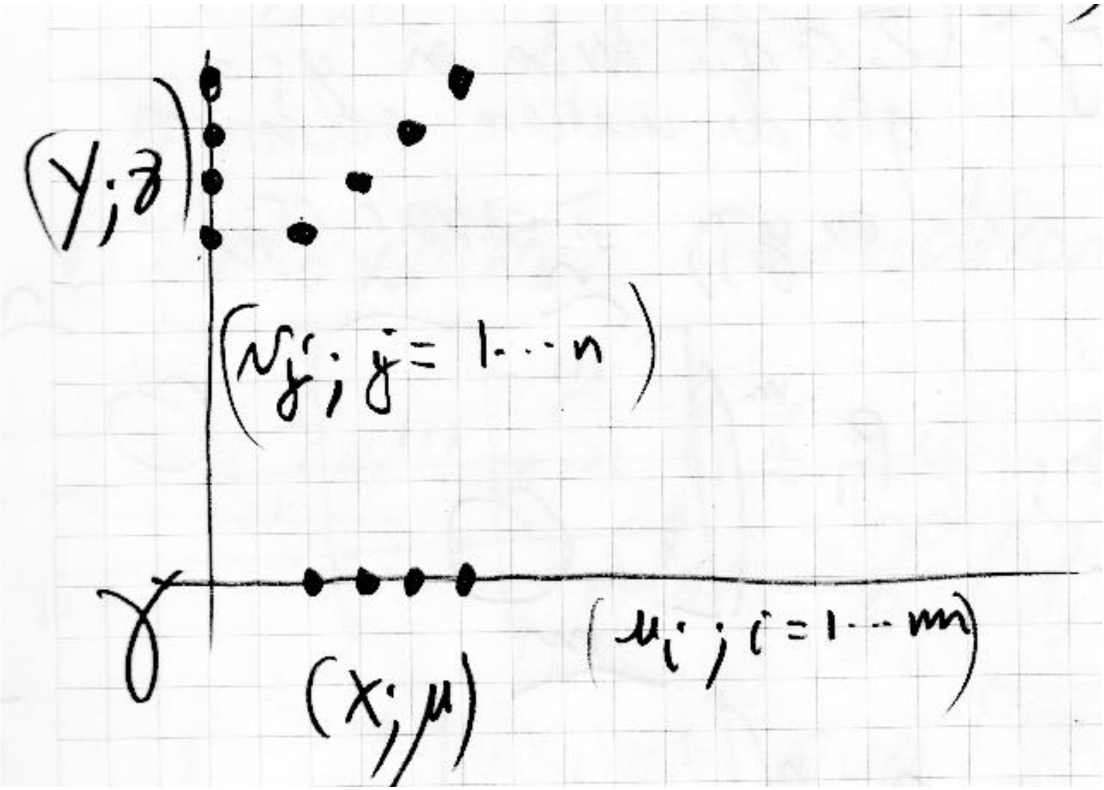
(DMK):

Min $\langle c, \gamma \rangle$

$$s.t. \begin{cases} P_1 \gamma = u \\ P_2 \gamma = v \\ \gamma \geq 0 \end{cases}$$

$$\underset{\in \mathbb{R}^{mn}}{\gamma} = \begin{bmatrix} \gamma_{11} \\ \gamma_{12} \\ \cdots \\ \gamma_{1n} \\ \gamma_{22} \\ \cdots \\ \gamma_{2n} \\ \cdots \\ \cdots \\ \gamma_{mn} \end{bmatrix}$$

Part. 2 Optimal Transport – Duality



(DMK):

$$\text{Min } \langle c, \gamma \rangle$$

$$s.t. \begin{cases} P_1 \gamma = u \\ P_2 \gamma = v \\ \gamma \geq 0 \end{cases}$$

$$\underset{\in \mathbb{R}^{mn}}{c} = \begin{bmatrix} c_{11} \\ c_{12} \\ \ldots \\ c_{1n} \\ c_{22} \\ \ldots \\ c_{2n} \\ \ldots \\ \ldots \\ c_{mn} \end{bmatrix} \qquad \underset{\in \mathbb{R}^{mn}}{\gamma} = \begin{bmatrix} \gamma_{11} \\ \gamma_{12} \\ \ldots \\ \gamma_{1n} \\ \gamma_{22} \\ \ldots \\ \gamma_{2n} \\ \ldots \\ \ldots \\ \gamma_{mn} \end{bmatrix}$$

Part. 2 Optimal Transport – Duality

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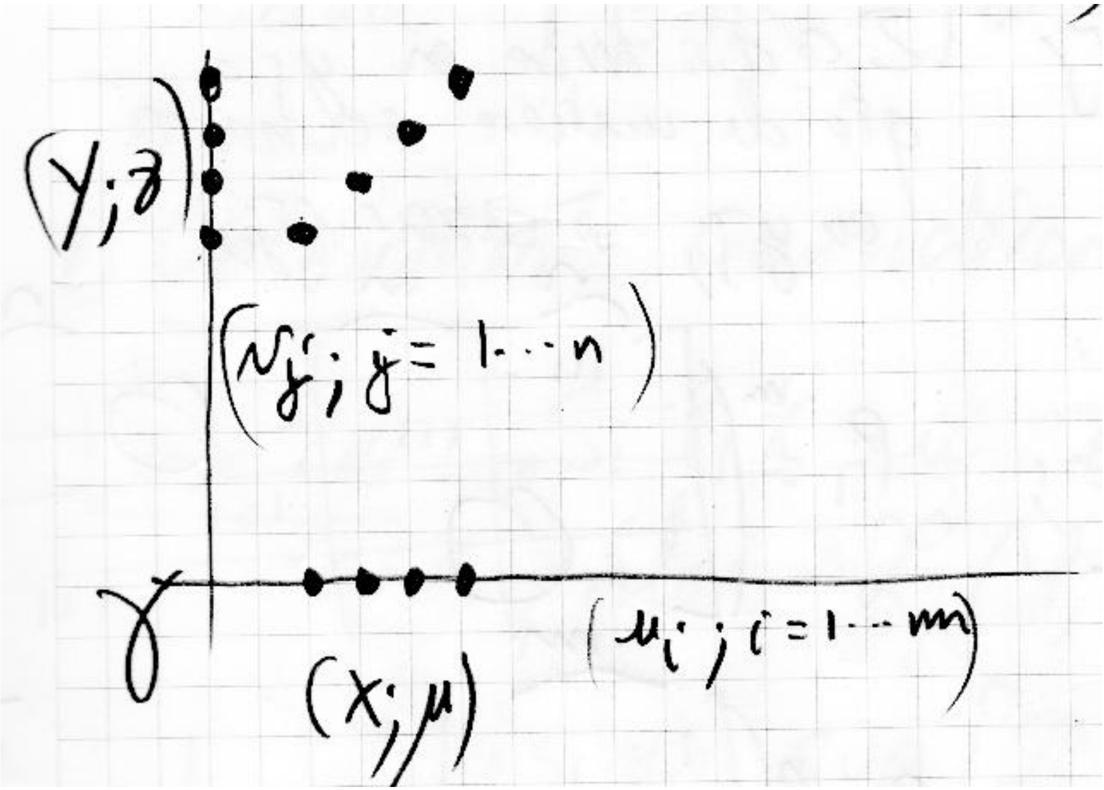


$$c = \begin{bmatrix} c_{11} \\ c_{12} \\ \dots \\ c_{1n} \\ c_{22} \\ \dots \\ c_{2n} \\ \dots \\ \dots \\ c_{mn} \end{bmatrix} \qquad \gamma = \begin{bmatrix} \gamma_{11} \\ \gamma_{12} \\ \dots \\ \gamma_{1n} \\ \gamma_{22} \\ \dots \\ \gamma_{2n} \\ \dots \\ \dots \\ \gamma_{mn} \end{bmatrix}$$

$c \in IR^{mn}$ $\quad$ $\gamma \in IR^{mn}$

$c_{ij} = || x_i - y_j ||^2$

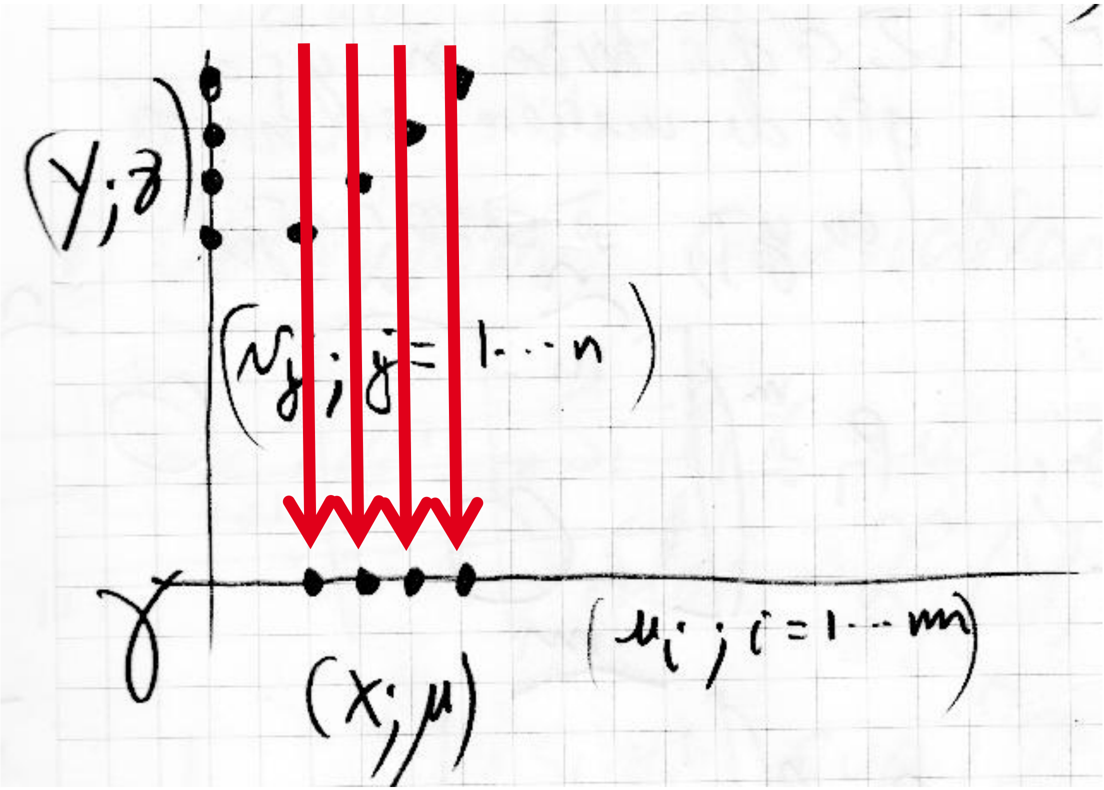
Part. 2 Optimal Transport – Duality

(DMK):

Min $\langle c, \gamma \rangle$

s.t. $\begin{cases} P_1 \gamma = u \\ P_2 \gamma = v \\ \gamma \geq 0 \end{cases}$

mn X m → P_1



$c = \begin{bmatrix} c_{11} \\ c_{12} \\ \dots \\ c_{1n} \\ c_{22} \\ \dots \\ c_{2n} \\ \dots \\ \dots \\ c_{mn} \end{bmatrix} \in \mathbb{R}^{mn}$ $\quad \gamma = \begin{bmatrix} \gamma_{11} \\ \gamma_{12} \\ \dots \\ \gamma_{1n} \\ \gamma_{22} \\ \dots \\ \gamma_{2n} \\ \dots \\ \dots \\ \gamma_{mn} \end{bmatrix} \in \mathbb{R}^{mn}$

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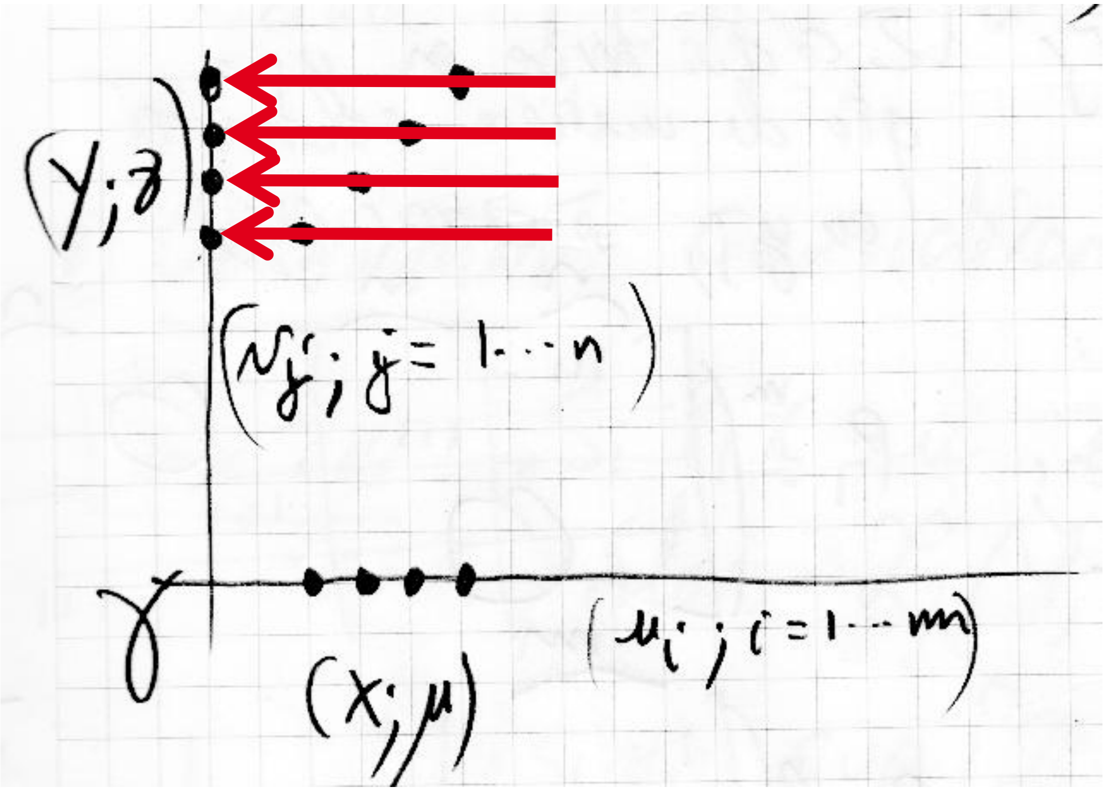
Part. 2 Optimal Transport – Duality



(DMK):

Min $\langle c, \gamma \rangle$

s.t.
- mn X m → $P_1 \gamma = u$
- **mn X n** → $\mathbf{P_2} \gamma = v$
- $\gamma \geq 0$

$$c = \begin{bmatrix} c_{11} \\ c_{12} \\ \dots \\ c_{1n} \\ c_{22} \\ \dots \\ c_{2n} \\ \dots \\ \dots \\ c_{mn} \end{bmatrix} \in \mathbb{R}^{mn} \qquad \gamma = \begin{bmatrix} \gamma_{11} \\ \gamma_{12} \\ \dots \\ \gamma_{1n} \\ \gamma_{22} \\ \dots \\ \gamma_{2n} \\ \dots \\ \dots \\ \gamma_{mn} \end{bmatrix} \in \mathbb{R}^{mn}$$

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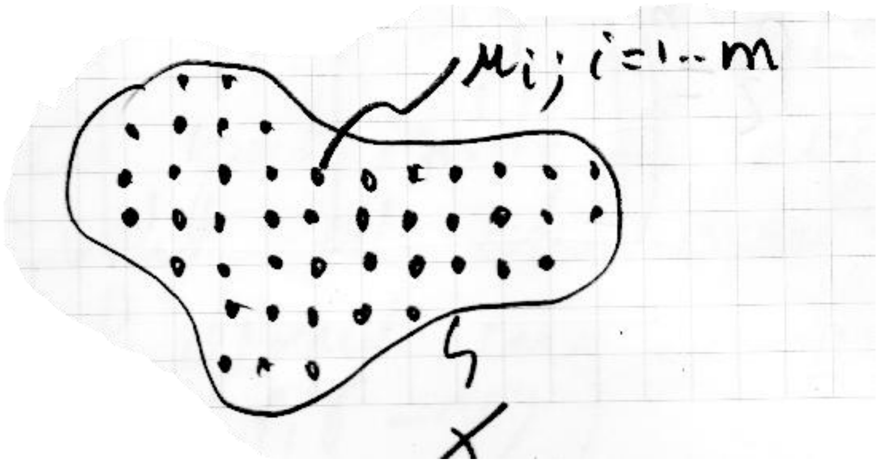
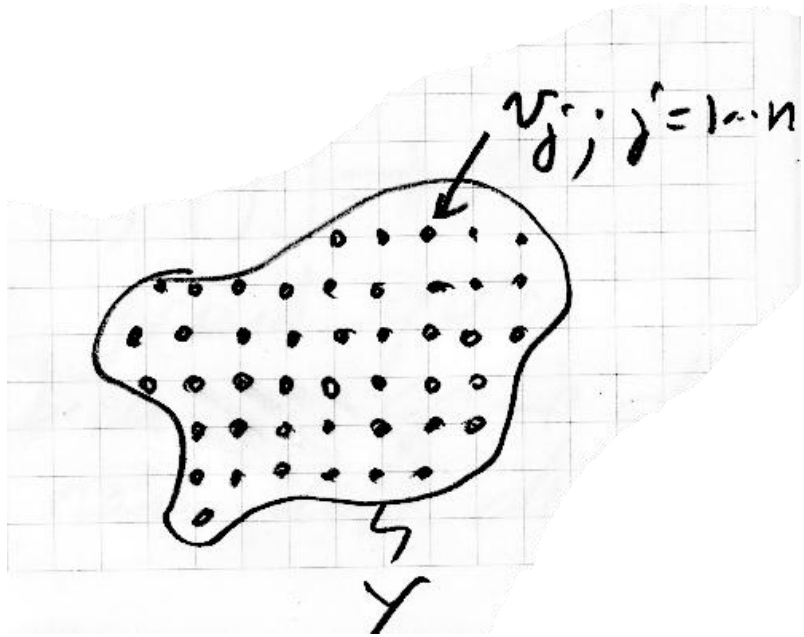
Part. 2 Optimal Transport – Duality





(DMK):

Min $\langle c, \gamma \rangle$

s.t.

mn X m → $P_1 \gamma = u$

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$\gamma \geq 0$

$$c = \begin{bmatrix} c_{11} \\ c_{12} \\ \dots \\ c_{1n} \\ c_{22} \\ \dots \\ c_{2n} \\ \dots \\ \dots \\ c_{mn} \end{bmatrix} \in \mathbb{R}^{mn} \qquad \gamma = \begin{bmatrix} \gamma_{11} \\ \gamma_{12} \\ \dots \\ \gamma_{1n} \\ \gamma_{22} \\ \dots \\ \gamma_{2n} \\ \dots \\ \dots \\ \gamma_{mn} \end{bmatrix} \in \mathbb{R}^{mn}$$

Part. 2 Optimal Transport – Duality

(DMK):

Min $<c, \gamma>$

$$s.t. \begin{cases} P_1 \gamma = u \\ P_2 \gamma = v \\ \gamma \geq 0 \end{cases}$$

< u, v > denotes the dot product between u and v

Consider $\mathcal{L}(\varphi,\psi) = <c, \gamma> - <\varphi, P_1 \gamma - u> - <\psi, P_2 \gamma - v>$

Part. 2 Optimal Transport – Duality

(DMK):

$$\text{Min } \langle c, \gamma \rangle \quad s.t. \begin{cases} P_1 \gamma = u \\ P_2 \gamma = v \\ \gamma \geq 0 \end{cases}$$

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Remark: $\sup_{\substack{\varphi \in \mathbb{R}^m \\ \psi \in \mathbb{R}^n}} [\, \mathcal{L}(\varphi,\psi)\,] = \langle c, \gamma \rangle$ if $P_1 \gamma = u$ and $P_2 \gamma = v$

Part. 2 Optimal Transport – Duality

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$= +\infty$ otherwise

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Remark: $\sup_{\substack{\varphi \in IR^m \\ \psi \in IR^n}} [\, \mathcal{L}(\varphi,\psi) \,] = \langle c, \gamma \rangle$ if $P_1 \gamma = u$ and $P_2 \gamma = v$

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Consider now: $\inf_{\gamma \geq 0} \left[\sup_{\substack{\varphi \in IR^m \\ \psi \in IR^n}} [\, \mathcal{L}(\varphi,\psi) \,] \right]$

Part. 2 Optimal Transport – Duality

(DMK):

$$\text{Min } \langle c, \gamma \rangle \quad s.t. \begin{cases} P_1 \gamma = u \\ P_2 \gamma = v \\ \gamma \geq 0 \end{cases}$$

Consider $\mathcal{L}(\varphi,\psi) = \langle c, \gamma \rangle - \langle \varphi, P_1 \gamma - u \rangle - \langle \psi, P_2 \gamma - v \rangle$

Remark: $\sup_{\varphi \in \mathbb{R}^m, \psi \in \mathbb{R}^n} [\mathcal{L}(\varphi,\psi)] = \langle c, \gamma \rangle$ if $P_1 \gamma = u$ and $P_2 \gamma = v$

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Part. 2 Optimal Transport – Duality

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Consider $\mathcal{L}(\varphi,\psi) = \langle c, \gamma \rangle - \langle \varphi, P_1 \gamma - u \rangle - \langle \psi, P_2 \gamma - v \rangle$

Remark: $\sup_{\varphi \in \mathbb{R}^m, \psi \in \mathbb{R}^n} [\mathcal{L}(\varphi,\psi)] = \langle c, \gamma \rangle$ if $P_1 \gamma = u$ and $P_2 \gamma = v$

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Part. 2 Optimal Transport – Duality

(DMK):

$$\text{Min } \langle c, \gamma \rangle \quad s.t. \begin{cases} P_1 \gamma = u \\ P_2 \gamma = v \\ \gamma \geq 0 \end{cases}$$

$$\underset{\gamma \geq 0}{\text{Inf}} \Big[\underset{\substack{\varphi \in \mathbb{R}^m \\ \psi \in \mathbb{R}^n}}{\text{Sup}} [\langle c, \gamma \rangle - \langle \varphi, P_1 \gamma - u \rangle - \langle \psi, P_2 \gamma - v \rangle] \Big]$$

Part. 2 Optimal Transport – Duality

(DMK):

Min $\langle c, \gamma \rangle$

$$s.t. \begin{cases} P_1 \gamma = u \\ P_2 \gamma = v \\ \gamma \geq 0 \end{cases}$$

$$\inf_{\gamma \geq 0} \Big[\sup_{\substack{\varphi \in \mathbb{R}^m \\ \psi \in \mathbb{R}^n}} [\ \langle c, \gamma \rangle - \langle \varphi, P_1 \gamma - u \rangle - \langle \psi, P_2 \gamma - v \rangle\ ] \Big]$$

Exchange Inf Sup

$$\sup_{\substack{\varphi \in \mathbb{R}^m \\ \psi \in \mathbb{R}^n}} \Big[\inf_{\gamma \geq 0} [\ \langle c, \gamma \rangle - \langle \varphi, P_1 \gamma - u \rangle - \langle \psi, P_2 \gamma - v \rangle\ ] \Big]$$

Part. 2 Optimal Transport – Duality

(DMK):

Min $\langle c, \gamma \rangle$

s.t. $\begin{cases} P_1 \gamma = u \\ P_2 \gamma = v \\ \gamma \geq 0 \end{cases}$

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Expand/Reorder/Collect

$$\sup_{\substack{\varphi \in \mathbb{R}^m \\ \psi \in \mathbb{R}^n}} \Big[\inf_{\gamma \geq 0} [\langle \gamma, c - P_1^t \varphi - P_2^t \psi \rangle + \langle \varphi, u \rangle + \langle \psi, v \rangle] \Big]$$

Part. 2 Optimal Transport – Duality

(DMK):

$$\text{Min } \langle c, \gamma \rangle \quad s.t. \begin{cases} P_1 \gamma = u \\ P_2 \gamma = v \\ \gamma \geq 0 \end{cases}$$

$$\inf_{\gamma \geq 0} \Big[\sup_{\varphi \in \mathbb{R}^m, \psi \in \mathbb{R}^n} [\ \langle c, \gamma \rangle - \langle \varphi, P_1 \gamma - u \rangle - \langle \psi, P_2 \gamma - v \rangle\ ] \Big]$$

Exchange Inf Sup

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Expand/Reorder/Collect

$$\sup_{\varphi \in \mathbb{R}^m, \psi \in \mathbb{R}^n} \Big[\inf_{\gamma \geq 0} [\ \langle \gamma, c - P_1^t \varphi - P_2^t \psi \rangle + \langle \varphi, u \rangle + \langle \psi, v \rangle\ ] \Big]$$

Interpret

Part. 2 Optimal Transport – Duality

(DMK):

$$\text{Min } \langle c, \gamma \rangle \quad s.t. \begin{cases} P_1 \gamma = u \\ P_2 \gamma = v \\ \gamma \geq 0 \end{cases}$$

$$\sup_{\substack{\varphi \in \mathbb{R}^m \\ \psi \in \mathbb{R}^n}} \Big[\inf_{\gamma \geq 0} \big[\langle \gamma, c - P_1^t \varphi - P_2^t \psi \rangle + \langle \varphi, u \rangle + \langle \psi, v \rangle \big] \Big]$$

Interpret

$$\sup_{\substack{\varphi \in \mathbb{R}^m \\ \psi \in \mathbb{R}^n \\ P_1^t \varphi + P_2^t \psi \leq c}} \big[\langle \varphi, u \rangle + \langle \psi, v \rangle \big] \qquad \textbf{(DDMK)}$$

Part. 2 Optimal Transport – Duality

(DMK):

Min $<c, \gamma>$

$$s.t. \begin{cases} P_1 \gamma = u \\ P_2 \gamma = v \\ \gamma \geq 0 \end{cases}$$

$$\operatorname*{Sup}_{\substack{\varphi \in IR^m \\ \psi \in IR^n}} \Big[\operatorname*{Inf}_{\gamma \geq 0} \big[< \gamma, c - P_1^t \varphi - P_2^t \psi > + <\varphi, u> + <\psi, v> \big] \Big]$$

Interpret

$$\operatorname*{Sup}_{\substack{\varphi \in IR^m \\ \psi \in IR^n \\ P_1^t \varphi + P_2^t \psi \leq c}} \Big[<\varphi, u> + <\psi, v> \Big]$$

(DDMK)

$\varphi_i + \psi_j \leq c_{ij} \quad \forall (i,j)$

Part. 2 Optimal Transport – Kantorovich dual

Kantorovich's problem:

Find a measure γ defined on X x Y

such that $\int_{x \text{ in } X} d\gamma(x,y) = d\mu(x)$

and $\int_{y \text{ in } Y} d\gamma(x,y) = d\nu(x)$

that minimizes $\iint_{X \times Y} \| x - y \|^2 \, d\gamma(x,y)$

Dual formulation of Kantorovich's problem (Continuous):

Find two functions φ in $L^1(\mu)$ and ψ in $L^1(\nu)$
Such that for all x,y, $\varphi(x) + \psi(y) \leq \frac{1}{2}\| x - y \|^2$

that maximize $\int_X \varphi d\mu + \int_Y \psi d\nu$

Part. 2 Optimal Transport – Kantorovich dual

Kantorovich's problem:

Find a measure γ defined on X x Y

such that $\int_{x \text{ in } X} d\gamma(x,y) = d\mu(x)$

and $\int_{y \text{ in } Y} d\gamma(x,y) = d\nu(x)$

that minimizes $\iint_{X \times Y} \| x - y \|^2 \, d\gamma(x,y)$

Your point of view:
Try to minimize transport cost

Dual formulation of Kantorovich's problem:

Find two functions φ in $L^1(\mu)$ and ψ in $L^1(\nu)$
Such that for all x,y, $\varphi(x) + \psi(y) \leq ½\| x - y \|^2$

that maximize $\int_X \varphi d\mu + \int_Y \psi d\nu$

Part. 2 Optimal Transport – Kantorovich dual

Kantorovich's problem:

Find a measure γ defined on $X \times Y$
such that $\int_{x \in X} d\gamma(x,y) = d\mu(x)$
and $\int_{y \in Y} d\gamma(x,y) = d\nu(x)$

that minimizes $\iint_{X \times Y} \| x - y \|^2 \, d\gamma(x,y)$

Your point of view:
Try to minimize transport cost

Dual formulation of Kantorovich's problem:

Find two functions φ in $L^1(\mu)$ and ψ in $L^1(\nu)$
Such that for all x,y, $\varphi(x) + \psi(y) \leq \frac{1}{2}\| x - y \|^2$

that maximize $\int_X \varphi d\mu + \int_Y \psi d\nu$

Point of view of a "transport company":
Try to maximize transport price

Part. 2 Optimal Transport – Kantorovich dual

Kantorovich's problem:

Find a measure γ defined on $X \times Y$

such that $\int_{x \text{ in } X} d\gamma(x,y) = d\mu(x)$

and $\int_{y \text{ in } Y} d\gamma(x,y) = d\nu(x)$

that minimizes $\iint_{X \times Y} \| x - y \|^2 \, d\gamma(x,y)$

Your point of view:
Try to minimize transport cost

Dual formulation of Kantorovich's problem:

Find two functions φ in $L^1(\mu)$ and ψ in $L^1(\nu)$
Such that for all x,y, $\varphi(x) + \psi(y) \leq ½\| x - y \|^2$

that maximize $\int_X \varphi(x) d\mu + \int_Y \psi(y) d\nu$

What they charge for loading at x

Part. 2 Optimal Transport – Kantorovich dual

Kantorovich's problem:

Find a measure γ defined on X x Y
such that $\int_{x \text{ in } X} d\gamma(x,y) = d\mu(x)$
and $\int_{y \text{ in } Y} d\gamma(x,y) = d\nu(x)$

that minimizes $\iint_{X \times Y} \| x - y \|^2 \, d\gamma(x,y)$

Your point of view:
Try to minimize transport cost

Dual formulation of Kantorovich's problem:

Find two functions φ in $L^1(\mu)$ and ψ in $L^1(\nu)$
Such that for all x,y, $\varphi(x) + \psi(y) \leq \frac{1}{2}\| x - y \|^2$

that maximize $\int_X \varphi(x) d\mu + \int_Y \psi(y) d\nu$

What they charge for loading at x

What they charge for unloading at y

Part. 2 Optimal Transport – Kantorovich dual

Kantorovich's problem:

Find a measure γ defined on X x Y

such that $\int_{x \text{ in } X} d\gamma(x,y) = d\mu(x)$

and $\int_{y \text{ in } Y} d\gamma(x,y) = d\nu(x)$

that minimizes $\iint_{X \times Y} || x - y ||^2 \, d\gamma(x,y)$

Your point of view:
Try to minimize transport cost

Dual formulation of Kantorovich's problem:

Find two functions φ in $L^1(\mu)$ and ψ in $L^1(\nu)$
Such that for all x,y, $\varphi(x) + \psi(y) \leq ½|| x - y ||^2$

that maximize $\int_X \varphi(x) d\mu + \int_Y \psi(y) d\nu$

Price (loading + unloading) cannot be greater than transport cost (else you do the job yourself)

What they charge for loading at x

What they charge for unloading at y

Part. 2 Optimal Transport – c-conjugate functions

Dual formulation of Kantorovich's problem:

Find two functions φ in $L^1(\mu)$ and ψ in $L^1(\nu)$
Such that for all x,y, $\varphi(x) + \psi(y) \leq \frac{1}{2}\| x - y \|^2$

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If we got two functions φ and ψ that satisfy the constraint

Then it is possible to obtain a better solution by replacing ψ with φ^c defined by:
For all y, $\varphi^c(y) = \inf_{x \text{ in } X} \frac{1}{2}\| x - y \|^2 - \varphi(y)$

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Then it is possible to obtain a better solution by replacing ψ with φ^c defined by:
For all y, $\varphi^c(y) = \inf_{x \in X} ½\| x - y \|^2 - \varphi(y)$

- φ^c is called the **c-conjugate** function of φ
- If there is a function φ such that $\psi = \varphi^c$ then ψ is said to be **c-concave**
- If ψ is c-concave, then $\psi^{cc} = \psi$

Part. 2 Optimal Transport – c-conjugate functions

Dual formulation of Kantorovich's problem:

Find a c-concave function ψ

that maximizes $\int_X \psi(x) d\mu + \int_Y \psi^c(y) d\nu$

Part. 2 Optimal Transport – c-conjugate functions

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Part. 2 Optimal Transport – c-subdifferential

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Part. 2 Optimal Transport – c-subdifferential

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ψ is called a **"Kantorovich potential"**

What about our initial problem ? (i.e., this is T() that we want to find …)

Part. 2 Optimal Transport – c-subdifferential

Theorem 1.

$$\forall (x, y) \in \partial_c \psi, \nabla \psi(x) - \nabla_x c(x, y) = 0$$

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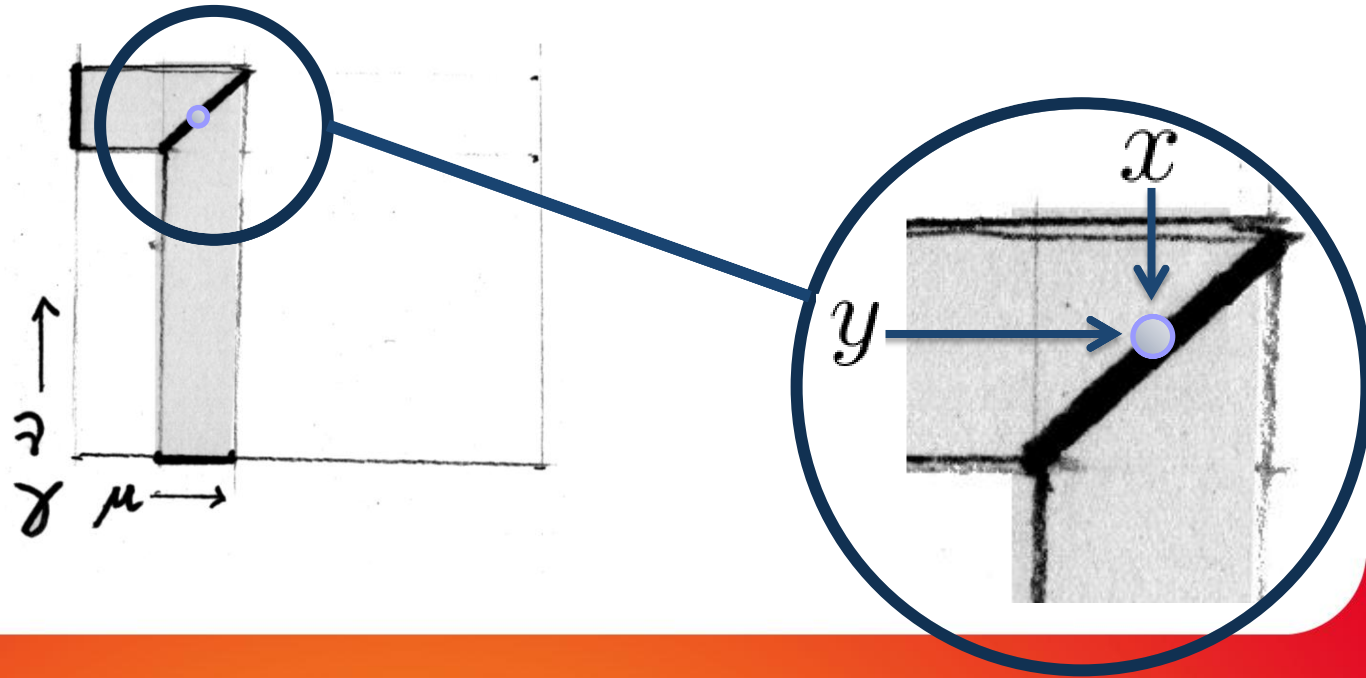

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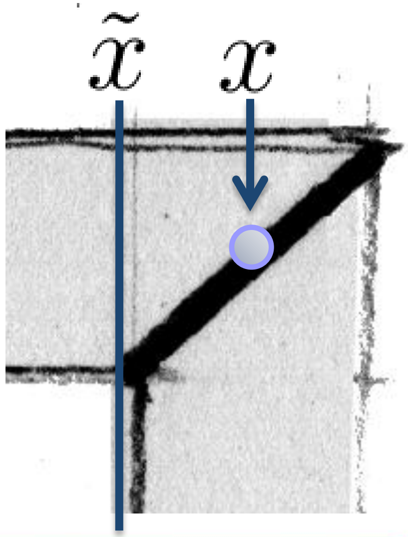

Part. 2 Optimal Transport – c-subdifferential

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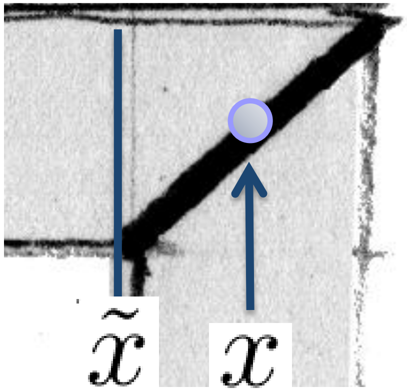

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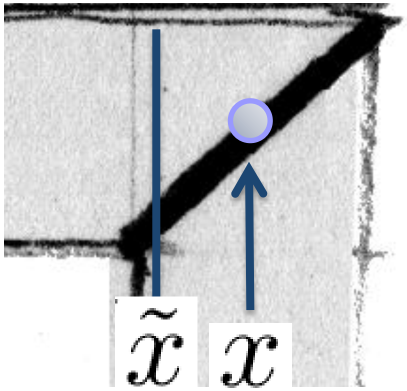

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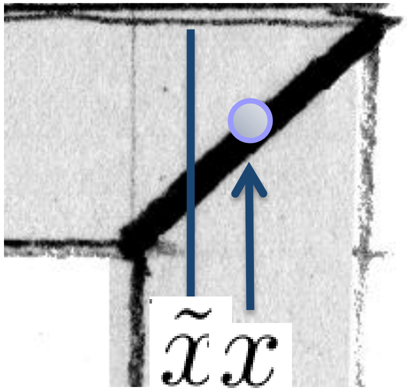

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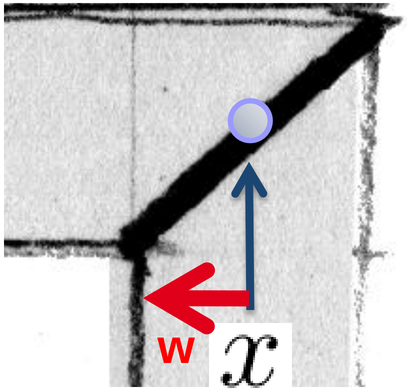
Thus we have $\nabla\psi(x) \cdot w \leq \nabla_x c(x,y) \cdot w$



Part. 2 Optimal Transport – c-subdifferential

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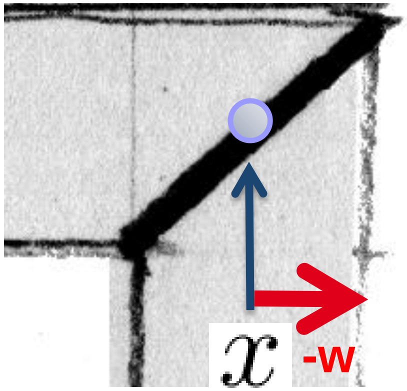
Thus we have $\nabla \psi(x) \cdot w \leq \nabla_x c(x,y) \cdot w$
The same derivation can be done with $-w$ instead of w, and one gets:
$\forall w, \nabla \psi(x) \cdot w = \nabla_x c(x,y) \cdot w$, thus $\forall (x,y) \in \partial_c \psi, \nabla \psi(x) - \nabla_x c(x,y) = 0$.



Part. 2 Optimal Transport – c-subdifferential

Dual formulation of Kantorovich's problem:

Find a c-concave function ψ

that maximizes $\int_X \psi(x)d\mu + \int_Y \psi^c(y)d\nu$

In the L_2 case, i.e. $c(x,y) = 1/2\|x-y\|^2$, we have $\forall (x,y) \in \partial_c\psi, \nabla\psi(x) + y - x = 0$, thus, whenever the optimal transport map T exists, we have $T(x) = x - \nabla\psi(x) = \nabla(\|x\|^2/2 - \psi(x))$.

Part. 2 Optimal Transport – c-subdifferential

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grad $\overline{\psi}(x)$ with $\overline{\psi}(x) := (\frac{1}{2} x^2 - \psi(x))$

Part. 2 Optimal Transport – convexity

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Part. 2 Optimal Transport – convexity

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grad $\overline{\psi}$(x) with $\overline{\psi}$(x) := (½ x²- ψ(x))

$\overline{\psi}$ is convex

Proof.

$$\begin{aligned}
\psi(x) &= \inf_y \frac{|x-y|^2}{2} - \phi(y) \\
&= \inf_y \frac{\|x\|^2}{2} - x\cdot y + \frac{\|y\|^2}{2} - \phi(y) \\
-\bar{\psi}(x) &= \phi(x) - \frac{\|x\|^2}{2} = \inf_y -x\cdot y + \left(\frac{\|y\|^2}{2} - \phi(y)\right) \\
\bar{\psi}(x) &= \sup_y x\cdot y - \left(\frac{\|y\|^2}{2} - \phi(y)\right)
\end{aligned}$$

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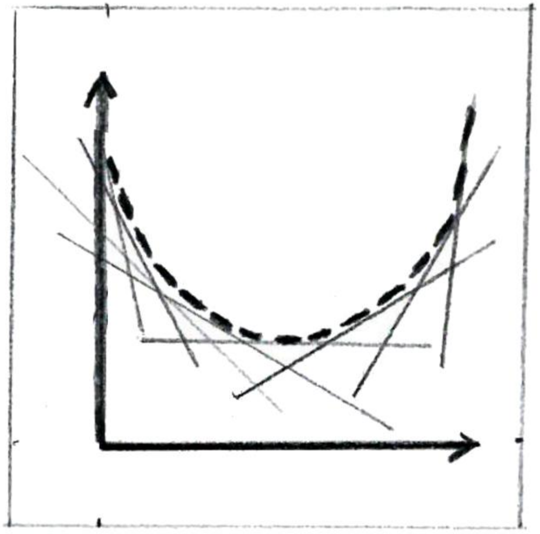

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Part. 2 Optimal Transport – no collision

Dual formulation of Kantorovich's problem:

Find a c-concave function ψ

that maximizes $\int_X \psi(x)d\mu + \int_Y \psi^c(y)d\nu$

If T(.) exists, then

$T(x) = x - \text{grad}\,\psi(x) = \text{grad}\,(\underbrace{\tfrac{1}{2}x^2 - \psi(x)}_{\text{grad}\,\overline{\psi}\,(x)})$

$\overline{\psi}$ is convex

↓

Two transported particles cannot "collide"

Part. 2 Optimal Transport – no collision

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Two transported particles cannot "collide"

Proof. By contradiction, suppose that you have $t \in (0,1)$ and $x_1 \neq x_2$ such that:

$$(1-t)x_1 + tT(x_1) = (1-t)x_2 + tT(x_2)$$

Part. 2 Optimal Transport – no collision

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$$\begin{array}{rcl} (1-t)x_1 + t\nabla\bar{\psi}(x_1) & = & (1-t)x_2 + t\nabla\bar{\psi}(x_2) \\ (1-t)(x_1 - x_2) + t(\nabla\bar{\psi}(x_1) - \nabla\bar{\psi}(x_2)) & = & 0 \\ \forall v, (1-t)v \cdot (x_1 - x_2) + tv \cdot (\nabla\bar{\psi}(x_1) - \nabla\bar{\psi}(x_2)) & = & 0 \\ \text{take } v = (x_1 - x_2) & & \\ (1-t)\|x_1 - x_2\|^2 + t(x_1 - x_2) \cdot (\nabla\bar{\psi}(x_1) - \nabla\bar{\psi}(x_2)) & = & 0 \end{array}$$

Part. 2 Optimal Transport – Monge-Ampere

Dual formulation of Kantorovich's problem:

Find a c-concave function ψ

that maximizes $\int_X \psi(x) d\mu + \int_Y \psi^c(y) dv$

What about our initial problem ? If T(.) exists, then one can show that:

$T(x) = x - \text{grad}\, \psi(x) = \text{grad}\, (\frac{1}{2} x^2 - \psi(x))$

grad $\overline{\psi}(x)$ with $\overline{\psi}(x) := (\frac{1}{2} x^2 - \psi(x))$

for all borel set A, $\int_A d\mu = \int_{T(A)} (|JT|)\, dv$ (change of variable)

Jacobian of T (1st order derivatives)

Part. 2 Optimal Transport – Monge-Ampere

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Det. of the Hessian of $\bar{\psi}$ (2^{nd} order derivatives)

Part. 2 Optimal Transport – Monge-Ampere

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When μ and ν have a density u and v, $(H\,\overline{\psi}(x)).\, v\big(\text{grad}\,\overline{\psi}(x)\big) = u(x)$ *Monge-Ampère equation*

Part. 2 Optimal Transport – summary

Find a transport map T that minimizes $C(T) = \int_X \| x - T(x) \|^2 d\mu(x)$

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After several rewrites and under some conditions….
(Kantorovich formulation, dual, c-convex functions)

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Solve $(H\,\overline{\psi}(x)).\, v\big(\mathrm{grad}\,\overline{\psi}(x)\big) = u(x)$ *Monge-Ampère equation*
(When μ and ν have a density u and v resp.)

Part. 2 Optimal Transport – summary

Find a transport map T that minimizes $C(T) = \int_X \| x - T(x) \|^2 d\mu(x)$

After several rewrites and under some conditions….
(Kantorovich formulation, dual, c-convex functions)

Solve $(H\,\overline{\psi}(x)).\, v\left(\text{grad}\,\overline{\psi}(x)\right) = u(x)$ *Monge-Ampère equation*
(When μ and ν have a density u and v resp.)

Brenier, Mc Cann, Trudinger: ***The optimal transport map is then given by:***
$T(x) = \text{grad}\,\overline{\psi}(x)$

Part. 2 Optimal Transport – Isoperimetric inequality

For a given volume,
ball is the shape that minimizes border area

Part. 2 Optimal Transport – Isoperimetric inequality

L_1 Sobolev inegality: Given f: $\mathbb{R}^n \rightarrow \mathbb{R}$ sufficiently regular

$$\int |\text{grad } f| \geq n \, \text{Vol}(B_2^n)^{1/n} \left(\int f^{\,n/(n-1)} \right)^{(n-1)/n}$$

Explanation in **[Dario Cordero Erauquin]** course notes

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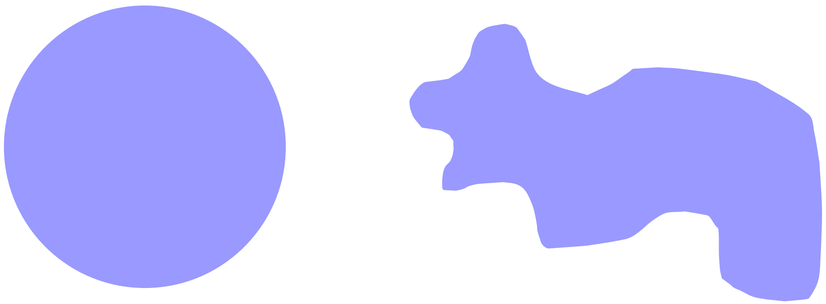

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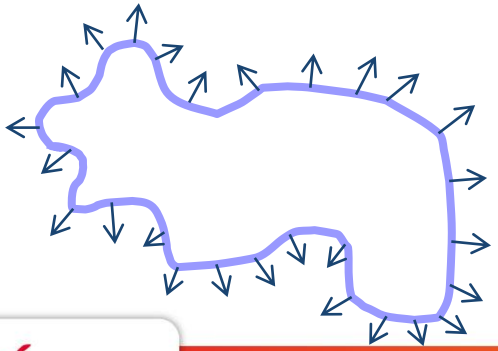

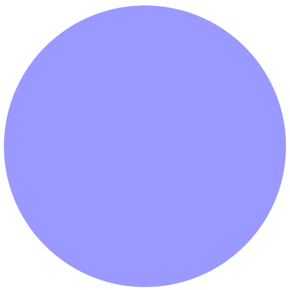

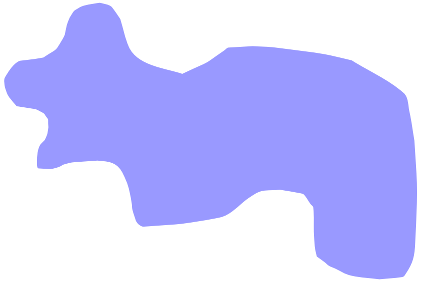

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$$\downarrow \qquad\qquad \downarrow \qquad\qquad \downarrow$$

$$Vol(\partial\Omega) \geq n\, Vol(B_2^3)^{1/3}\; Vol(B_2^3)^{2/3}$$

$$Vol(\partial\Omega) \geq 4\,\pi = Vol(\partial B_2^3)$$

Part. 2 Optimal Transport – Isoperimetric inequality

L_1 Sobolev inegality: a proof with OT [Gromov]

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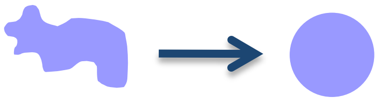

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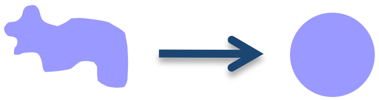

Monge-Ampère equation: $\mathrm{Vol}(B_2^n)\, f^{n/(n-1)}(x) = \det \mathrm{Hess}\, \overline{\Psi}$

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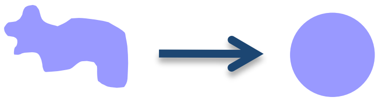

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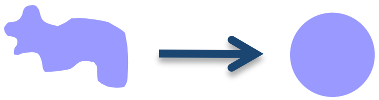

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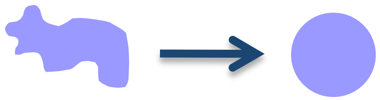

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$$\int | \mathrm{grad}\ f | \geq n\, \mathrm{Vol}(B_2^n)^{1/n} \ \blacksquare$$

3

Semi-Discrete Optimal Transport

Part. 3 Optimal Transport – how to program ?

Continuous

(X;μ)

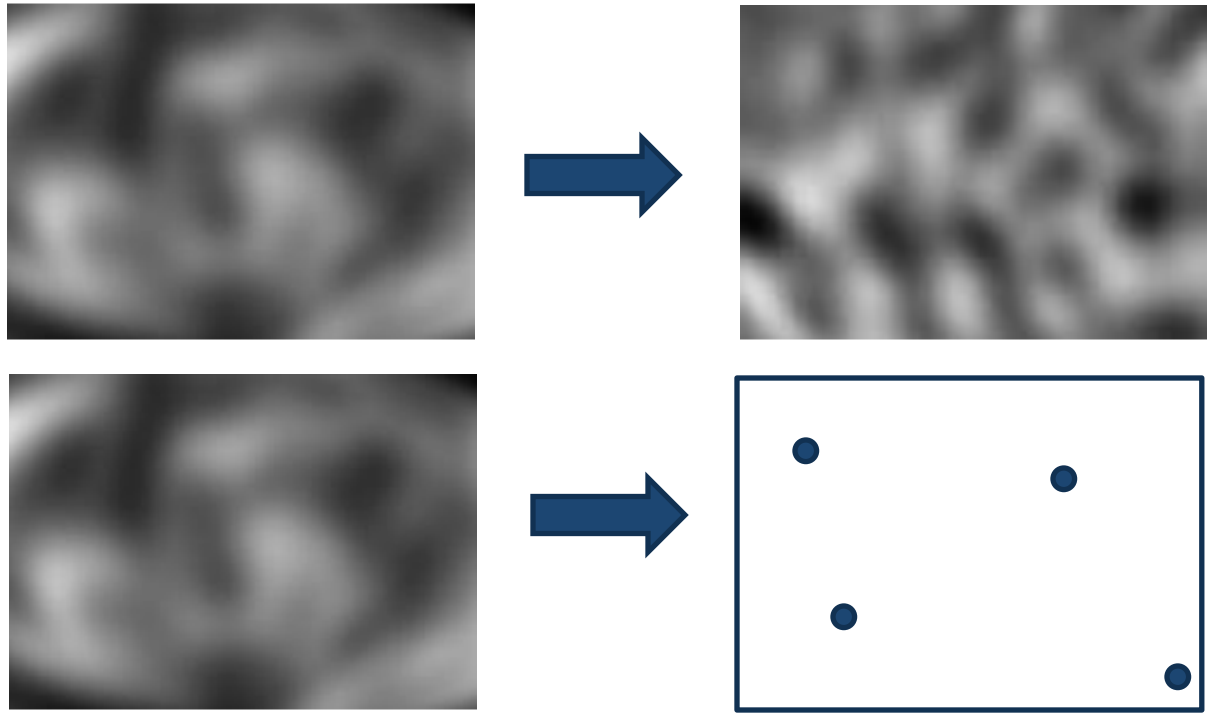
(Y;ν)

Part. 3 Optimal Transport – how to program ?

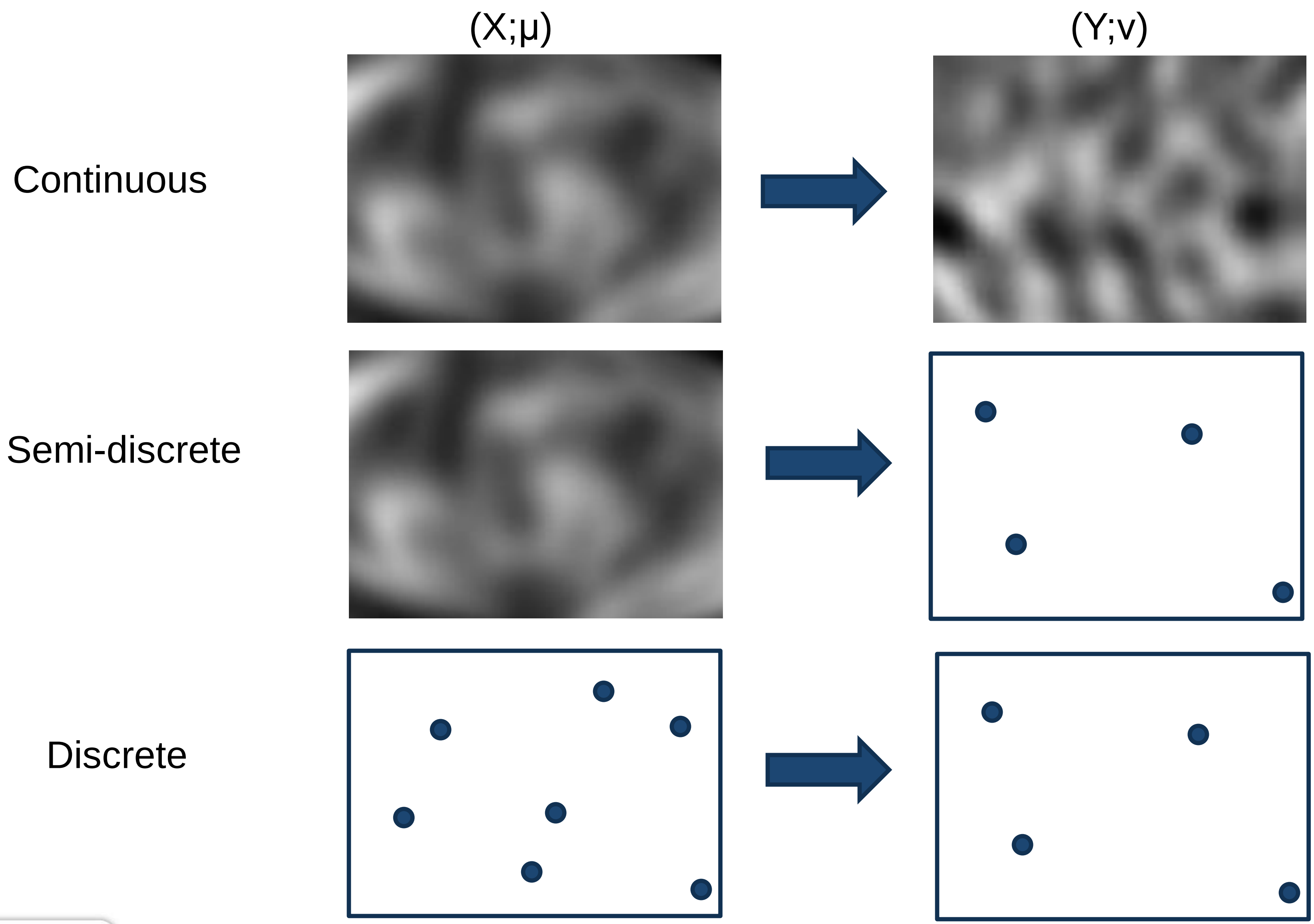
(X;μ) (Y;ν)

Continuous

Semi-discrete



Part. 3 Optimal Transport – how to program ?



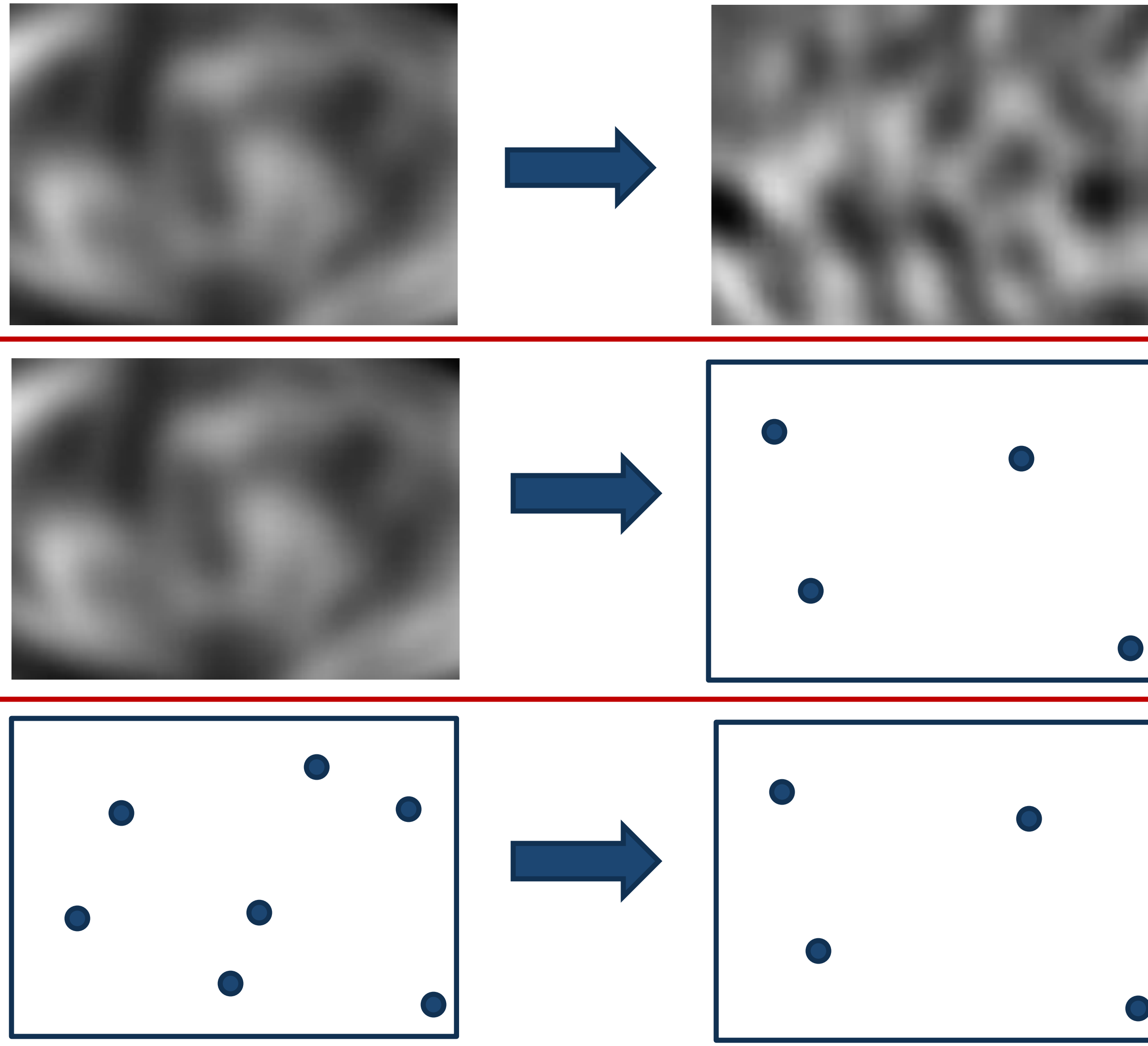
Part. 3 Optimal Transport – how to program ?

(X;μ) (Y;ν)

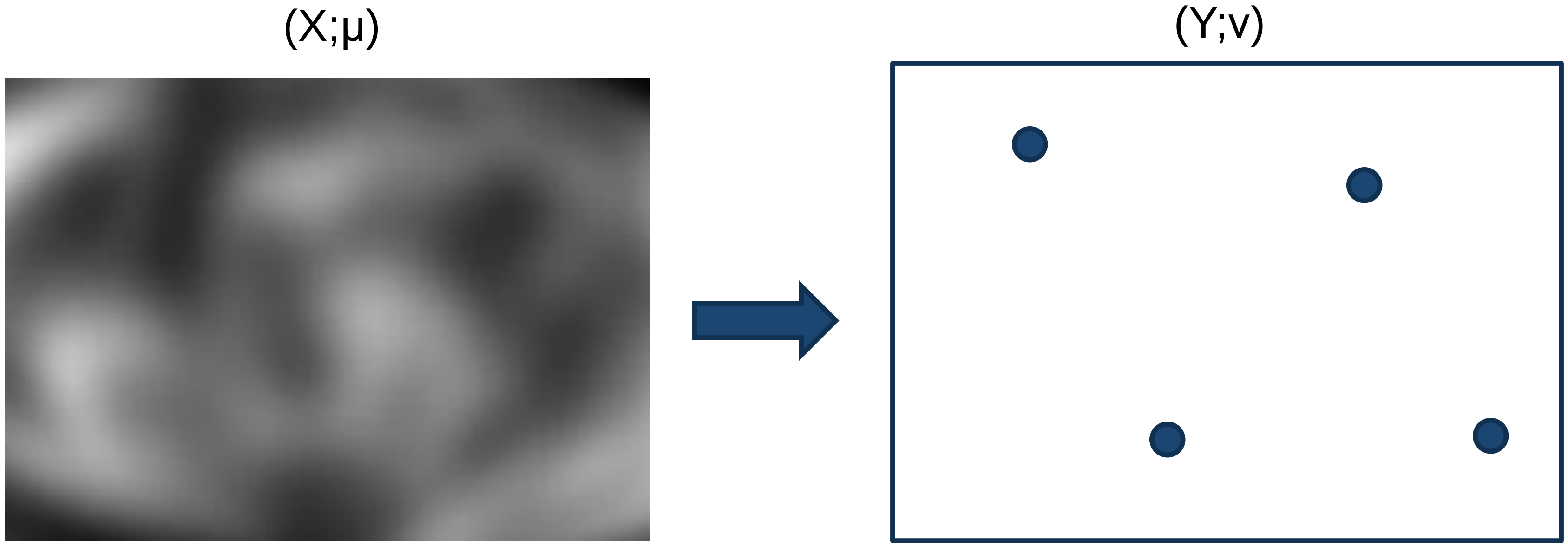
Continuous

Semi-discrete

Discrete

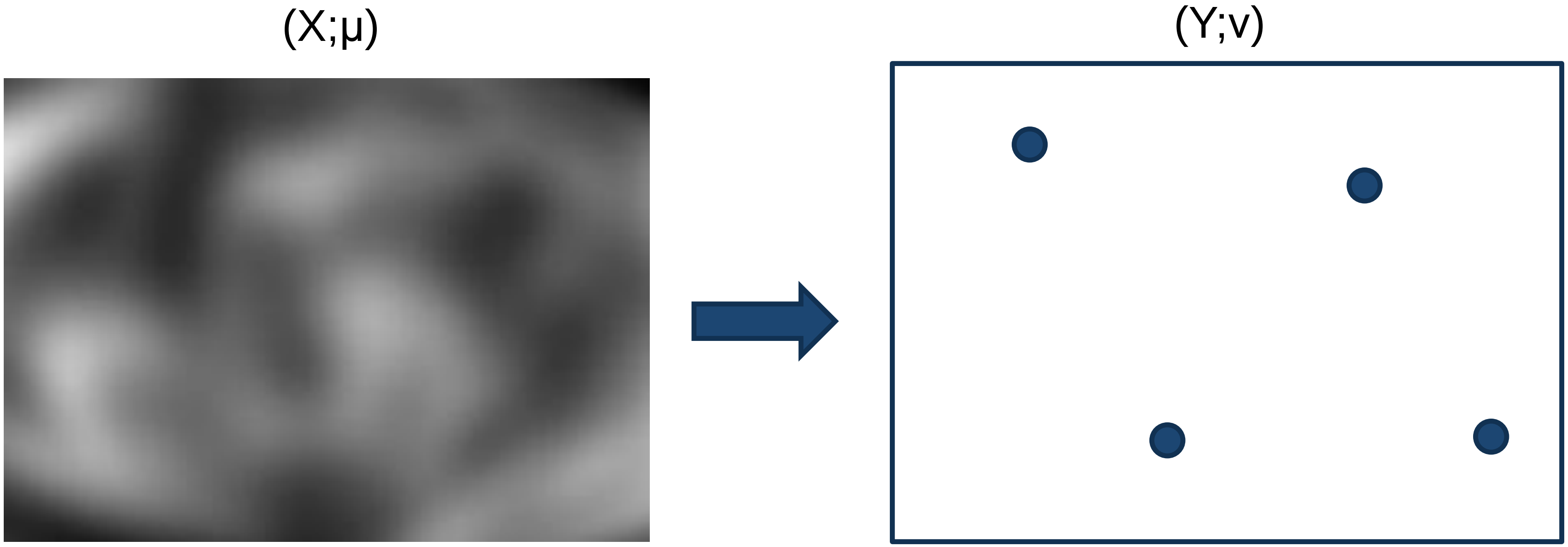


Part. 3 Optimal Transport – semi-discrete



(DMK) $$\sup_{\psi \in \Psi^c} \int_X \psi^c(x)\,d\mu + \int_Y \psi(y)\,d\nu$$

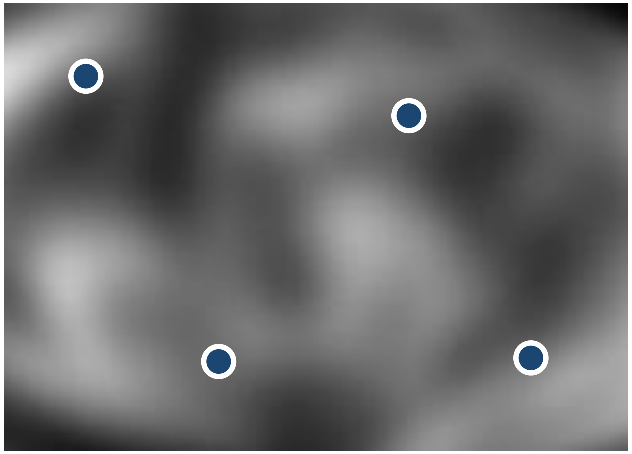
Part. 3 Optimal Transport – semi-discrete



(DMK) $$\sup_{\psi \in \psi^c} \int_X \psi^c(x)d\mu + \int_Y \psi(y)dv$$

$$\sum_j \psi(y_j)\, v_j$$

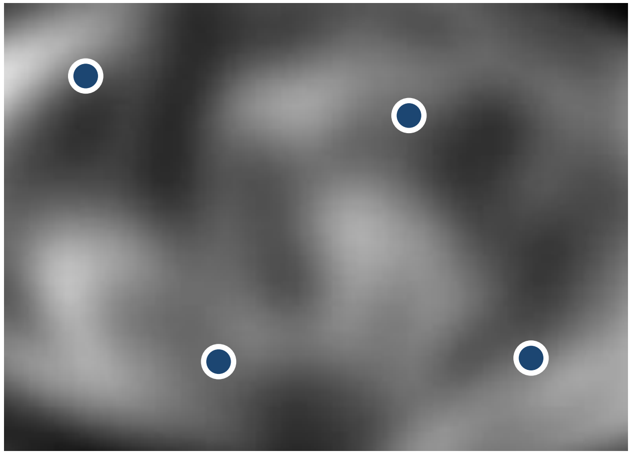
Part. 3 Optimal Transport – semi-discrete



(DMK) $$\sup_{\psi \in \Psi^c} \int_X \psi^c(x)d\mu + \int_Y \psi(y)d\nu$$

$$\to \sum_j \psi(y_j)\, \nu_j$$

Part. 3 Optimal Transport – semi-discrete

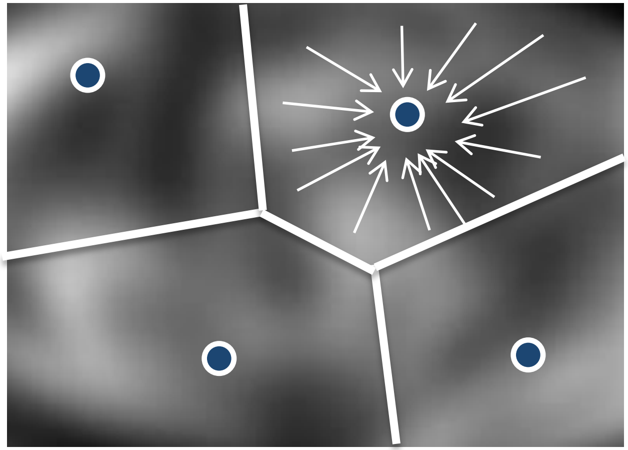


(DMK) $\sup_{\psi \in \Psi^c} \int_X \psi^c(x) d\mu + \int_Y \psi(y) d\nu$

$\int_X \inf_{y_j \in Y} [\, \| x - y_j \|^2 - \psi(y_j) \,] \, d\mu$

$\sum_j \psi(y_j) \, \nu_j$

Part. 3 Optimal Transport – semi-discrete



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$\sum_j \int_{Lag_\psi(y_j)} \| x - y_j \|^2 - \psi(y_j) \, d\mu$

$\sum_j \psi(y_j) \, v_j$

Part. 3 Optimal Transport – semi-discrete

(DMK) $$\sup_{\psi \in \Psi^c} G(\psi) = \sum_j \int_{Lag_{\psi}(y_j)} \| x - y_j \|^2 - \psi(y_j)\, d\mu + \sum_j \psi(y_j)\, v_j$$

Where: $Lag_{\psi}(y_j) = \left\{ x \mid \| x - y_j \|^2 - \psi(y_j) < \| x - y_{j'} \|^2 - \psi(y_{j'}) \right\}$ for all $j' \neq j$

Part. 3 Optimal Transport – semi-discrete

(DMK) $\sup_{\psi \in \Psi^c} G(\psi) = \sum_j \int_{Lag\ \psi(yj)} || x - y_j ||^2 - \psi(y_j)\, d\mu \;+\; \sum_j \psi(y_j)\, v_j$

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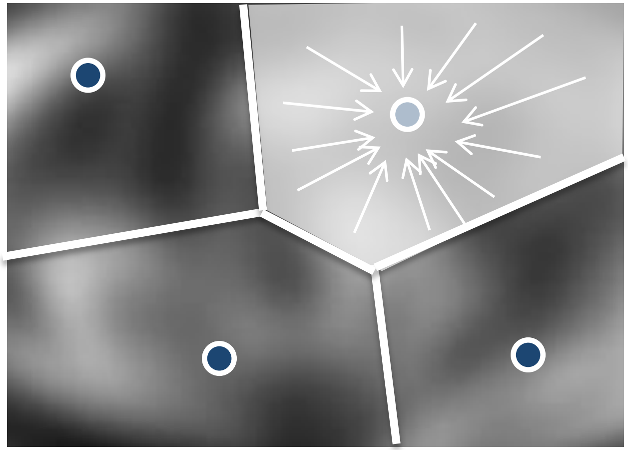
Laguerre diagram of the y_j's
(with the L_2 cost $|| x - y ||^2$ used here, Power diagram)



Part. 3 Optimal Transport – semi-discrete

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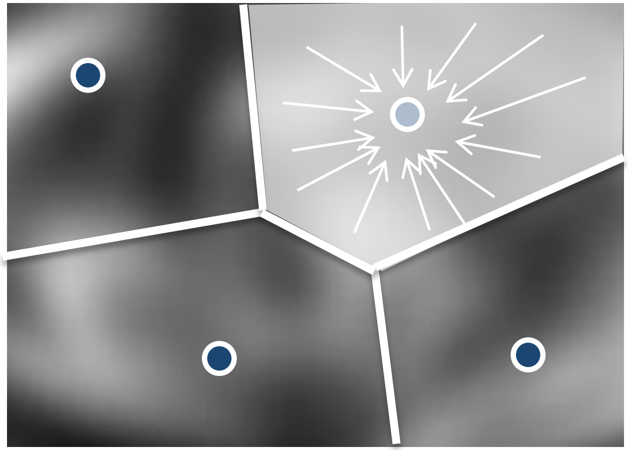
Weight of y_j in the power diagram



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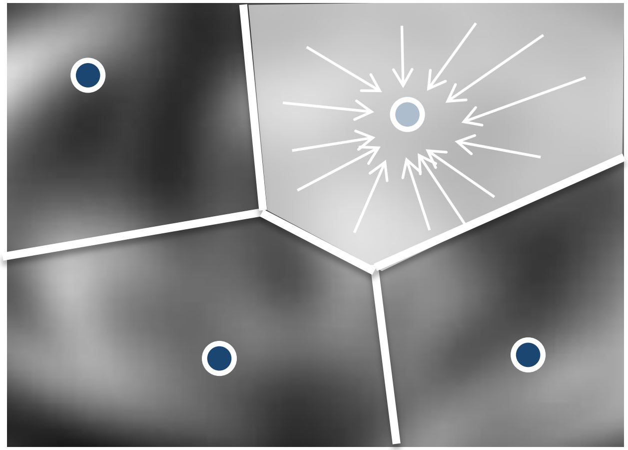

ψ is determined by the
weight vector $[\psi(y_1)\ \psi(y_2) \ldots \psi(y_m)]$

Part. 3 Optimal Transport – semi-discrete

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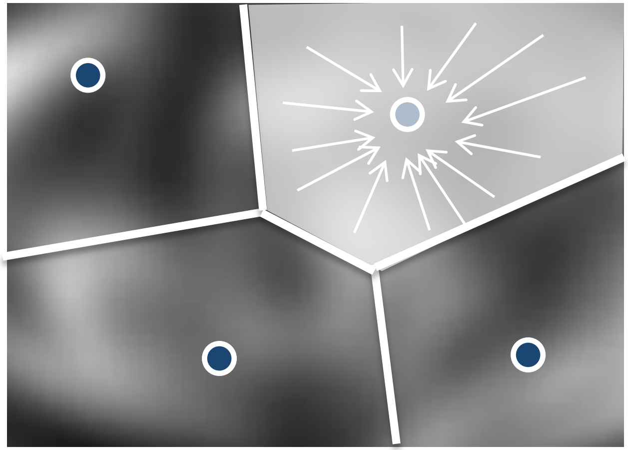

ψ is determined by the **weight vector** $[\psi(y_1)\ \psi(y_2) \dots \psi(y_m)]$

For all weight vector, ψ is c-concave

Part. 3 Power Diagrams

Voronoi diagram: $Vor(x_i) = \{ x \mid d^2(x,x_i) \quad < d^2(x,x_j) \quad \}$

Part. 3 Power Diagrams

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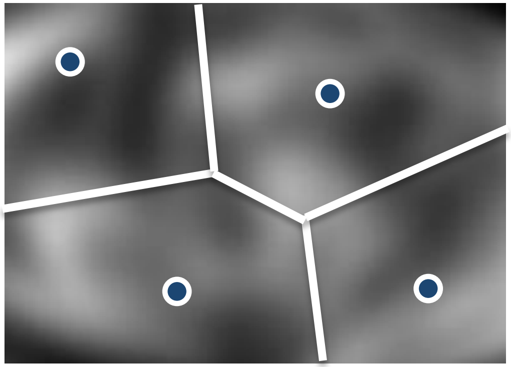
Power diagram: $\text{Pow}(x_i) = \{ x \mid d^2(x,x_i) - \psi_i < d^2(x,x_j) - \psi_j \}$

Part. 3 Power Diagrams

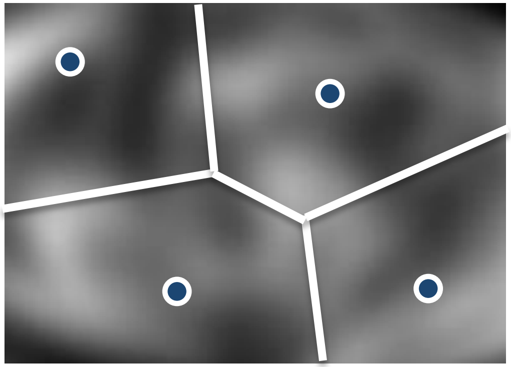
Part. 3 Optimal Transport



Theorem: *(direct consequence of MK duality*
alternative proof in [Aurenhammer, Hoffmann, Aronov 98]):

Given a measure μ with density, a set of points (y_j), a set of positive coefficients v_j such that $\sum v_j = \int d\mu(x)$, it is possible to find the weights $W = [\psi(y_1)\ \psi(y_2)\ \dots\ \psi(y_m)]$ such that the map T_S^W is the unique optimal transport map between μ and $v = \sum v_j\, \delta(y_j)$

Part. 3 Optimal Transport



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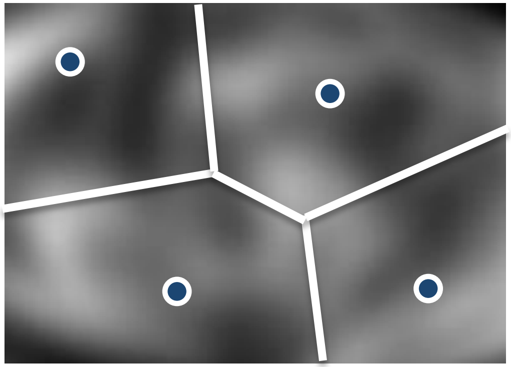
Proof: $G(\psi) = \sum_j \int_{Lag\ \psi(yj)} \| x - y_j \|^2 - \psi(y_j)\, d\mu \ + \ \sum_j \psi(y_j)\, v_j$

Is a concave function of the weight vector $[\psi(y_1)\ \psi(y_2) \ldots \psi(y_m)]$

Part. 3 Optimal Transport



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Part. 3 Optimal Transport – the AHA paper

Idea of the proof

Consider the function $$f_T(W) = \int \left(\| x - T(x) \|^2 - \psi\left(T(X)\right) \right) d\mu(x)$$

The (unknown) weights $W = [\psi(y_1)\ \psi(y_2)\ \ldots\ \psi(y_m)]$

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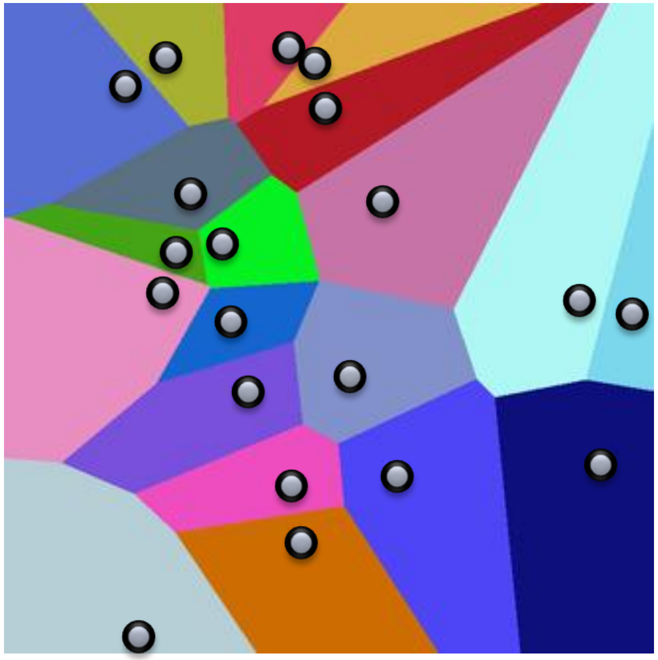
Consider the function $f_T(W) = \int \left(\| x - T(x) \|^2 - \psi\left(T(X)\right) \right) d\mu(x)$

T : an arbitrary but fixed assignment.



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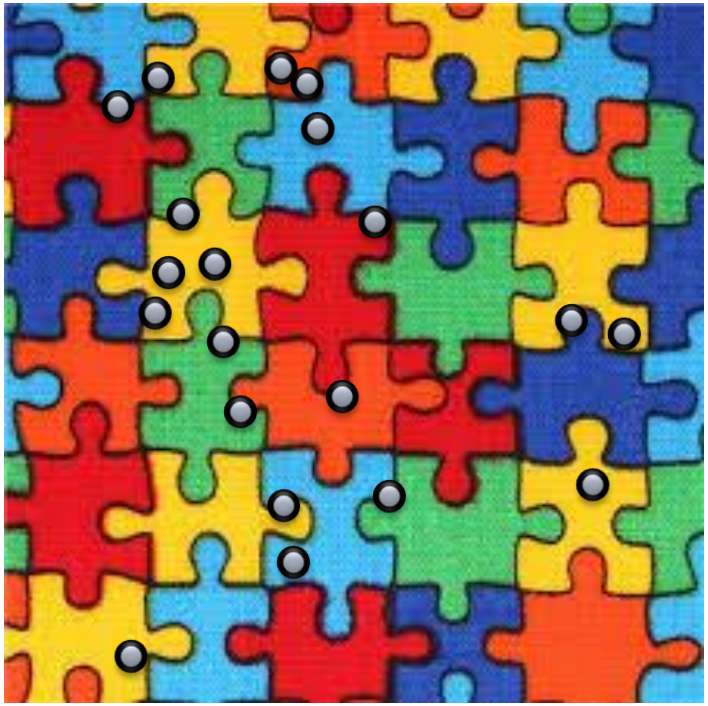

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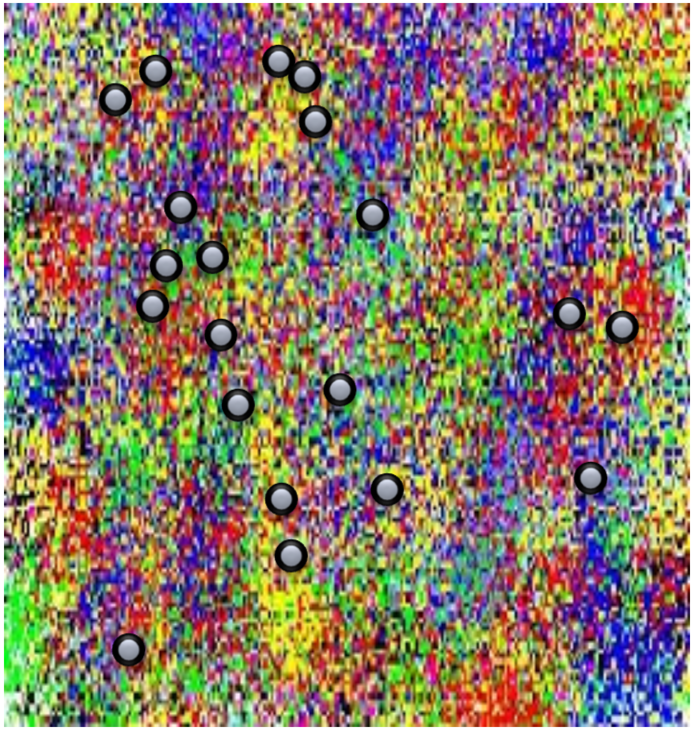

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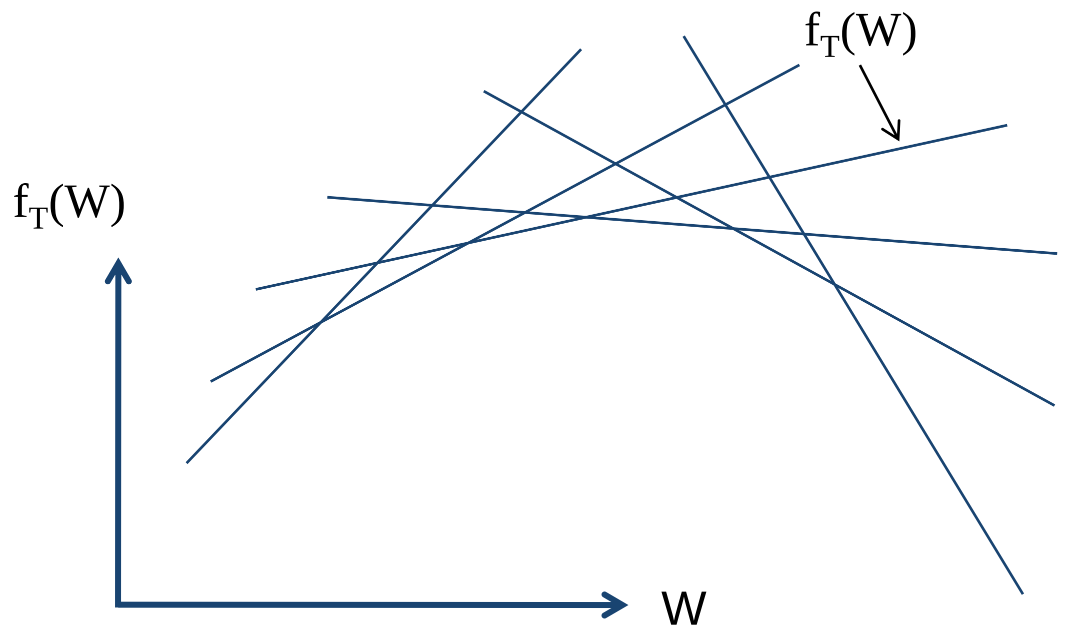

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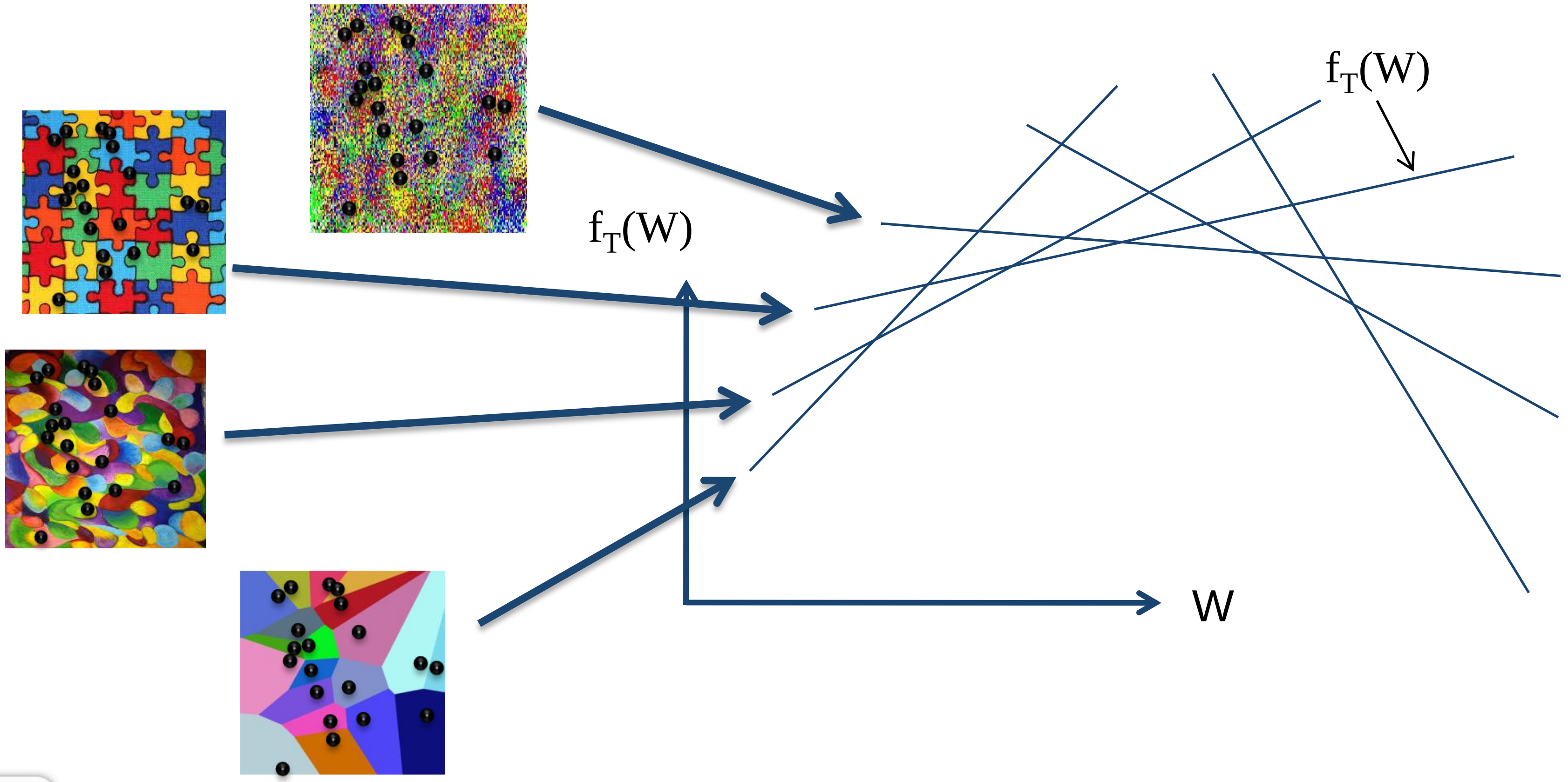

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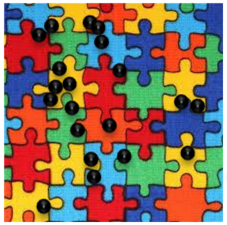

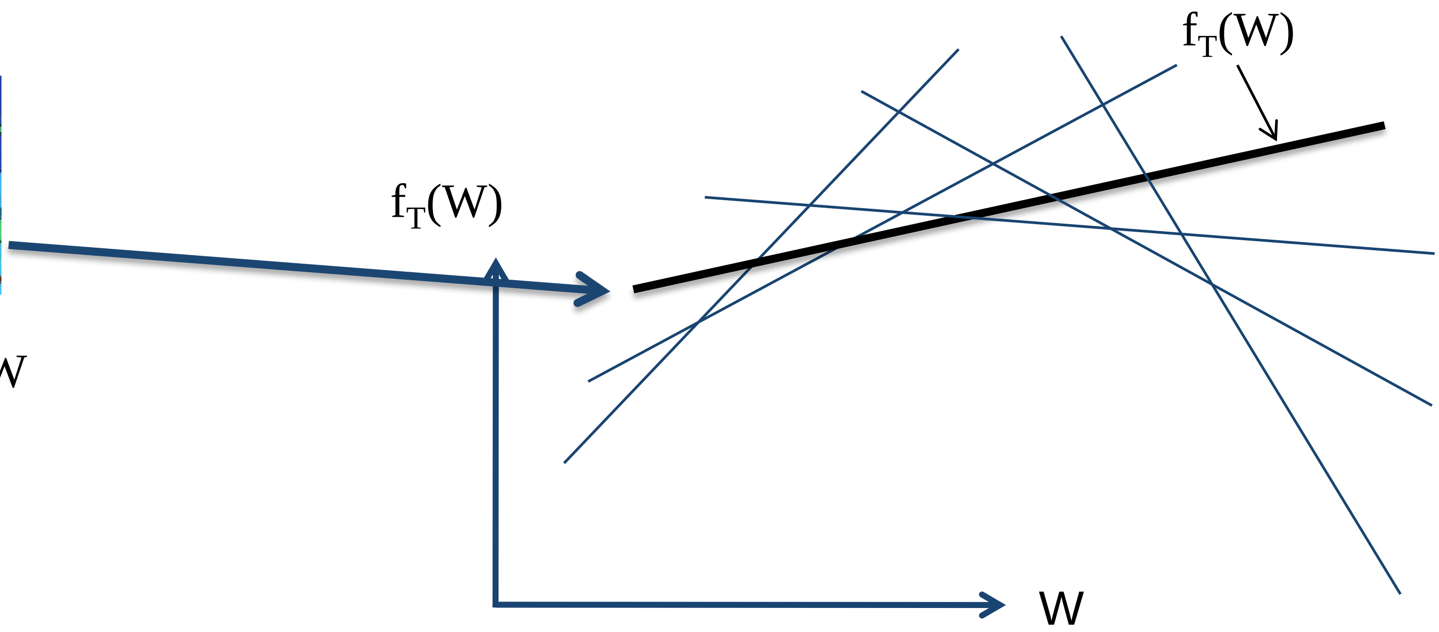

$f_T(W)$ is linear in W

Part. 3 Optimal Transport – the AHA paper

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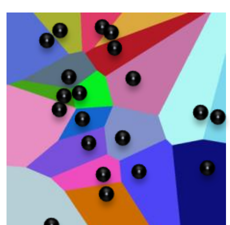
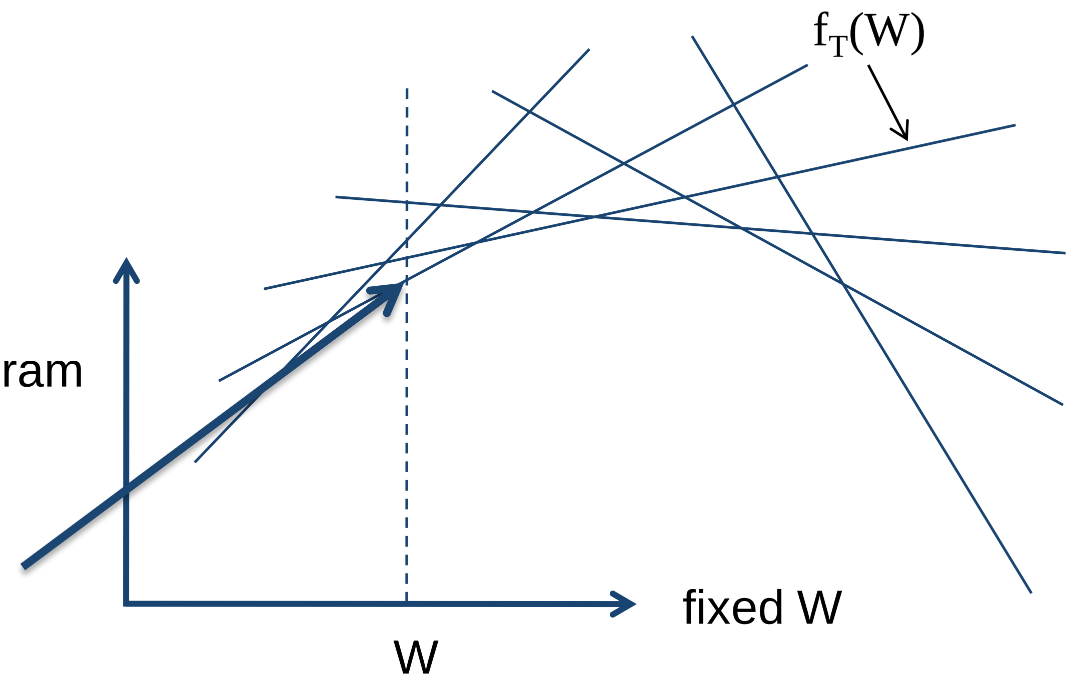
$f_T(W)$ is linear in W

$f_{T_W}(W)$: defined by Laguerre diagram





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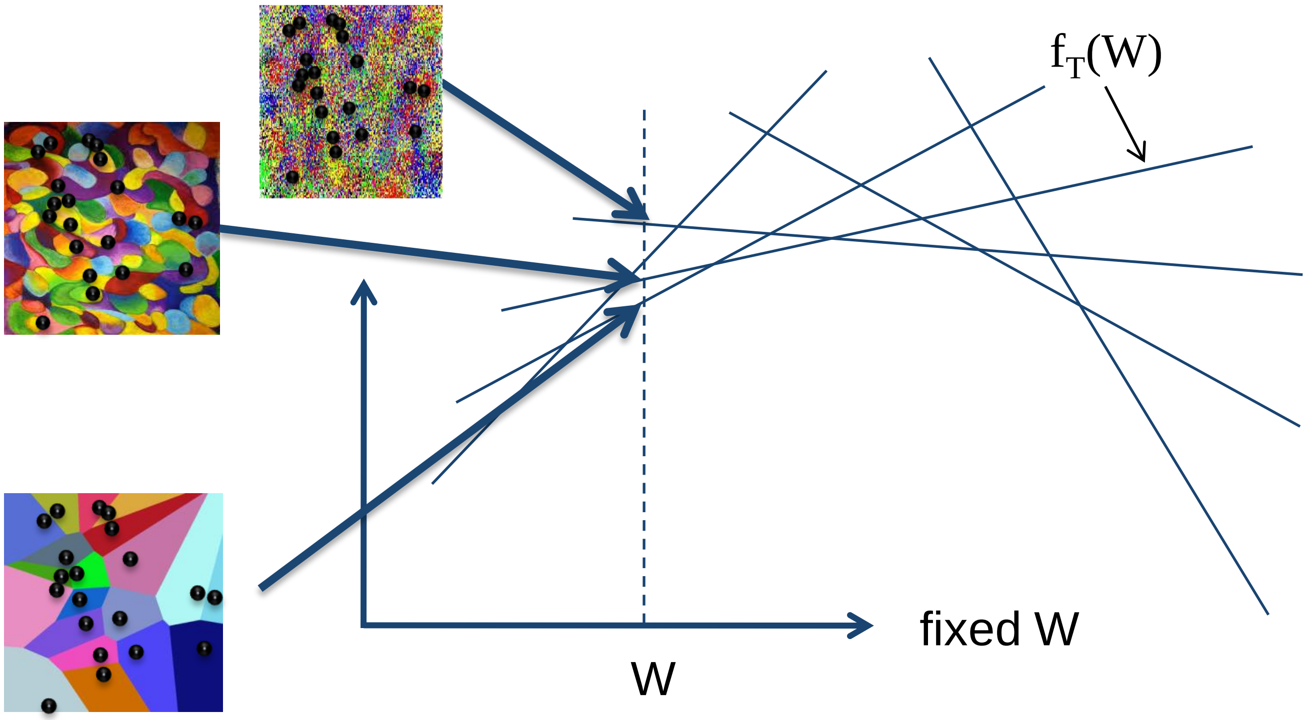
$f_{T_W}(W) = \min_T f_T(W)$



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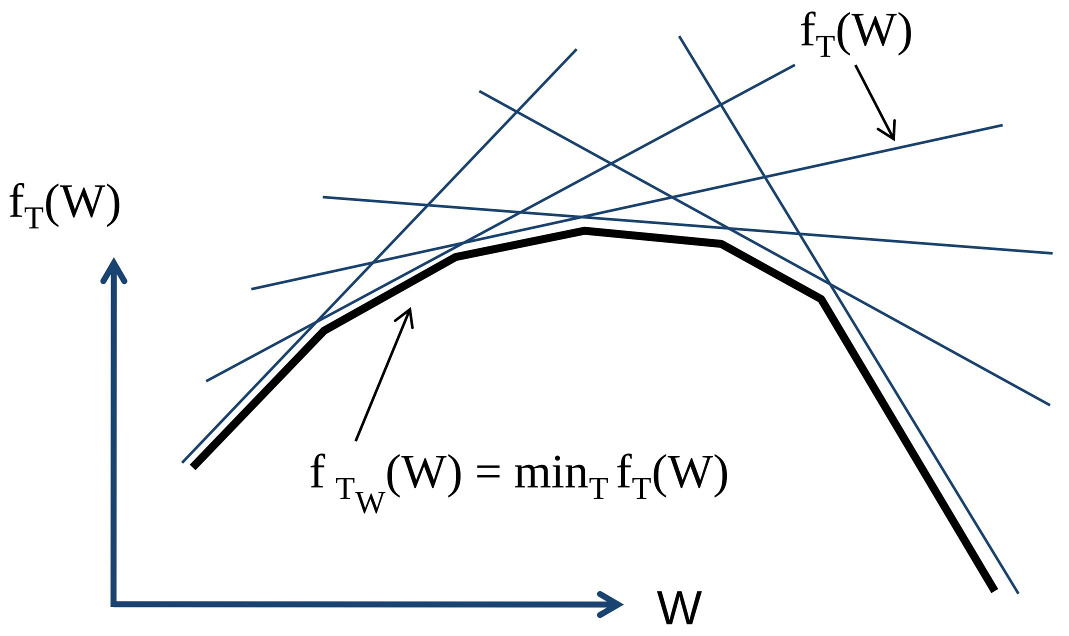
f: $W \rightarrow f_{T_W}(W)$ is **concave !!**

(because its graph is the lower enveloppe of linear functions)



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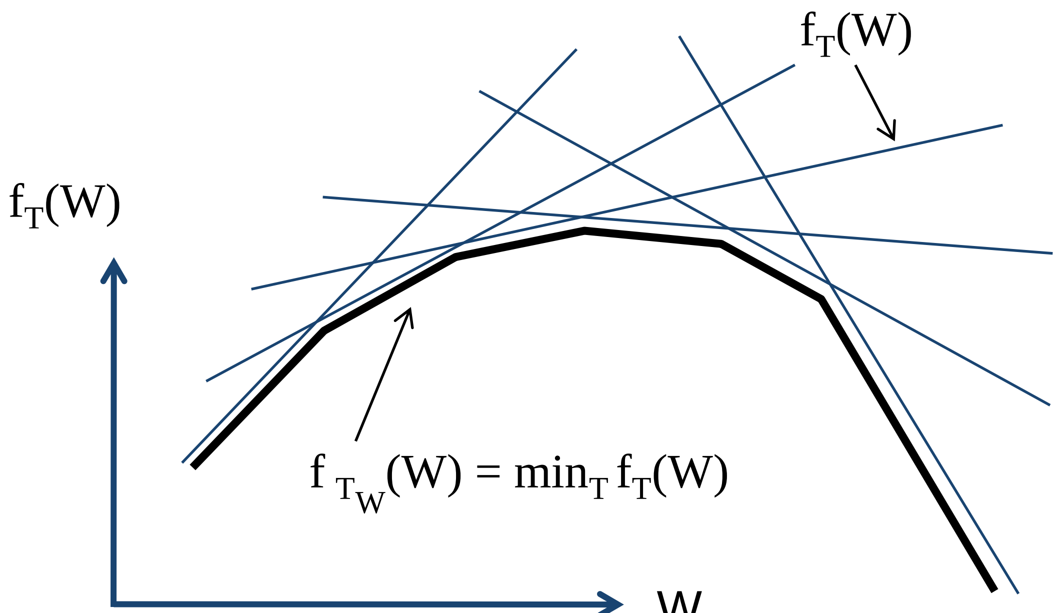

$f_T(W)$ is linear in W

$f: W \rightarrow f_{T_W}(W)$ is concave (because its graph is the lower enveloppe of linear functions)

Consider $g(W) = f_{T_W}(W) + \sum v_j \psi_j$

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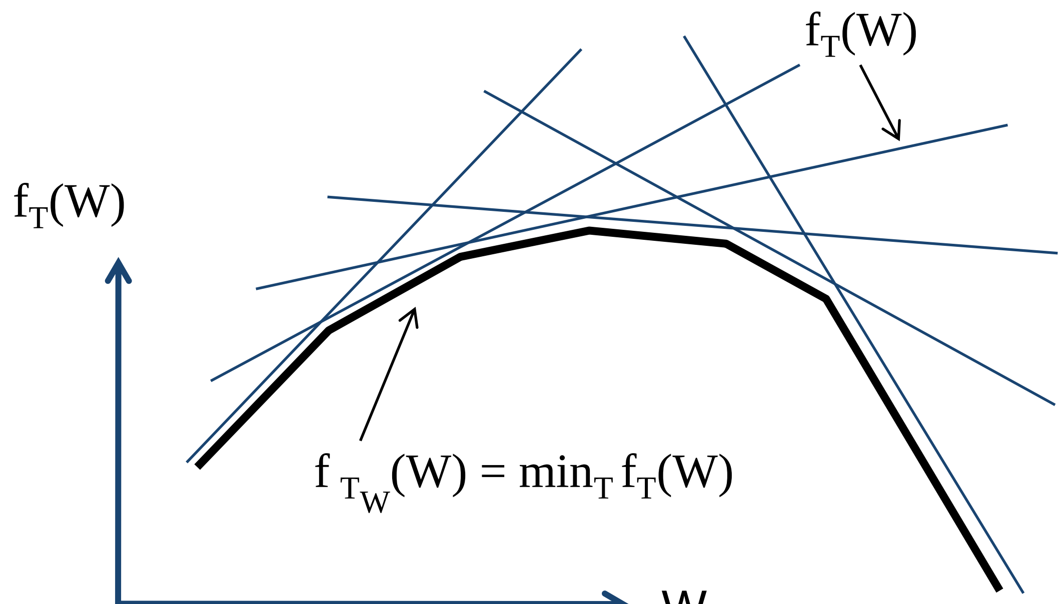

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Consider $g(W) = f_{T_W}(W) + \sum v_j \psi_j$

$$\partial g / \partial \psi_j = v_j - \int_{Lag^{\psi}(yj)} d\mu(x)$$ and g is concave.

Part. 3 Optimal Transport – the algorithm

Semi-discrete OT Summary:

(DMK) $$\sup_{\psi \in \Psi^c} G(\psi) = \int_X \psi^c(x)d\mu + \int_Y \psi(y)d\nu$$

Part. 3 Optimal Transport – the algorithm

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Part. 3 Optimal Transport – the algorithm

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$$\partial G / \partial \psi_j = v_j - \int_{Lag(yj)} d\mu(x) \quad (= 0 \text{ at the maximum})$$

Part. 3 Optimal Transport – the algorithm

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Desired mass at y_j

Mass transported to y_j

Part. 3 Optimal Transport – the Hessian

$$\partial G / \partial \psi_j = V_j - \int_{Lag(yj)} d\mu(x)$$

Part. 3 Optimal Transport – the Hessian

$$\partial G / \partial \Psi_j = v_j - \int_{Lag(yj)} d\mu(x)$$

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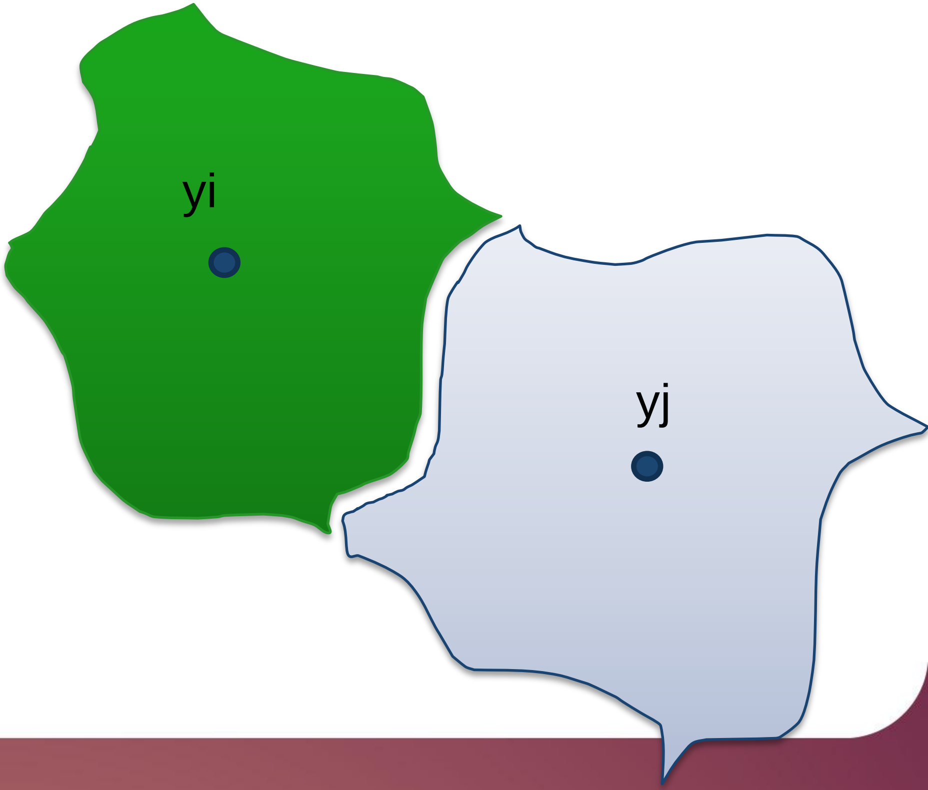

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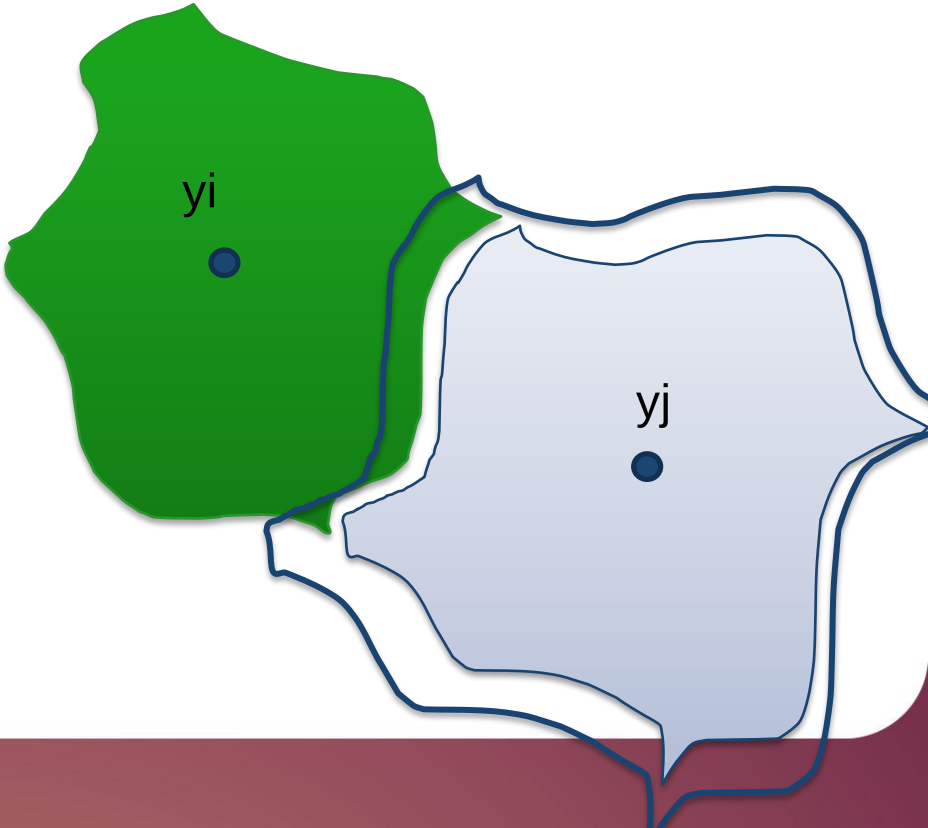

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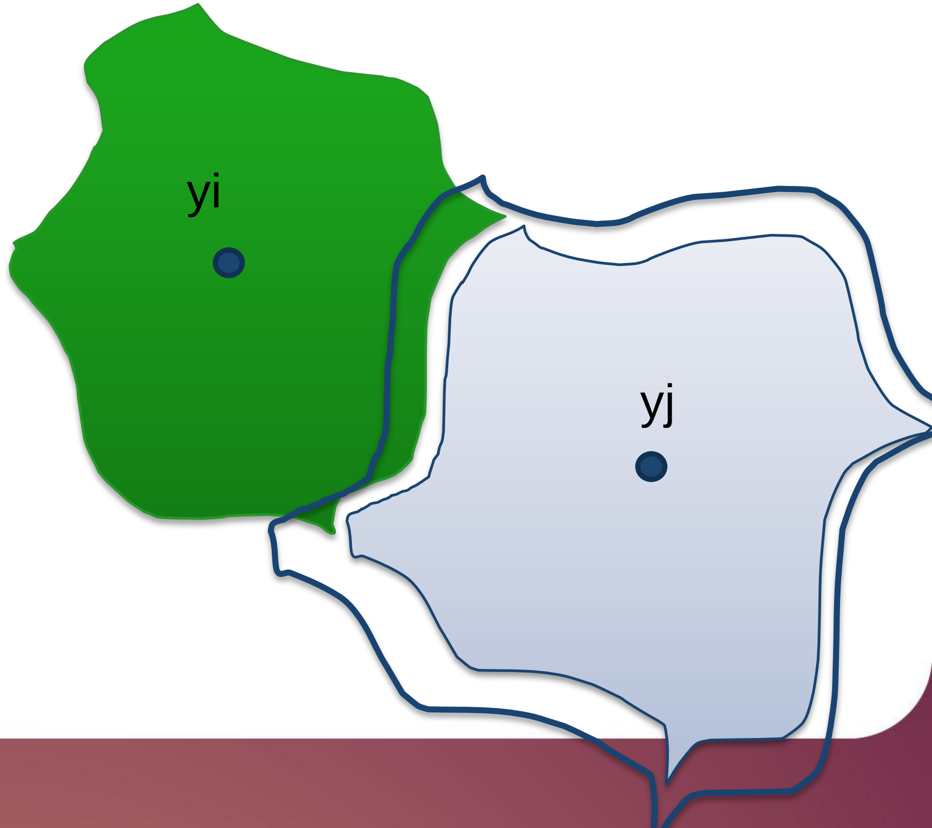
Reynold's thm:

$$\partial / \partial \psi_j \int_{Lag(yj)} d\mu(x) = \int_{\partial Lag(yj)} v.n \, d\mu(x)$$



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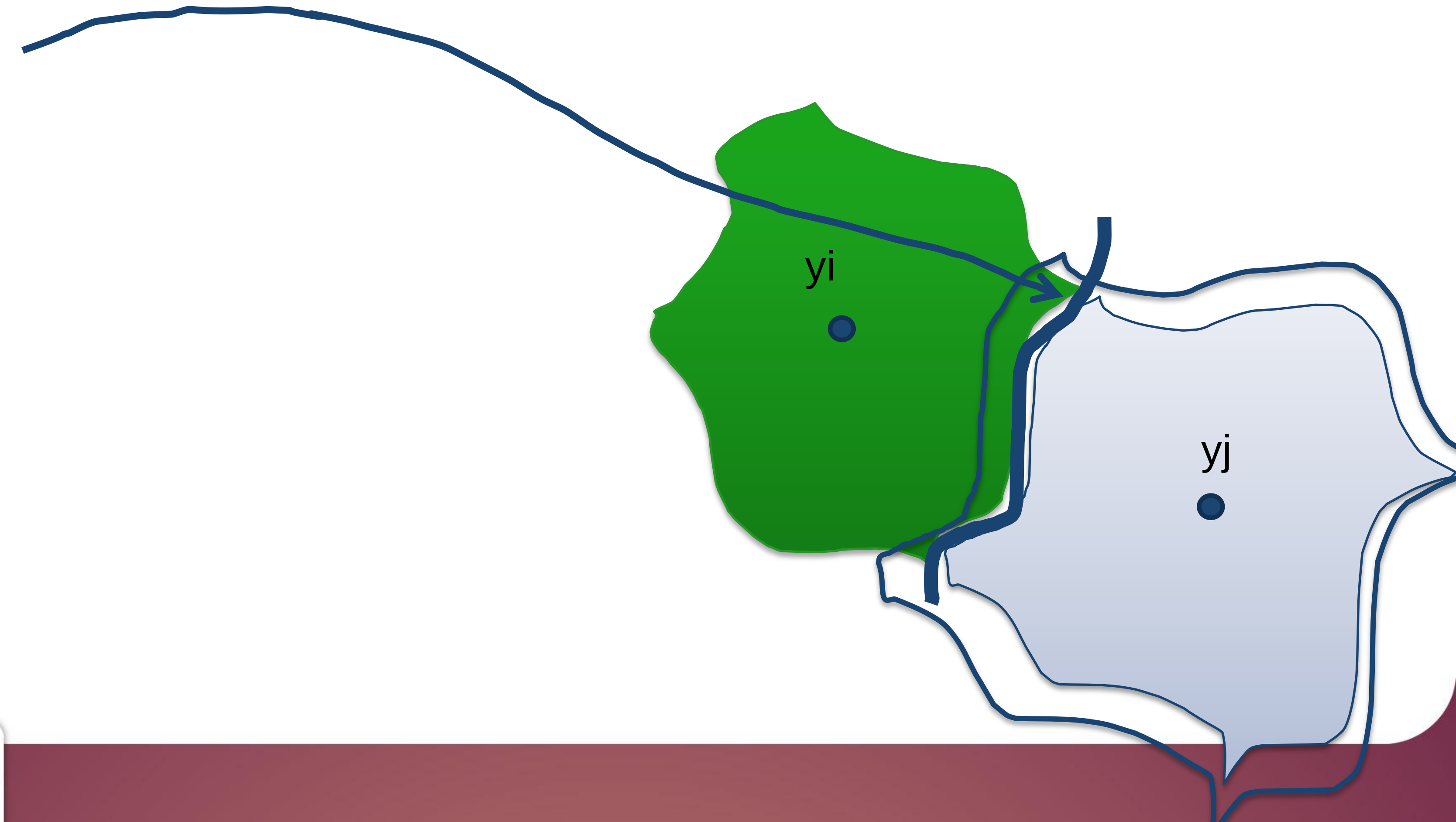

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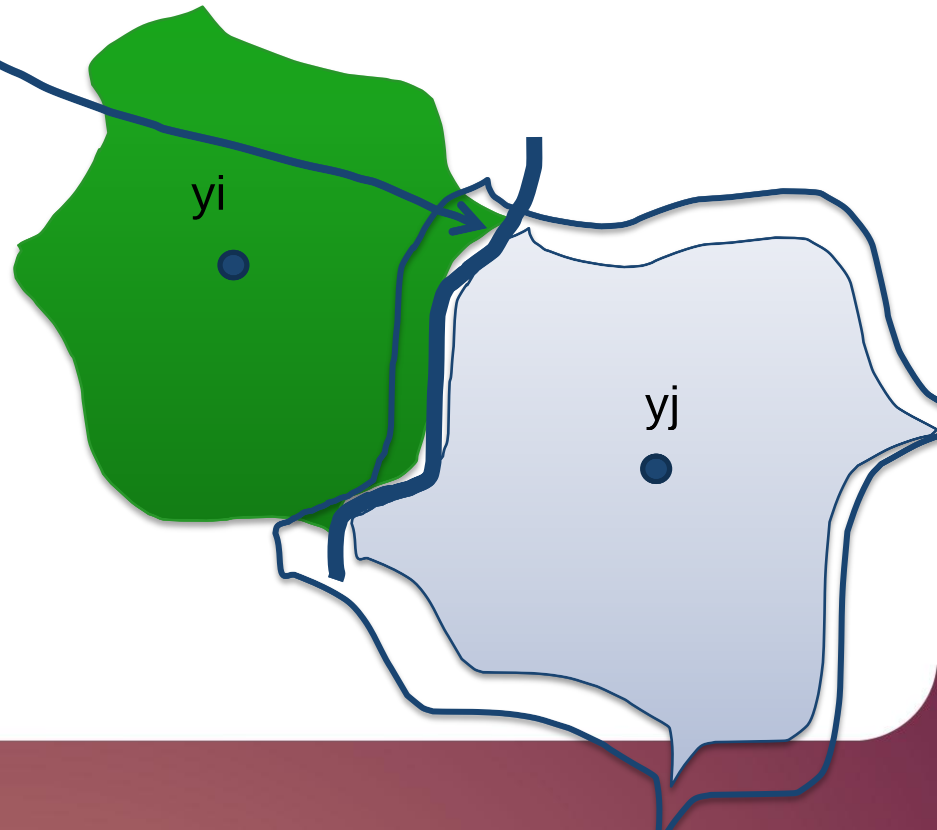

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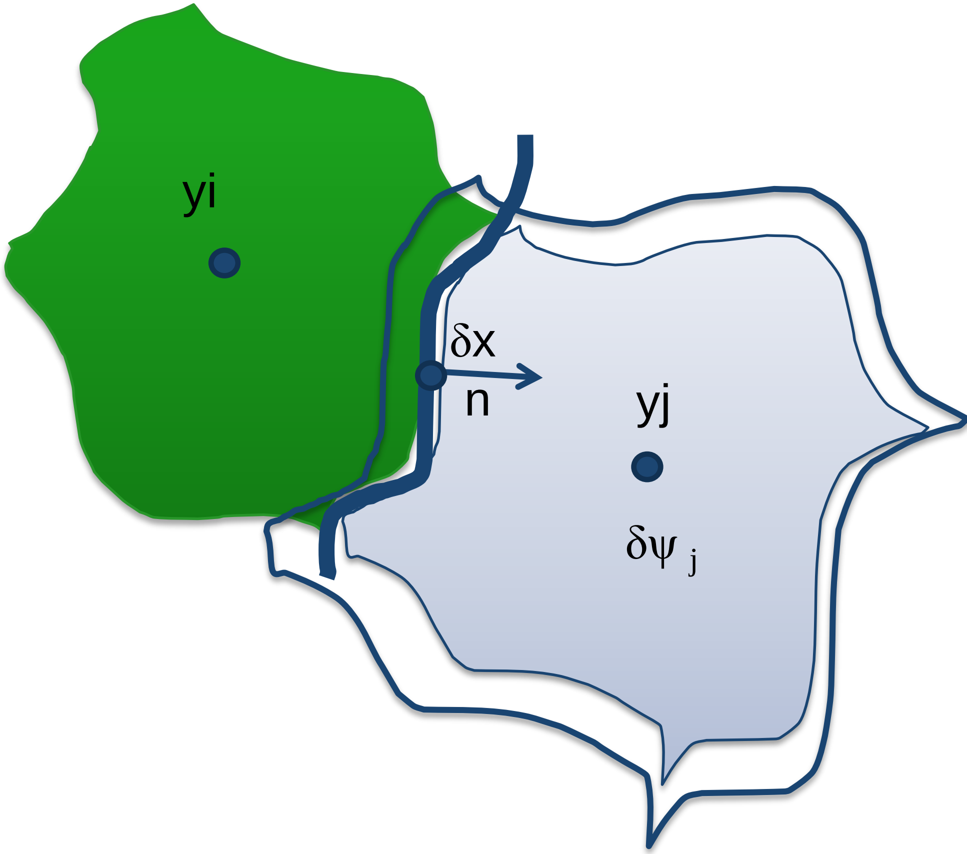

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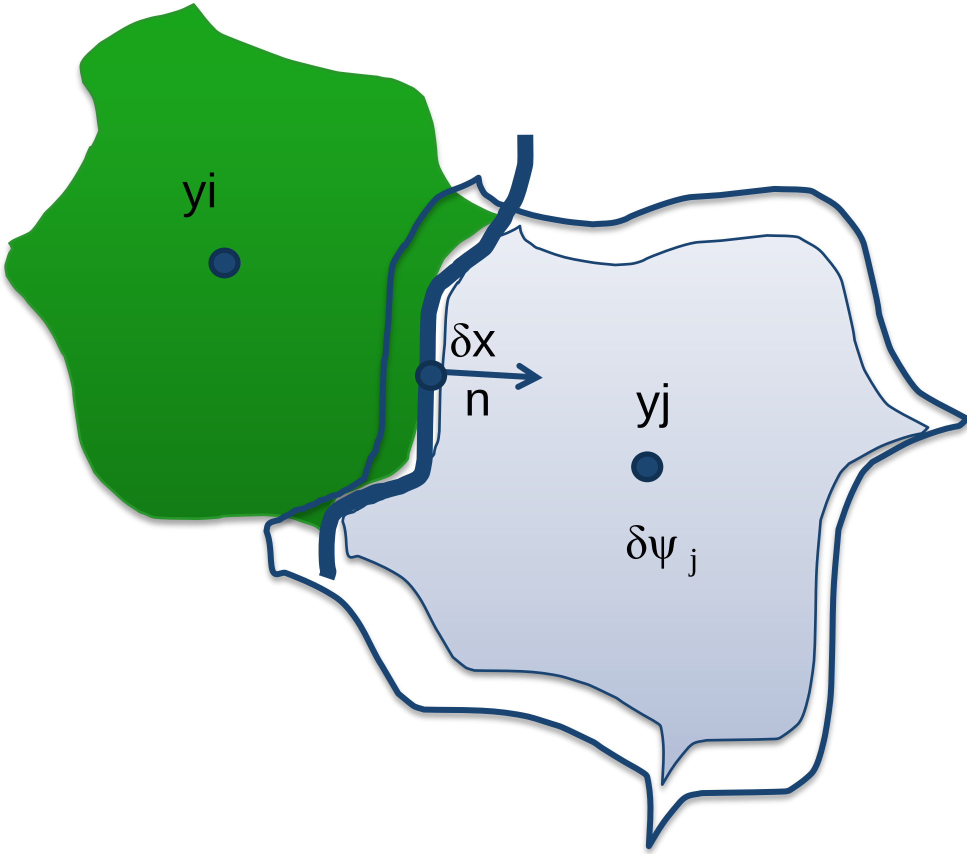

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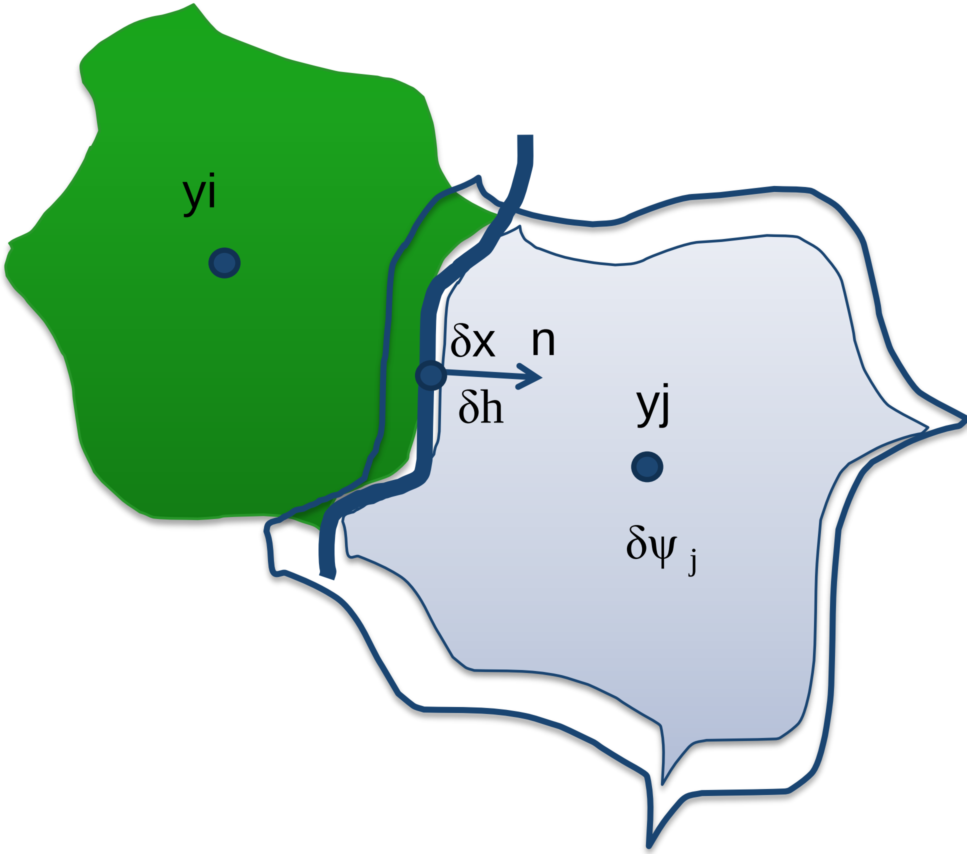

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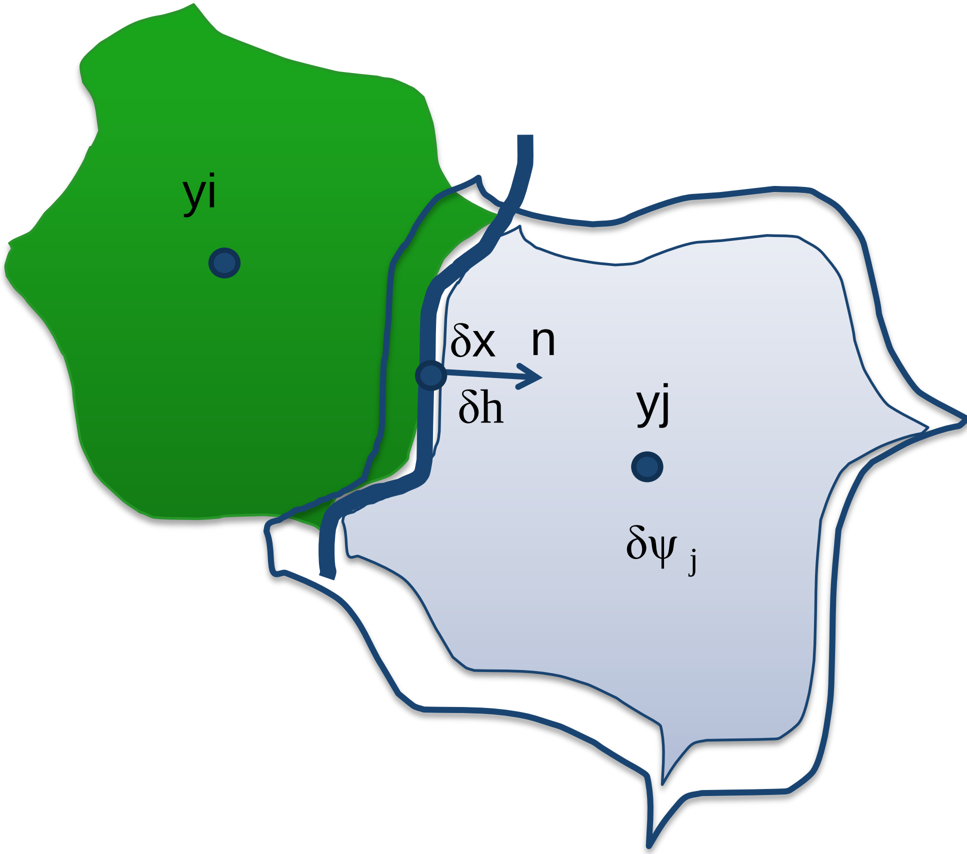
$$\partial h / \partial \psi_j = -1/ \| grad_x c(x,y_i) - grad_x c(x,y_j) \|$$



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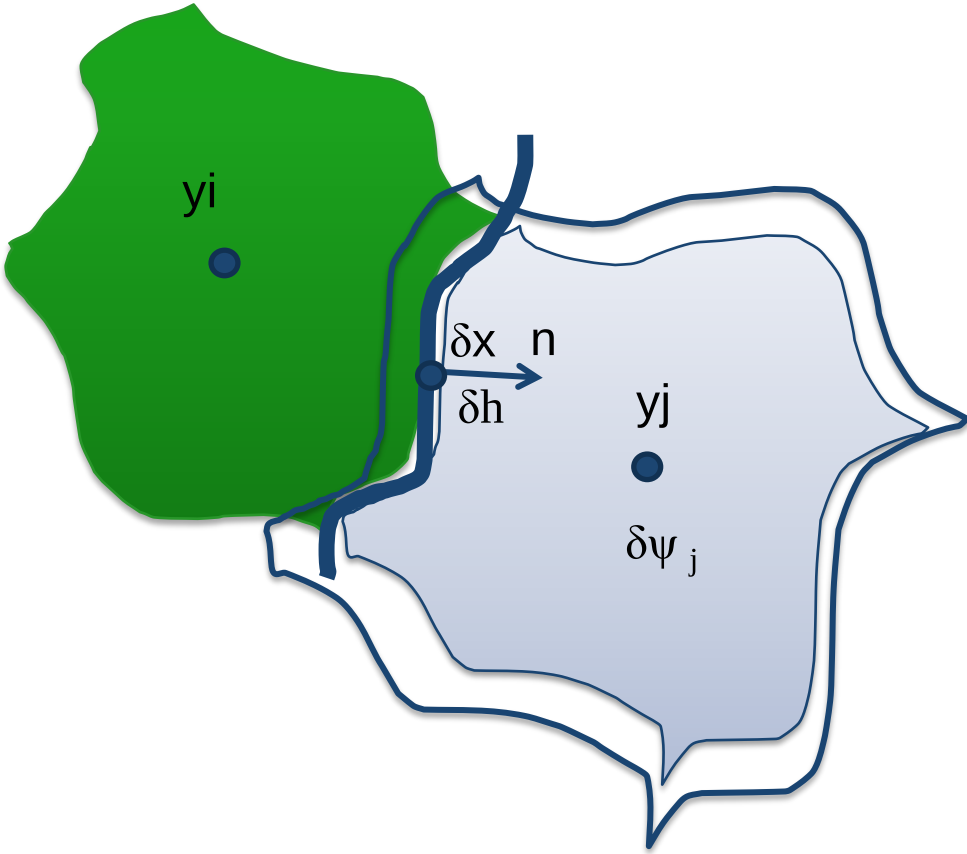

$$\partial / \partial \psi_j \int_{Lag(yj)} d\mu(x) = \int_{Lag(yi) \cap Lag(yj)} -1/\| \mathrm{grad}_x c(x,y_i) - \mathrm{grad}_x c(x,y_j) \| d\mu(x)$$

Part. 3 the Hessian

$$\partial^2 / \partial\psi_i \partial\psi_j F = \int_{Lag(yi) \cap Lag(yj)} -1/\| \text{grad}_x c(x,y_i) - \text{grad}_x c(x,y_j) \| d\mu(x)$$

$$\partial^2 / \partial\psi_i^2 F = -\sum \partial^2 / \partial\psi_i \partial\psi_j$$

Part. 3 the Hessian

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$c(x,y) = \| x - y \|^2$

$$\partial^2 / \partial \psi_i \partial \psi_j F = \int_{Lag(yi) \cap Lag(yj)} 1 / \| xj - xi \| \, d\mu(x)$$

Part. 3 the Hessian

$$\partial^2 / \partial \psi_i \partial \psi_j F = \int_{Lag(yi) \cap Lag(yj)} -1/\| grad_x \, c(x,y_i) - grad_x \, c(x,y_j) \| d\mu(x)$$

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IP_1 FEM Laplacian (not a big surprise)

Part. 3 Optimal Transport – the algorithm

The [AHA] paper summary:

- The optimal weights minimize a convex function
- The gradient of this convex function is easy to compute

Note: the weight w(s) correspond to the Kantorovich potential $\psi(x)$
(solves a "discrete Monge-Ampere" equation)

The algorithm:

Input: two tetrahedral meshes M_1 and M_2
Output: a morphing between M_1 and M_2

Step 1: sample M_2 with N points $(s_1 \dots s_N)$
Step 2: initialize the weights $(w_1 \dots w_N) = (0 \dots 0)$
Step 3: minimize $g(w_1 \dots w_N)$ with a quasi-Newton algorithm:

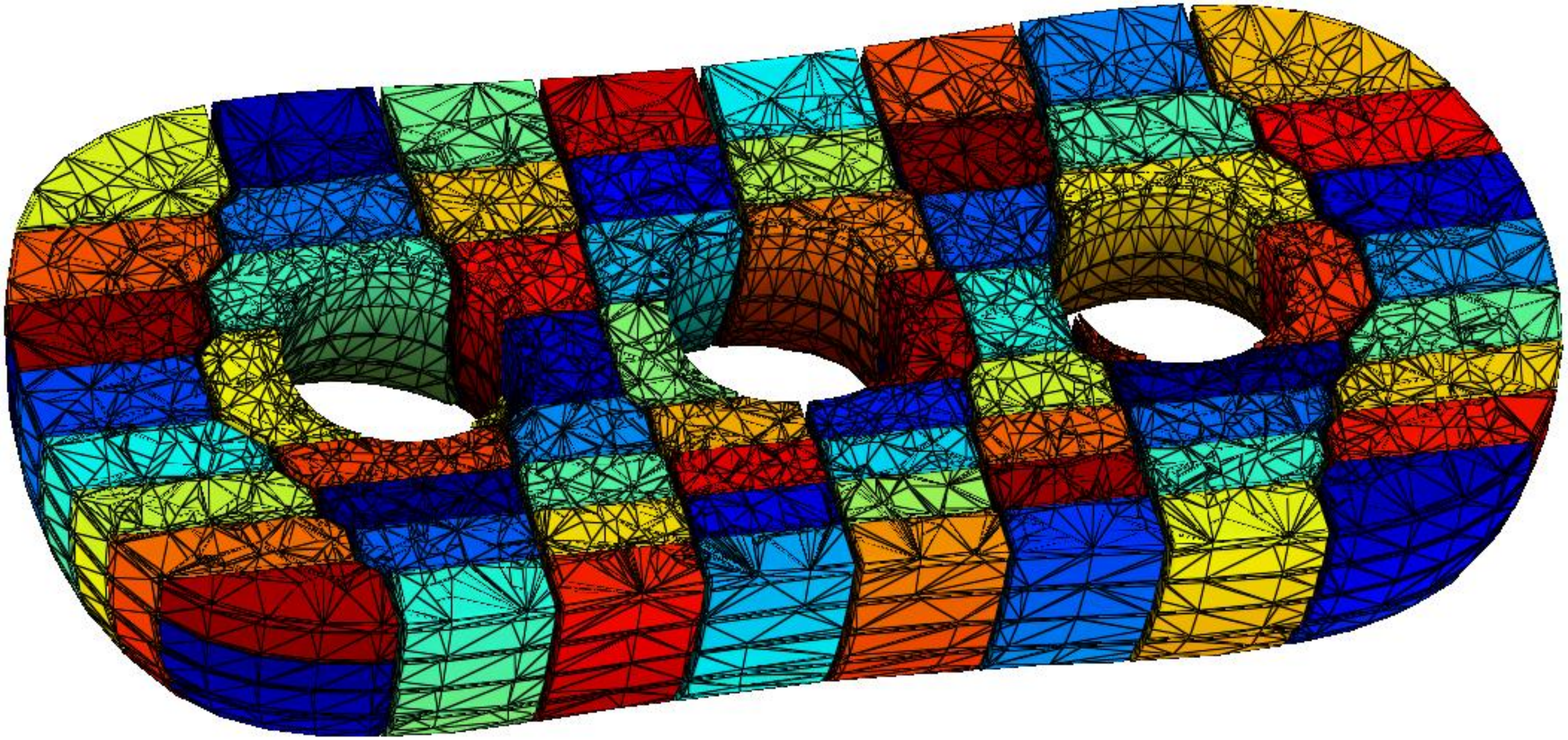
For each iterate $(s_1 \dots s_N)^{(k)}$:

Compute $\mathrm{Pow}\big((w_i, s_i)\big) \cap M_1$ [Nivoliers, **L** 2014, Curves and Surfaces]

Compute g, grad g, Hg

Damped Newton algorithm, [Kitagawa, Mérigot, Thibert]

Part. 3 Optimal Transport – the algorithm



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- The gradient and Hessian of this convex function is easy to compute

Note: the weight w(s) correspond to the Kantorovich potential $\psi(x)$
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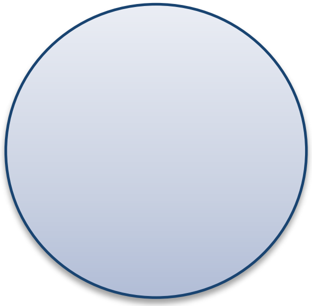
The algorithm:

Summary:

The algorithm computes the weights w_i such that the power cells associated with the Diracs correspond to the preimages of the Diracs.



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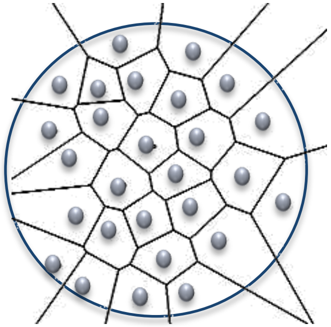

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Part. 3 Optimal Transport – the algorithm

The [AHA] paper summary:

- The optimal weights minimize a convex function
- The gradient and Hessian of this convex function is easy to compute

Note: the weight w(s) correspond to the Kantorovich potential $\psi(x)$
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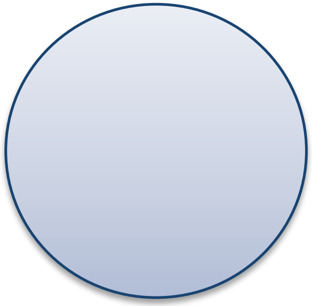

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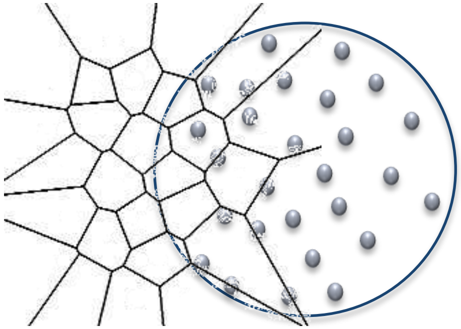

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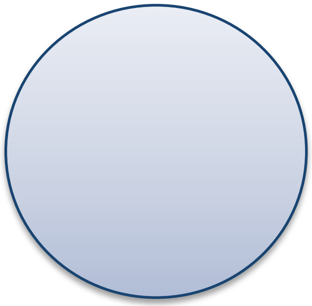

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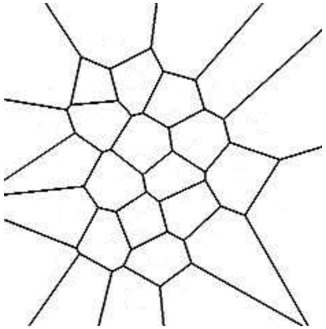

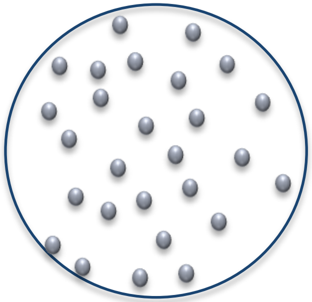

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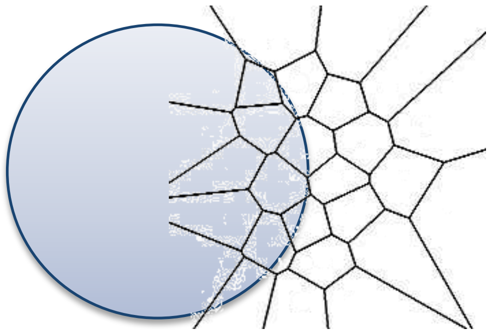

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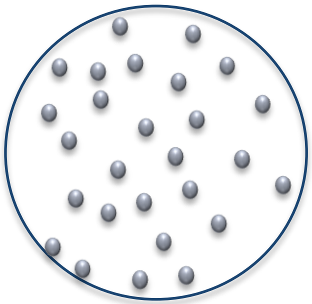

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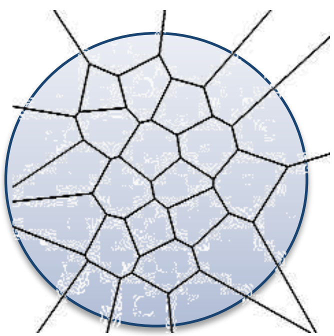

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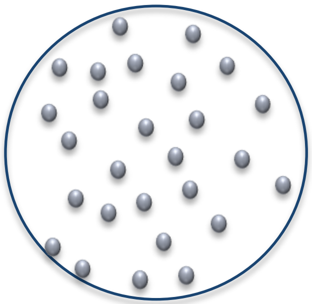

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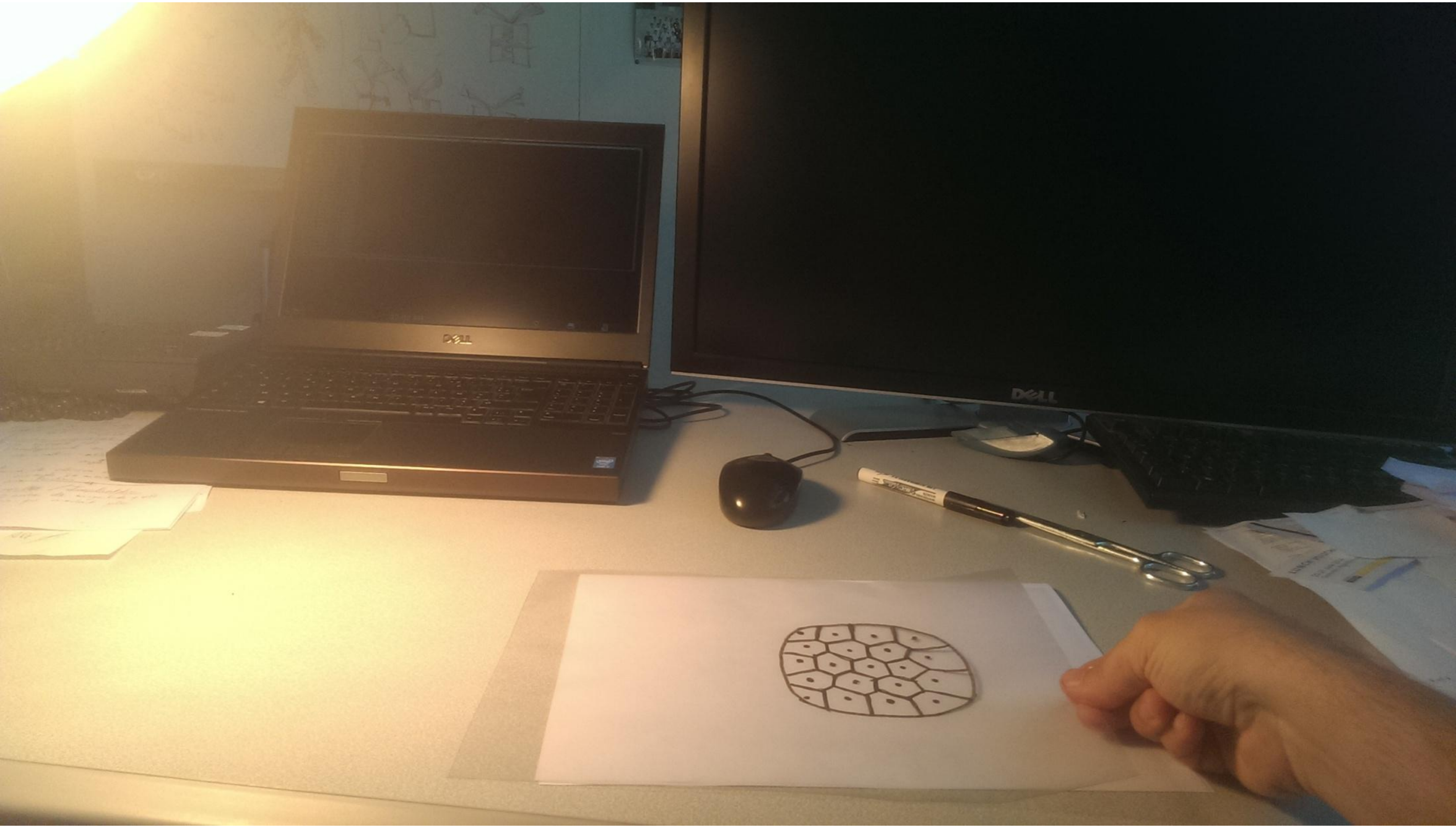
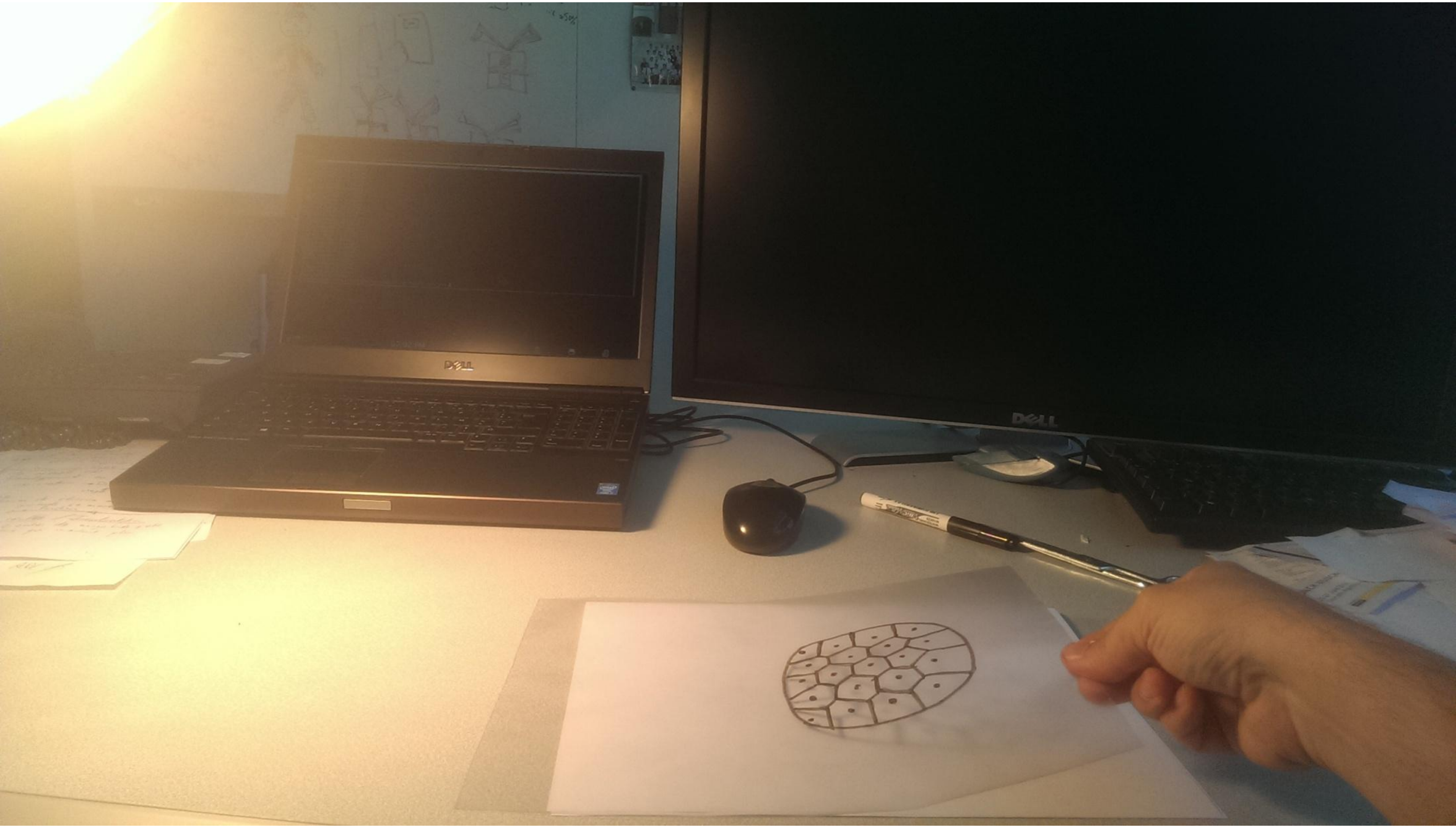
Part. 3 Power Diagrams & Transport



Part. 3 Power Diagrams & Transport



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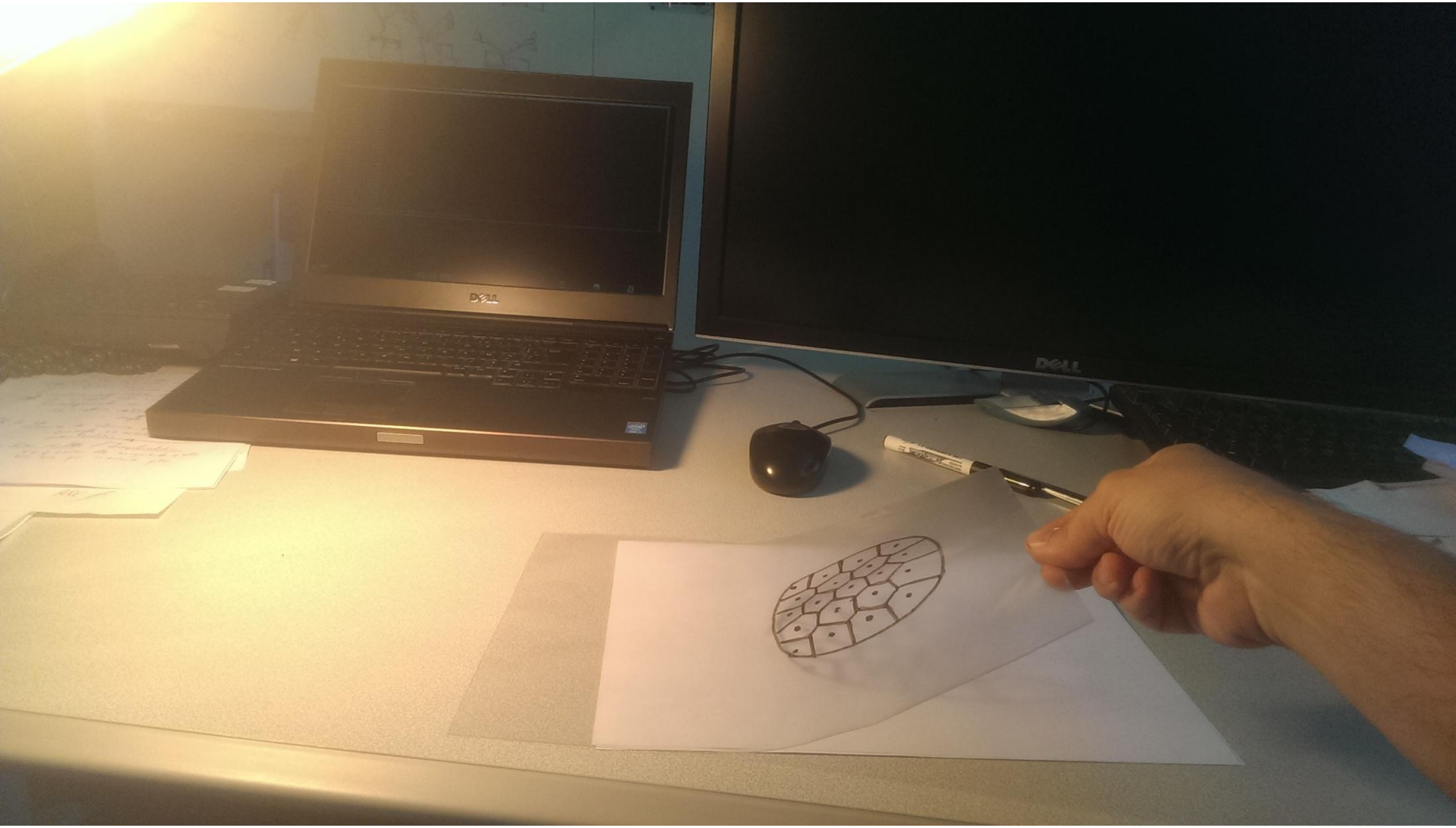

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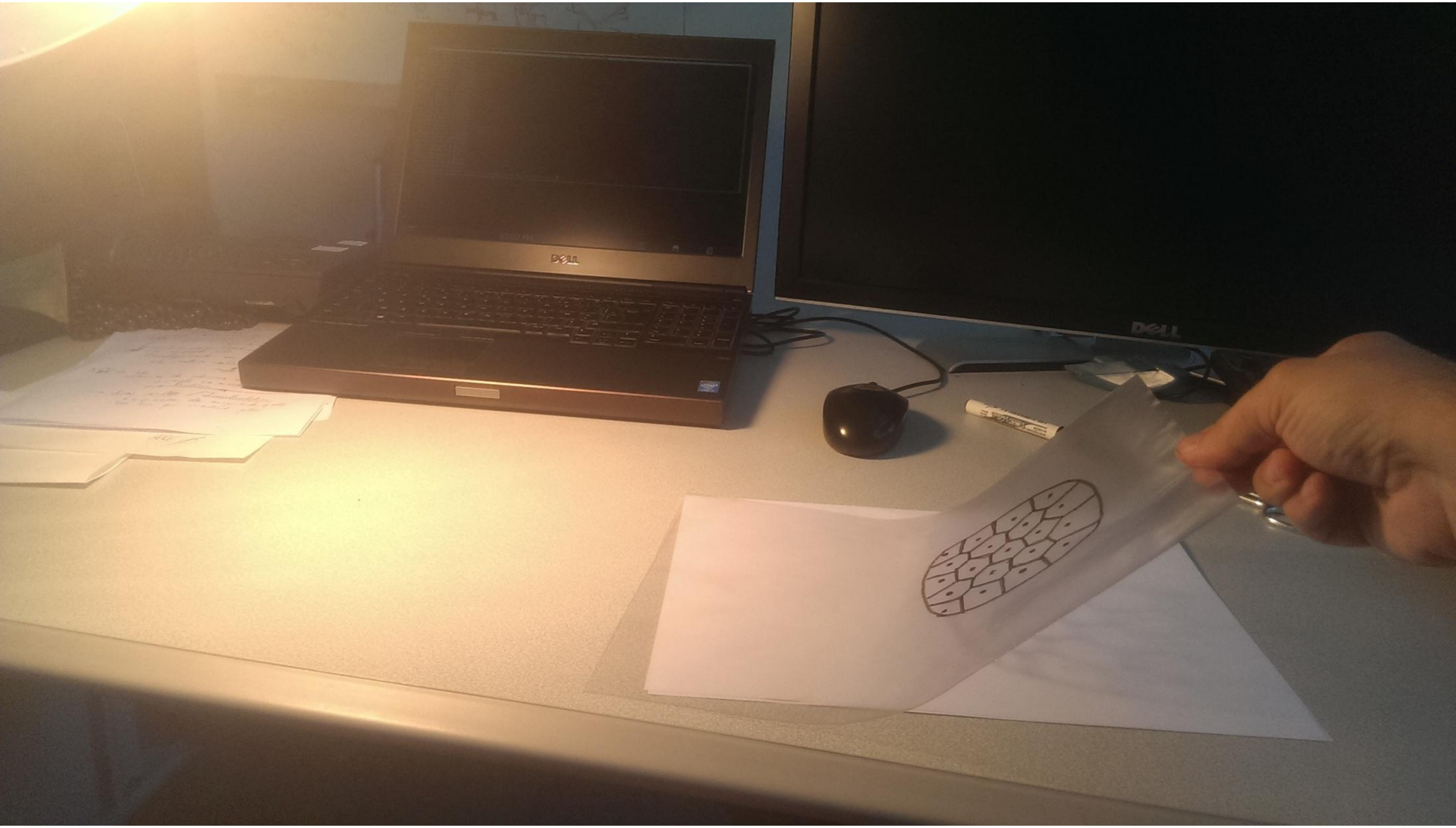

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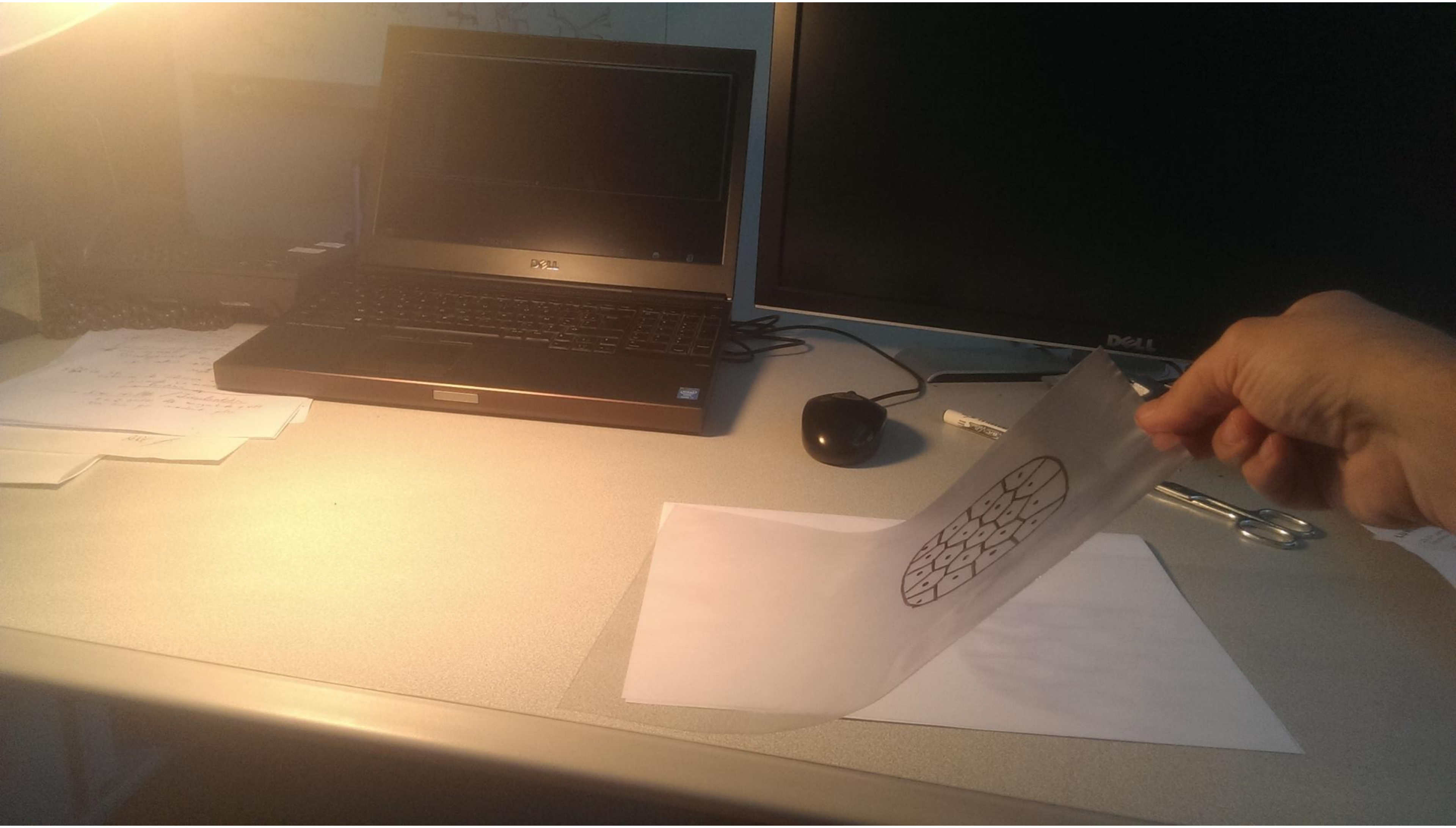

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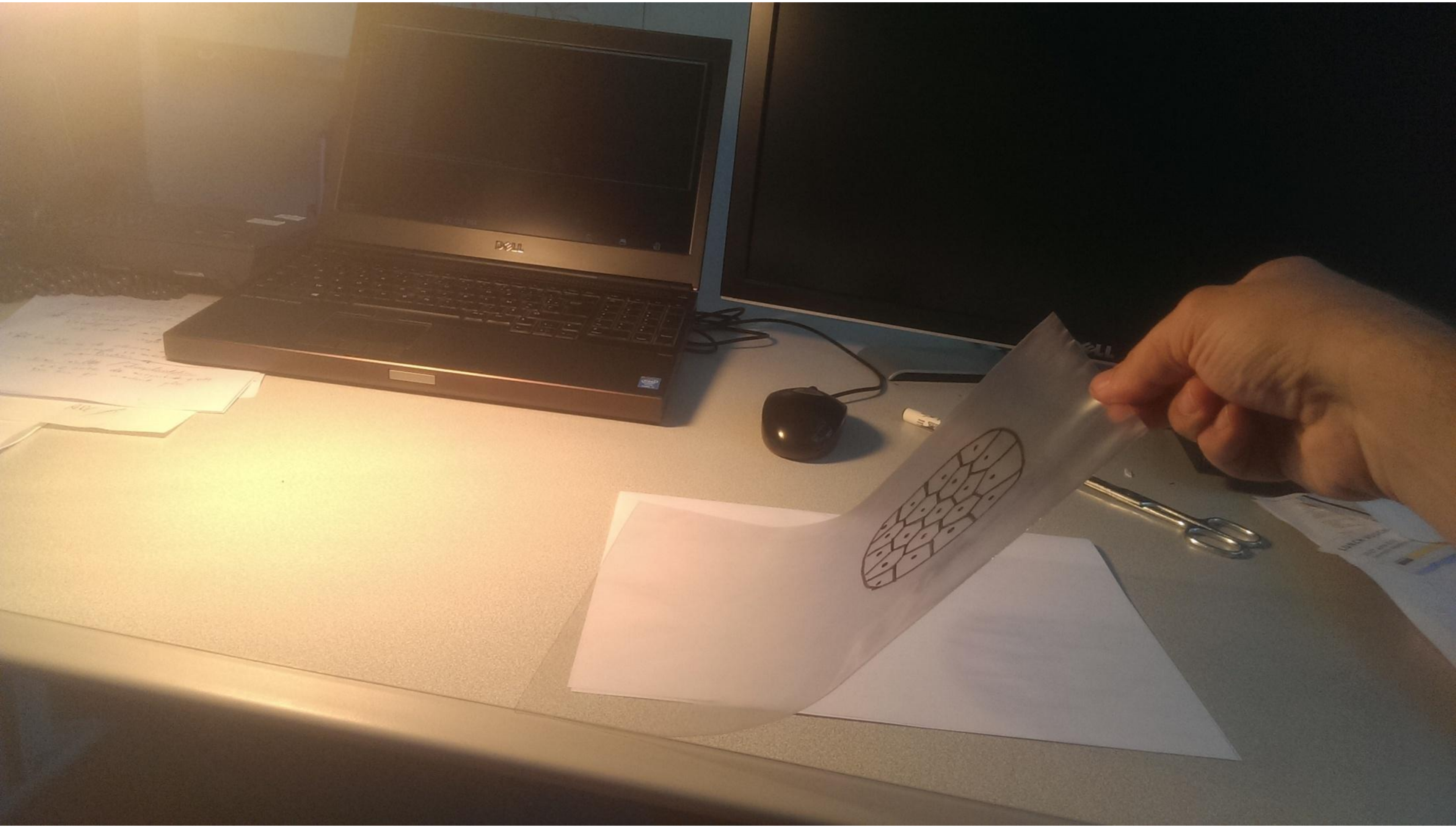

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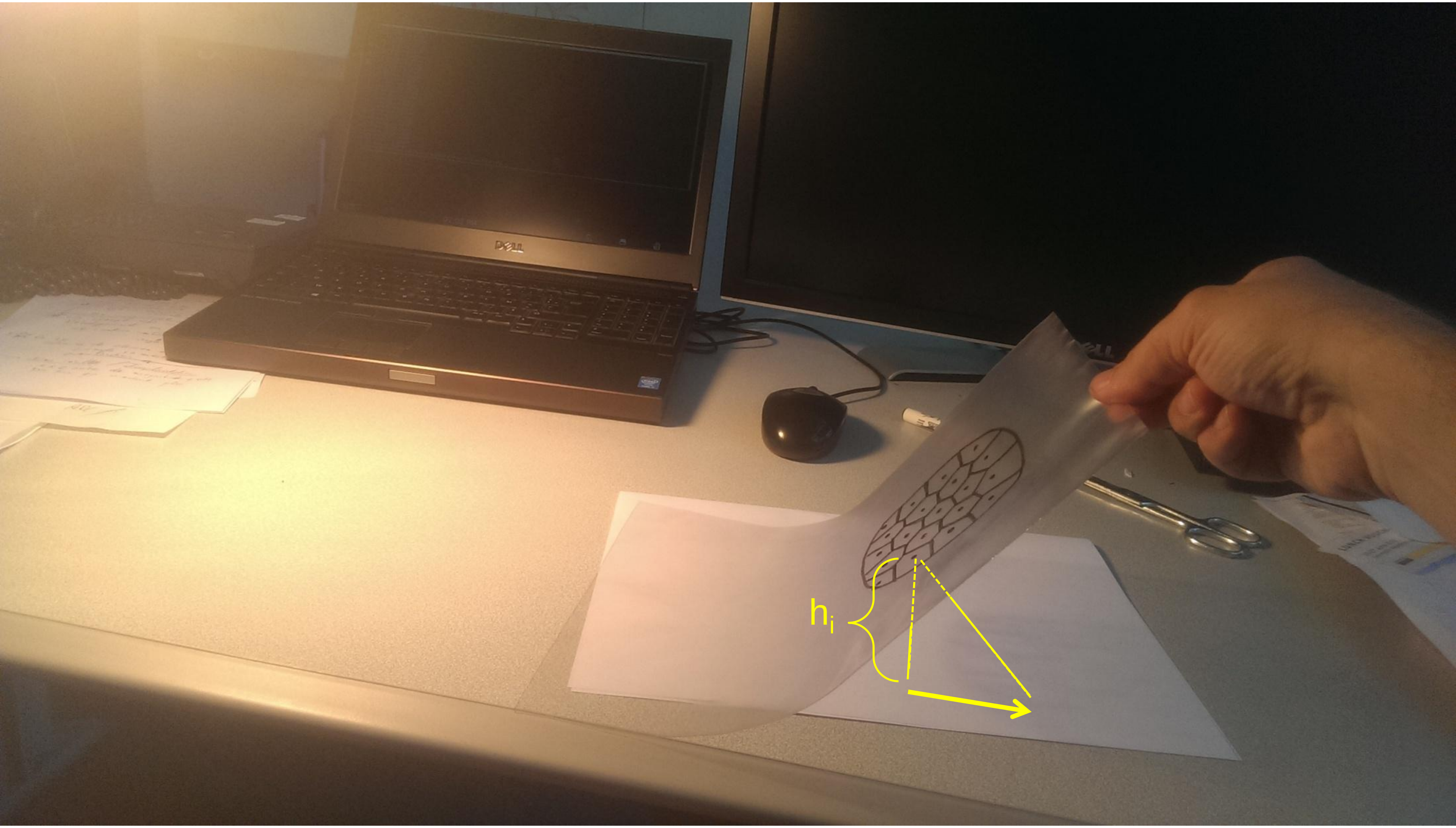
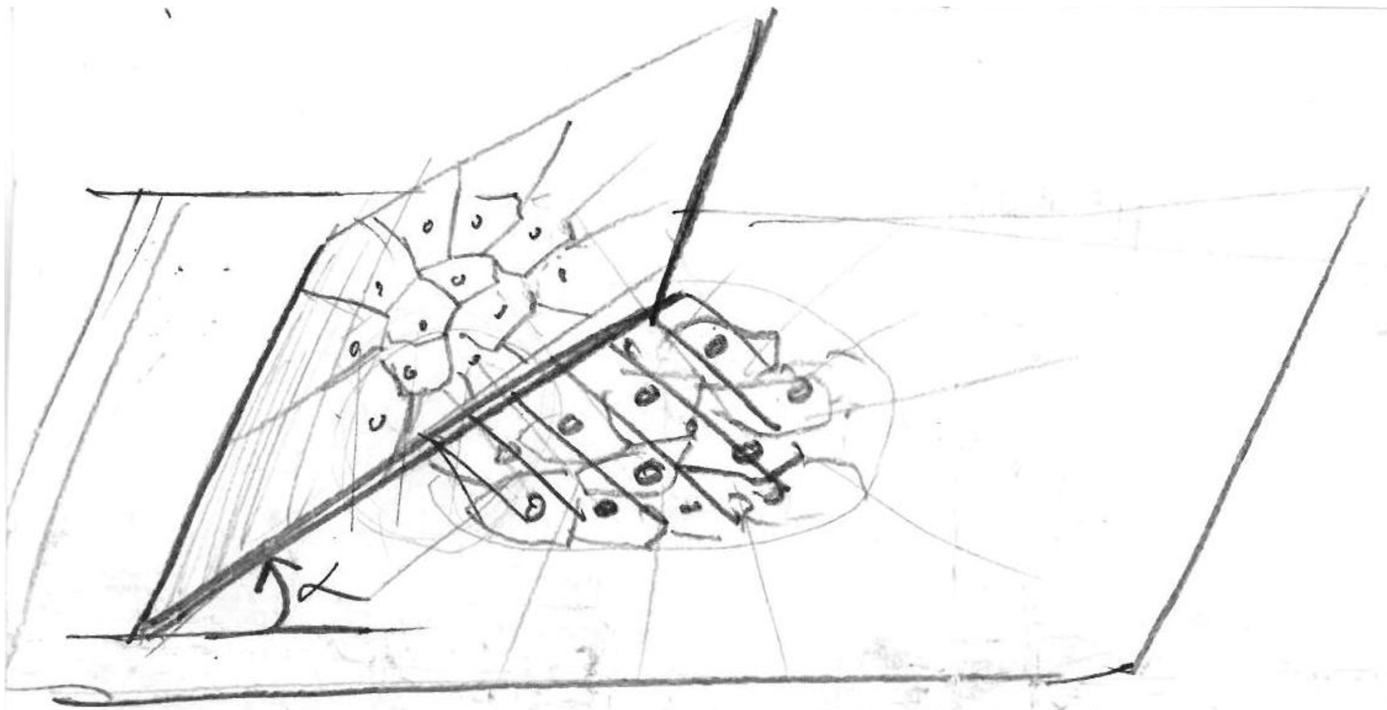


Part. 3 Power Diagrams & Transport

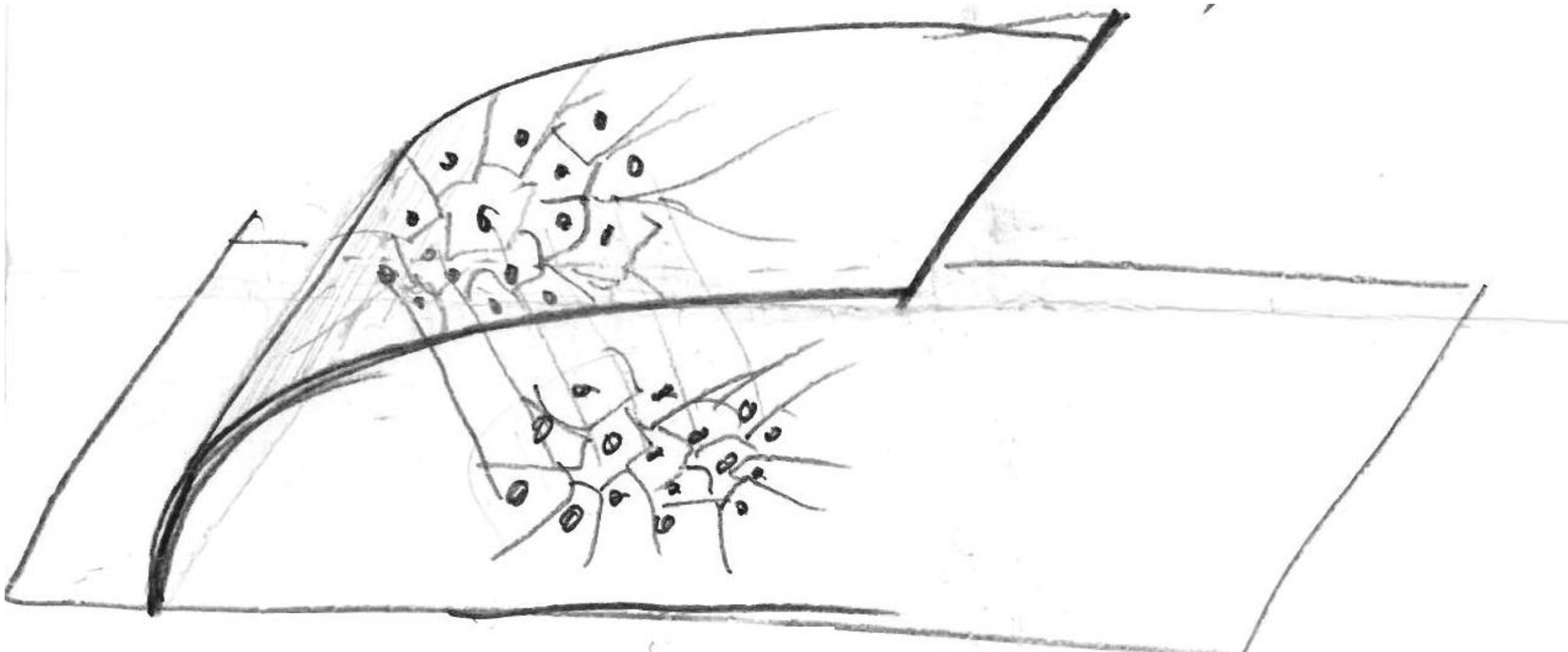


Translating a Voronoi diagram.

1st Try : linear lifting

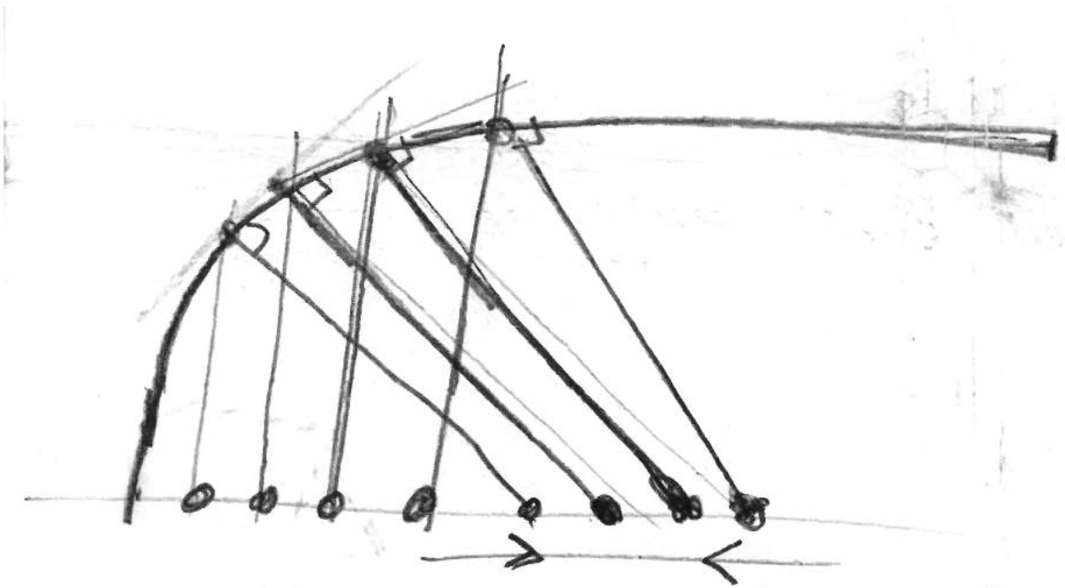
(FAIL : scales by 1/cos(α))

Part. 3 Power Diagrams & Transport



2nd Try : Curved lifting

Part. 3 Power Diagrams & Transport



"converging beams" can compensate the 1/cos(α) expansion by "re-concentrating" the points

Part. 3 Power Diagrams & Transport

$$d^2(p_i, q) \begin{array}{l} + h_i^2 \\ - w_i \end{array} < d^2(p_j, q) \begin{array}{l} + h_i^2 \\ - w_j \end{array} \quad \forall j$$

$$d^2(p_i, q - T) < d^2(p_j, q - T) \quad \forall j$$

$$(p_i - q + T)^2 < (p_j - q + T)^2 \quad \forall j$$

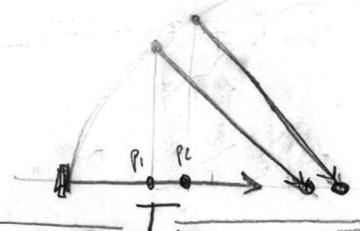
$$d^2(p_i, q) + 2T \cdot (p_i - q) + T^2 < d^2(p_j, q) + 2T(p_j - q) + T^2 \quad \forall j$$

$$d^2(p_i, q) + 2T \cdot p_i < d^2(p_j, q) + 2T \cdot p_j$$

$$\begin{array}{l} h_i^2 \\ w_i \end{array} \Big| = -2T \cdot p_i + cte$$

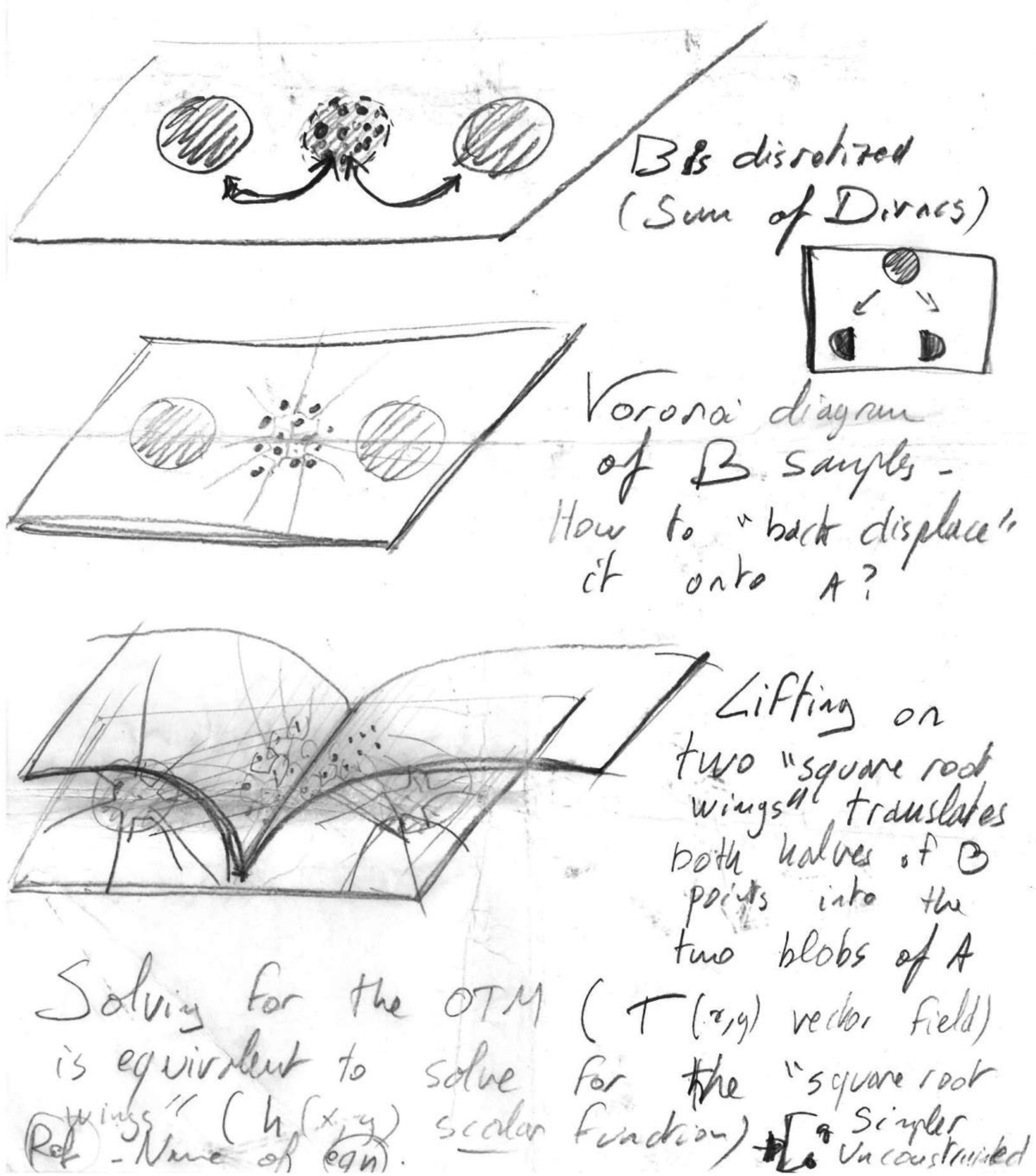
$$h_i^2 = (2T \cdot p_i + Cte)$$

$$h_i = \sqrt{2T \cdot p_i - \min_i (T \cdot p_i)}$$



Translation d'un diagramme de Voronoï sectionnel - Relèvement en racine carrée -

Part. 3 Power Diagrams and Transport



Part. 3 Optimal Transport – 2D examples

Numerical Experiment: *A disk becomes two disks*

4

Optimal Transport

applications in computational physics

Part. 4 Optimal Transport – 3D examples

Numerical Experiment: *A sphere becomes two spheres*

Part. 4 Optimal Transport – 3D examples

Numerical Experiment: *Armadillo to sphere*

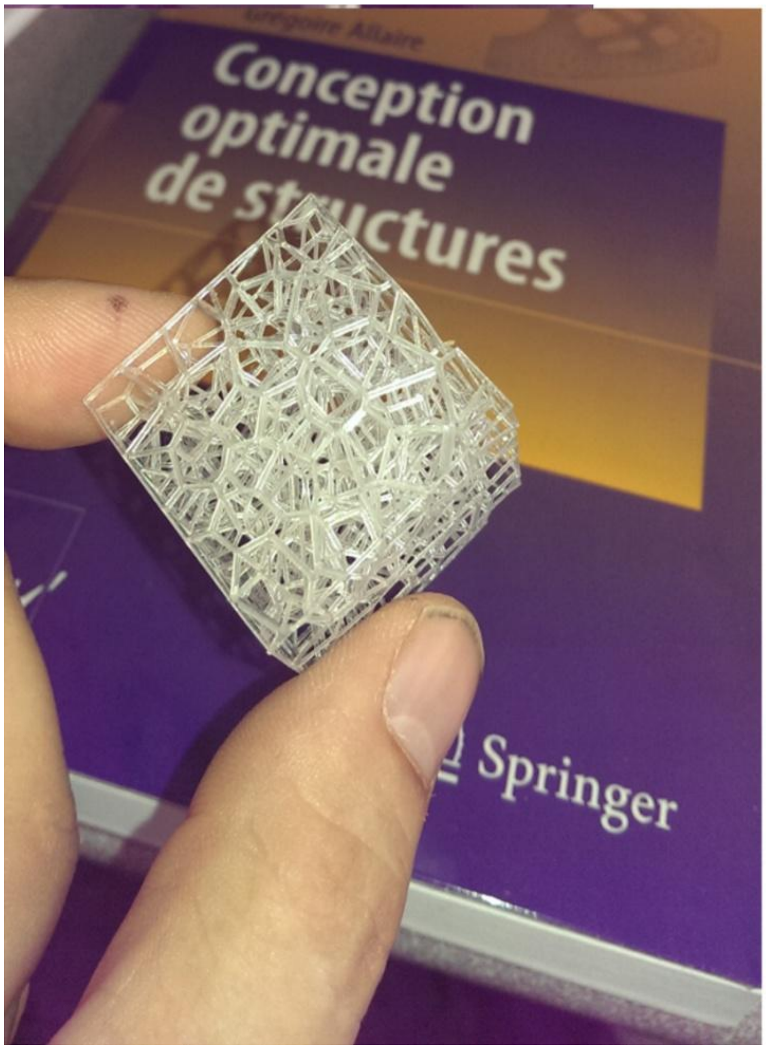
Part. 4 Optimal Transport – 3D examples

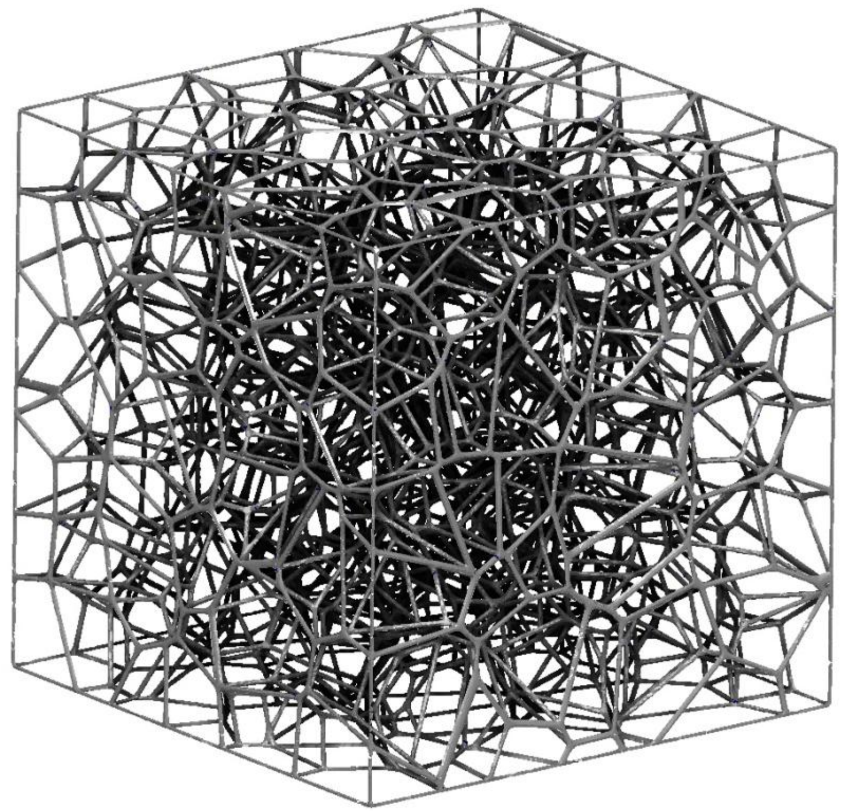
Numerical Experiment: *Other examples*

Computing singularity set…

Part. 4 Optimal Transport – 3D examples

Numerical Experiment: *Other examples*





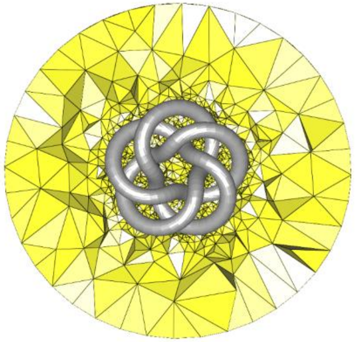
Inria

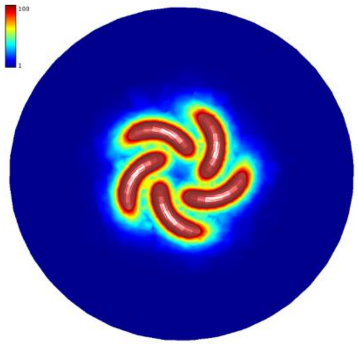
Part. 4 Optimal Transport – 3D examples

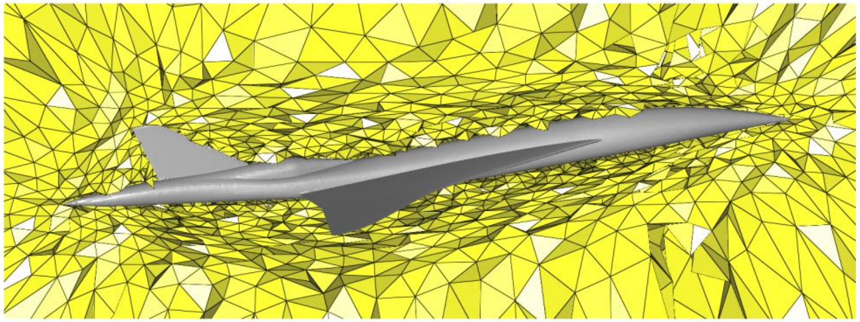
Numerical Experiment: *Varying density*

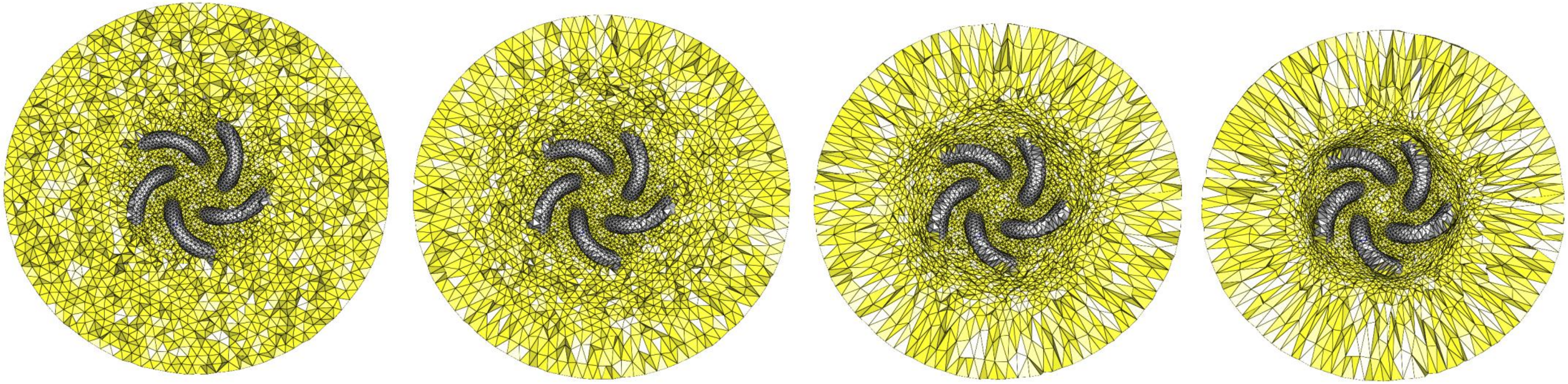
Part. 4 Optimal Transport – 3D examples

Numerical Experiment: *Varying density*

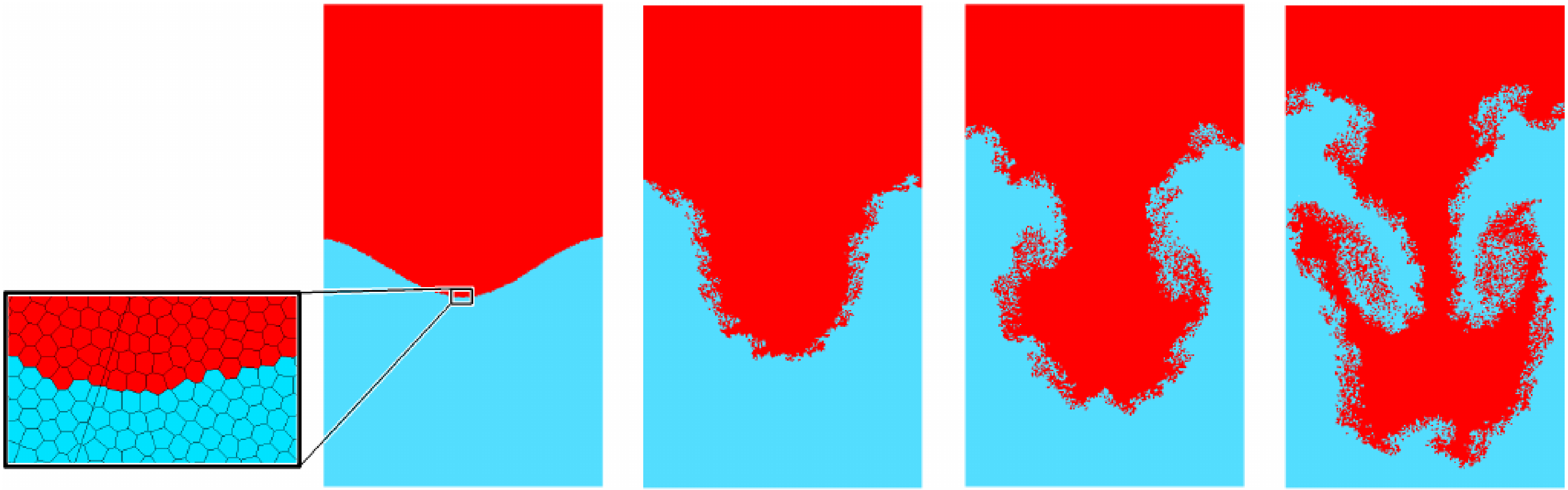








Part. 4 Optimal Transport – Fluids



Le schéma [Mérigot-Gallouet]
Applications en graphisme: [De Goes et.al] (power particles)

Part. 4 Optimal Transport – Fluids

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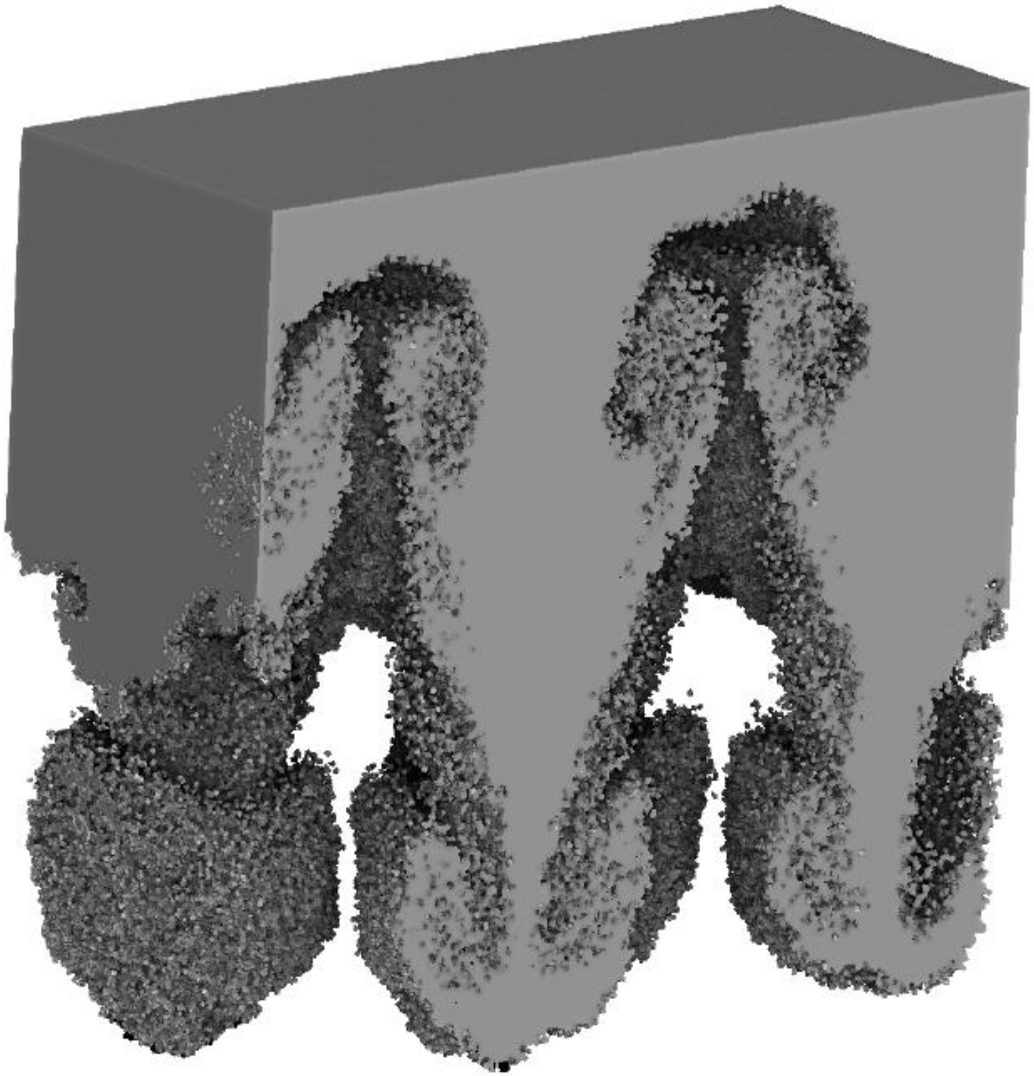
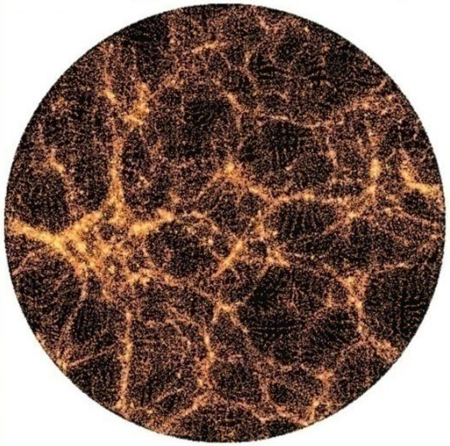


Part. 4 Optimal Transport – Fluids

Part. 4 Optimal Transport – 3D examples

Numerical Experiment: *Performances*



2002: several hours of supercomputer time were needed for computing OT with a few thousand Dirac masses, with a com algorithm in $O(n^2 \log(n))$

Part. 4 Optimal Transport – 3D examples
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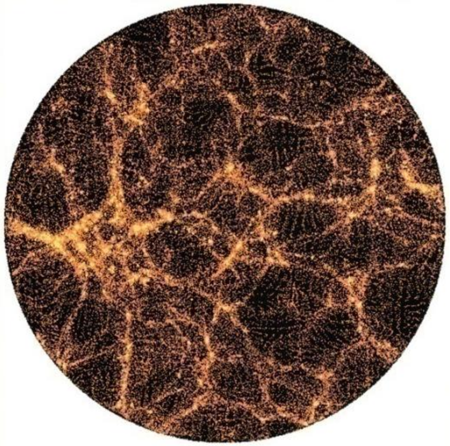

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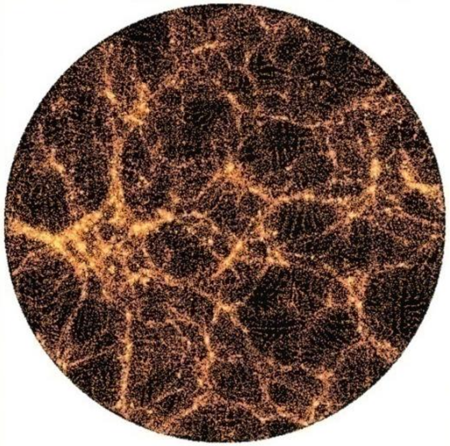
nb masses	1000	2000	5000	10000	30000	50000	10^5	3×10^5	5×10^5	10^6
time (s)	1.45	3.2	7.3	17.3	55	154	187	671	1262	2649

TABLE 4. Statistics for the Armadillo → sphere optimal transport with varying number of masses (see third row of Figure 12). Timings are given in seconds. The multi-level algorithm with BRIO pre-ordering and degree 2 regressions is used.

3D version of [Mérigot] (multilevel + BFGS) + several tricks [**L** 2015]

Part. 4 Optimal Transport – 3D examples

Numerical Experiment: *Performances*



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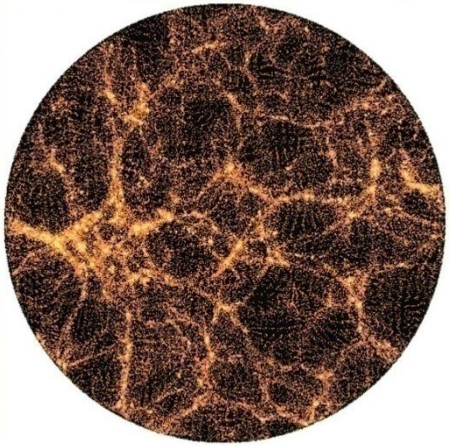

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2016: Damped Newton [Mérigot, Thibert] + several tricks for 3D:
1 million Dirac masses in 240 seconds

Part. 4 Optimal Transport – 3D examples

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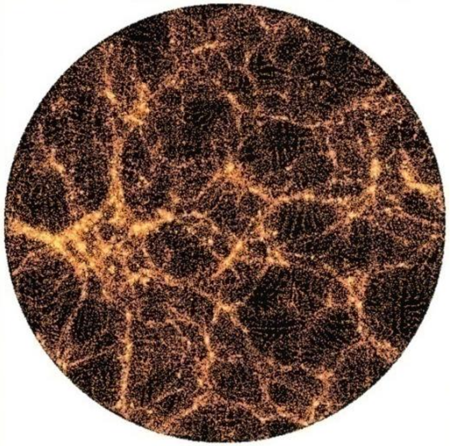

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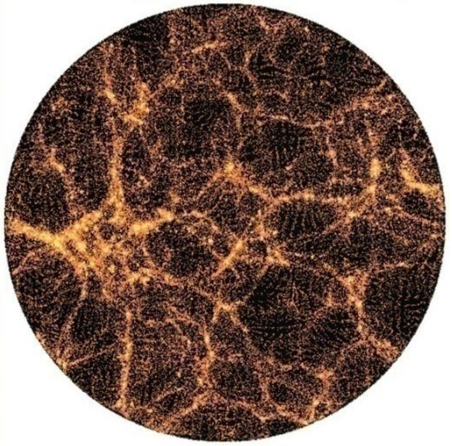
2016: Damped Newton [Mérigot, Thibert] + several tricks for 3D:

1 million Dirac masses in 240 seconds

10 million Dirac masses in 90 minutes

Part. 4 Optimal Transport – 3D examples

Numerical Experiment: *Performances*



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Semi-discrete OT is now scalable ! (new tool in Num. Ana. Toolbox)

Conclusions – Open questions

* **Connections with physics, Legendre transform and entropy ?**

[Cuturi & Peyré] – regularized discrete optimal transport – why does it work ?

Hint 1: Minimum action principle subject to conservation laws

Hint 2: Entropy = dual of temperature ; Legendre = Fourier[(+,*) → (Max,+)]…

*** More continuous numerical algorithms ?**

[Benamou & Brenier] fluid dynamics point of view – very elegant, but 4D problem !!

FEM-type adaptive discretization of the subdifferential (graph of T) ?

*** Can we characterize OT in other semi-discrete settings ?**

measures supported on unions of spheres

piecewise linear densities

*** Connections with computational geometry ?**

Singularity set **[Figalli]** = set of points where T is discontinuous

Looks like a “mutual power diagram”, anisotropic Voronoi diagrams

Conclusions - References

A Multiscale Approach to Optimal Transport,
Quentin Mérigot, Computer Graphics Forum, 2011

Variational Principles for Minkowski Type Problems, Discrete Optimal Transport, and Discrete Monge-Ampere Equations
Xianfeng Gu, Feng Luo, Jian Sun, S.-T. Yau, ArXiv 2013

Minkowski-type theorems and least-squares clustering
AHA! (Aurenhammer, Hoffmann, and Aronov), SIAM J. on math. ana. 1998

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Optimal Transport Old and New, 2008
Cédric Villani

Conclusions - References

Polar factorization and monotone rearrangement of vector-valued functions
Yann Brenier, Comm. On Pure and Applied Mathematics, June 1991

A computational fluid mechanics solution of the Monge-Kantorovich mass transfer problem, **J.-D. Benamou, Y. Brenier**, Numer. Math. 84 (2000), pp. 375-393

Pogorelov, Alexandrov – Gradient maps, Minkovsky problem (older than AHA paper, some overlap, in slightly different context, formalism used by Gu & Yau)

Rockafeller – Convex optimization – Theorem to switch inf(sup()) – sup(inf()) with convex functions (used to justify Kantorovich duality)

Filippo Santambrogio – Optimal Transport for Applied Mathematician, Calculus of Variations, PDEs and Modeling – Jan 15, 2015

Gabriel Peyré, Marco Cuturi, Computational Optimal Transport, 2018

Online resources

All the sourcecode/documentation available from:
http://alice.loria.fr/software/geogram
Demo: www.loria.fr/~levy/GLUP/vorpaview

* **L.**, A numerical algorithm for semi-discrete L2 OT in 3D, ESAIM Math. Modeling and Analysis, 2015

* **L.** and E. Schwindt, Notions of OT and how to implement them on a computer, Computer and Graphics, 2018.