Symposium on Geometry Processing – Paris – 2018

Course on Numerical Optimal Transport – Bruno Lévy

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

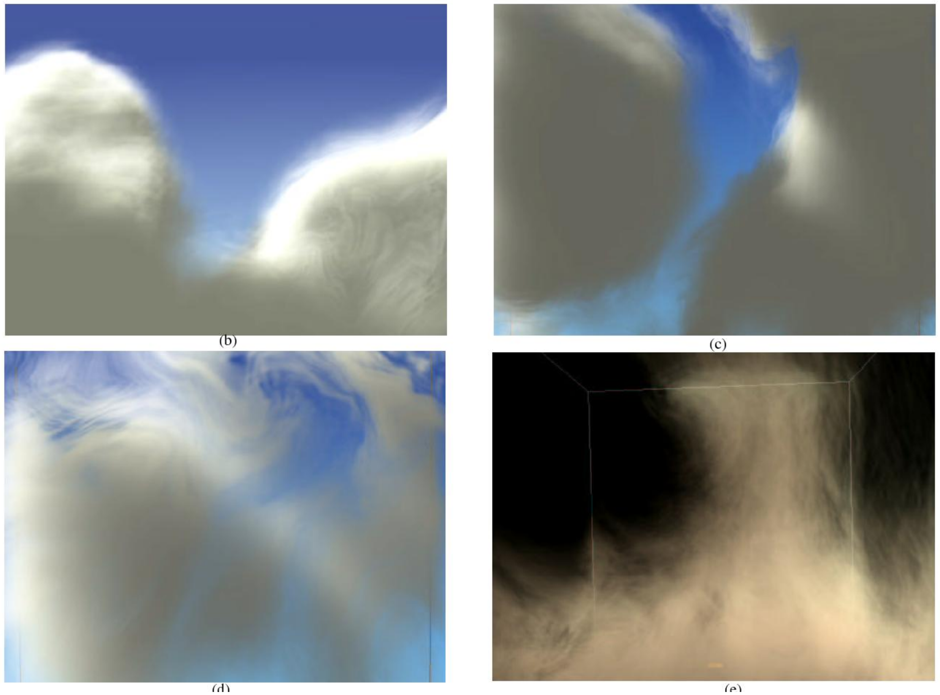
Goal #1: “**Understanding**”

Goal #1: "**Understanding**"

What I can't create
I don't understand

Richard Feynman

Goal #1: “**Understanding**”



Jos Stam,
Stable Fluids, 1999
The art of fluid sim.

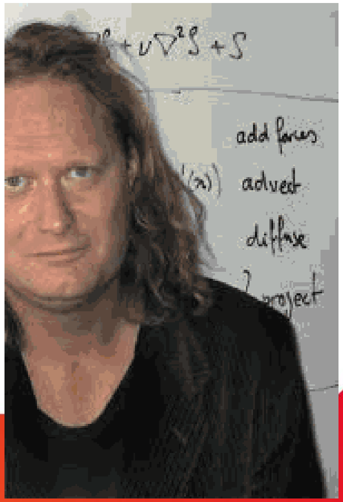
Understand fluids
Explain
Program

Goal #1: "**Understanding**"

I have no formal background in fluid dynamics. I am not an engineer nor do I have a specialized degree in the mathematics or physics of fluids. I am fortunate that I did not have to carry that baggage around. On the other hand, I *do* have degrees in pure mathematics and computer science and have an artsy background. More importantly, I have written computer code that animates fluids.*

I wrote code. That is the bottom line.

I wrote code



Goal #1: “**Understanding**”

Your mission statement:

1. Understand the stuff

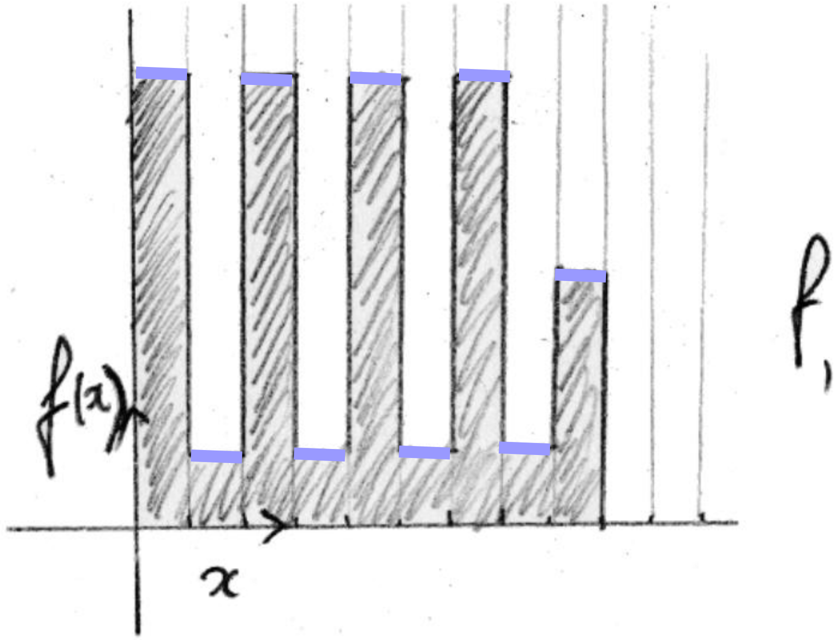
2. Explain it **in simple terms**

   Be a good teacher, to others and to yourself
   Know what you know and what you don’t know
   Try to know what you don’t know

3. Program it

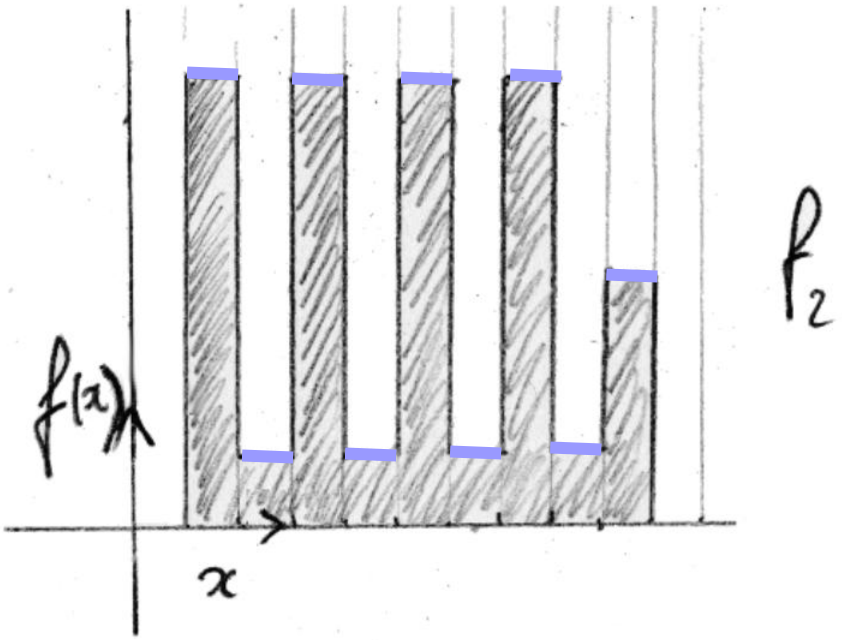
Part. 1 Optimal Transport

Measuring distances between functions



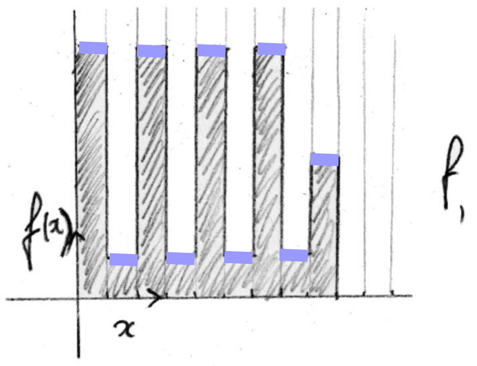
Part. 1 Optimal Transport

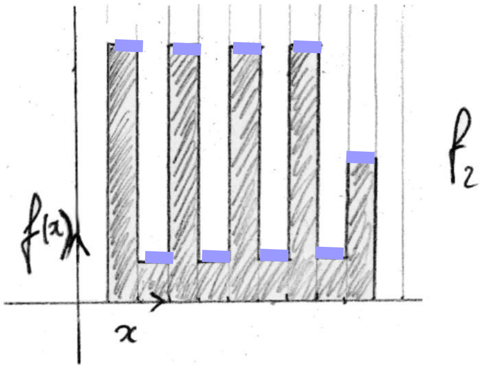
Measuring distances between functions



Part. 1 Optimal Transport

Measuring distances between functions

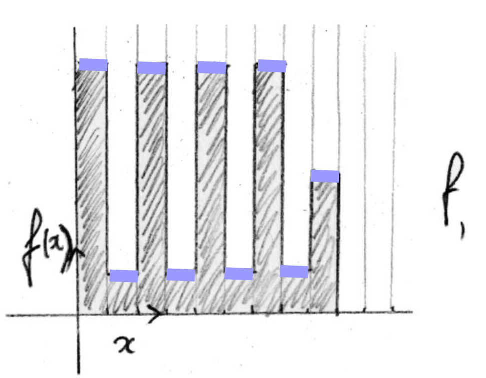


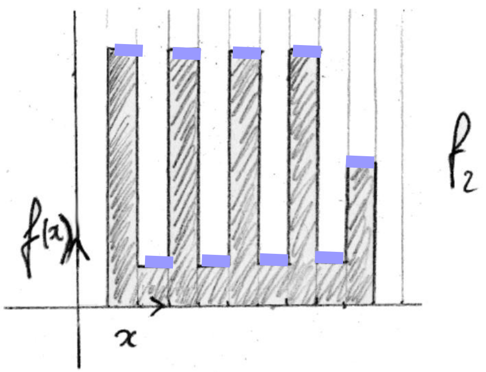


$$d_{L_2}(f_1, f_2) = \int (f_1(x) - f_2(x))^2 \, dx$$

Part. 1 Optimal Transport

Measuring distances between function





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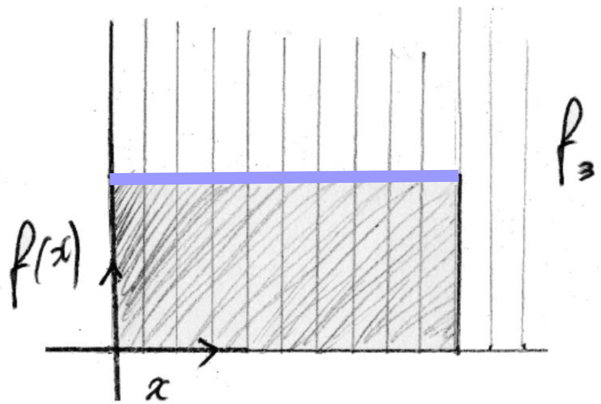
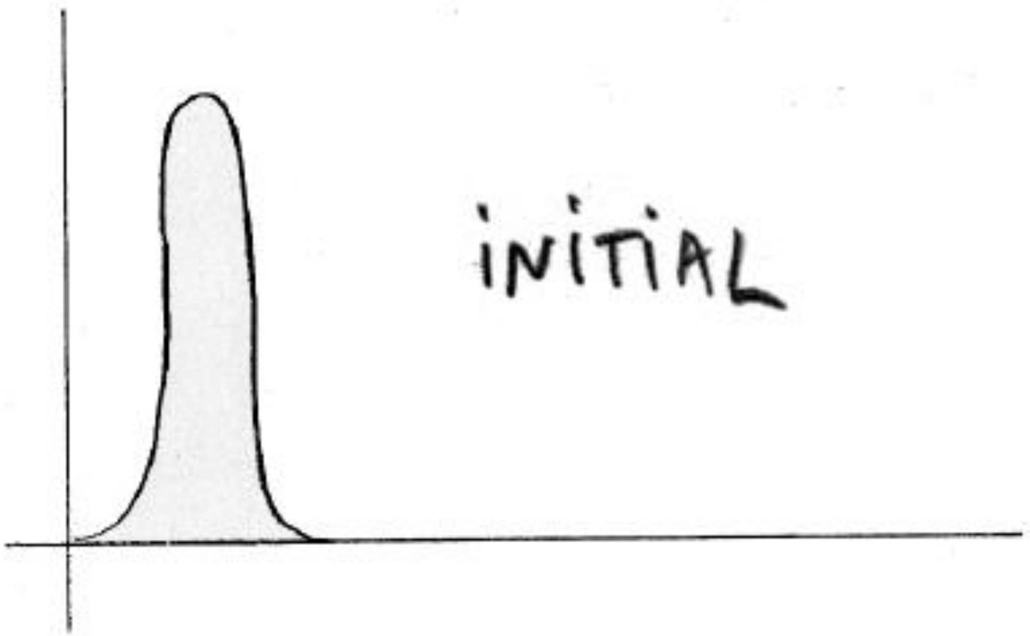


Inria

Part. 1 Optimal Transport
Interpolating functions



Part. 1 Optimal Transport

Interpolating functions

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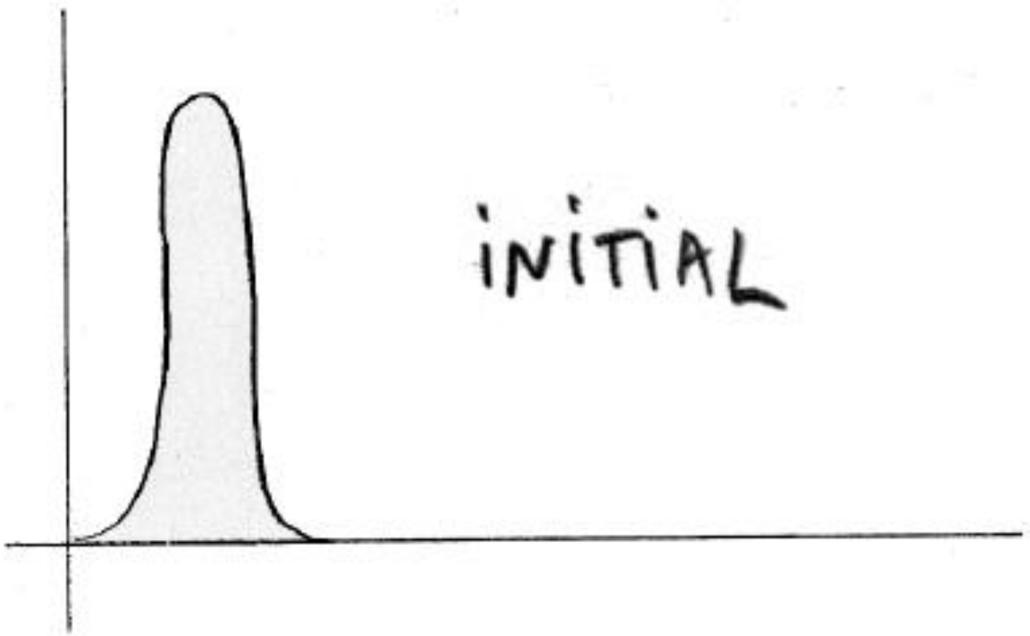
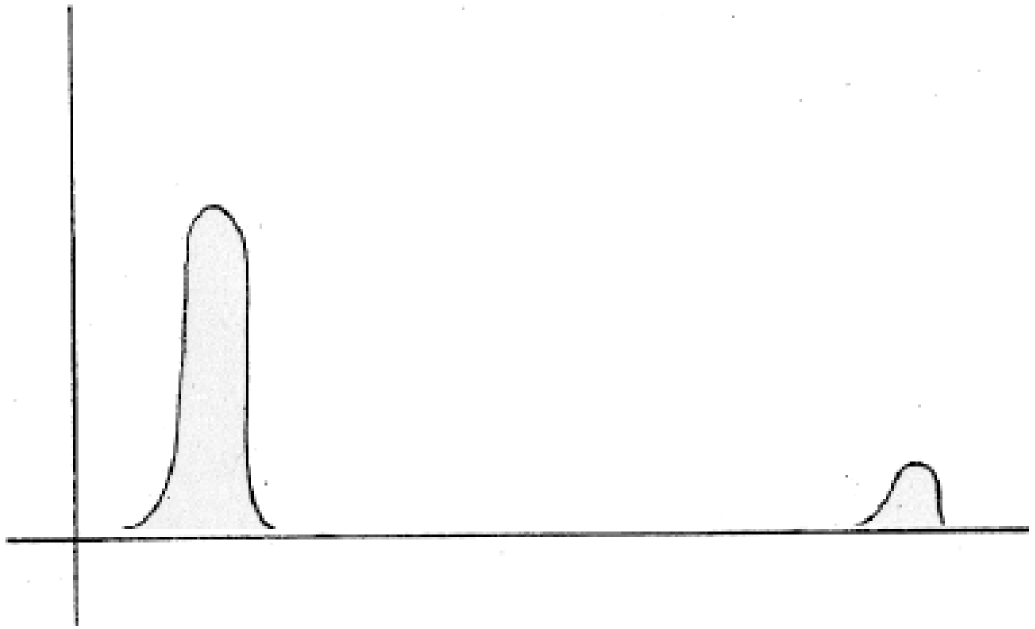


LINEAR INTERPOLATION

Part. 1 Optimal Transport

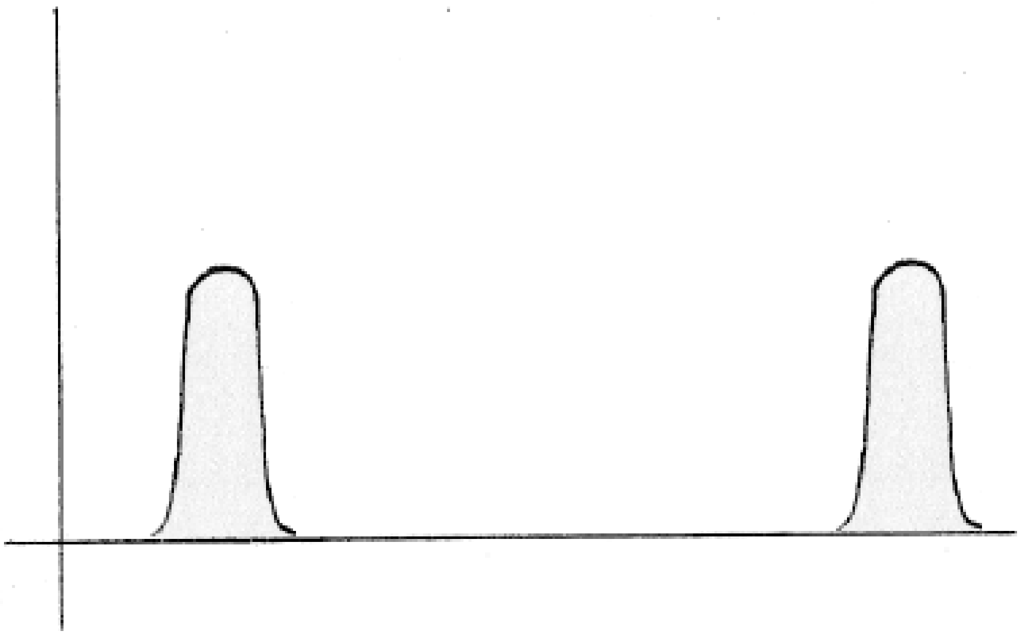
Interpolating functions



LINEAR INTERPOLATION

Part. 1 Optimal Transport

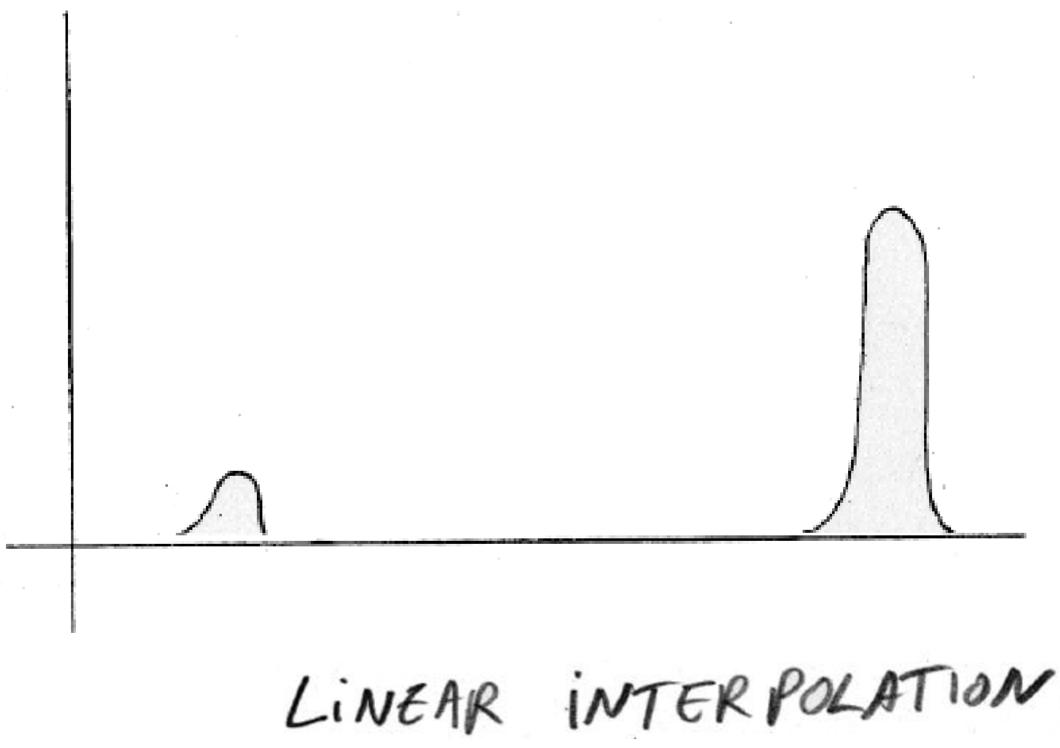
Interpolating functions



LINEAR INTERPOLATION

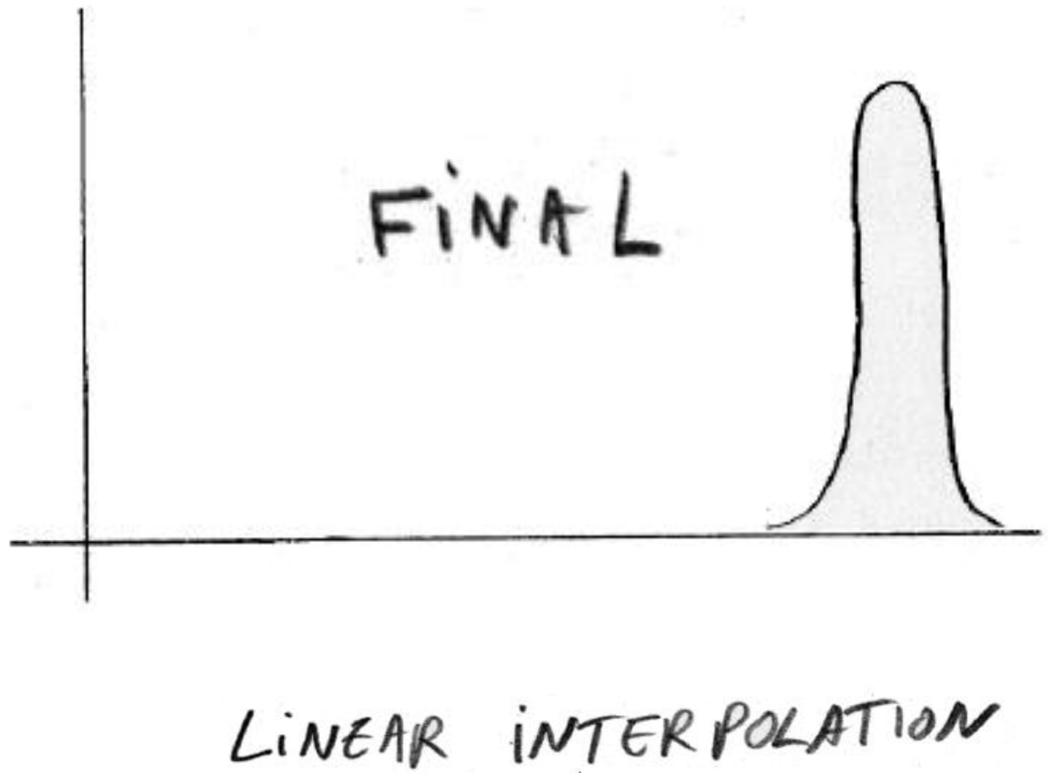
Part. 1 Optimal Transport

Interpolating functions



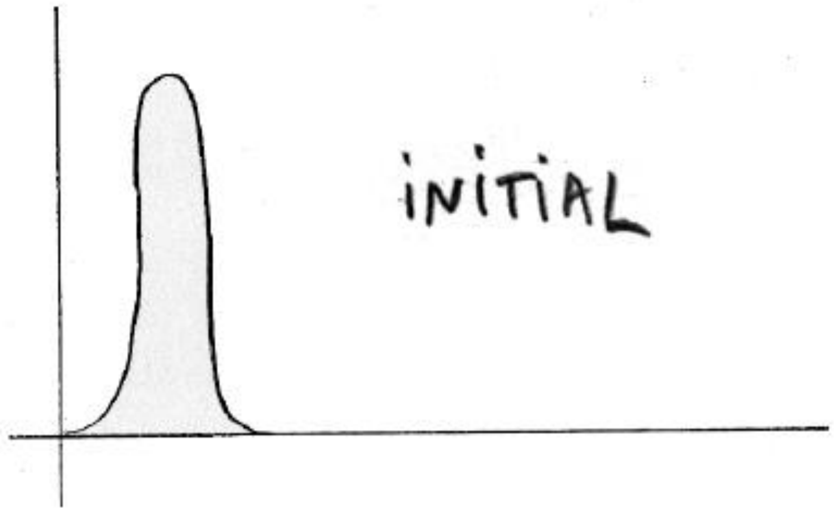
Part. 1 Optimal Transport

Interpolating functions



Part. 1 Optimal Transport

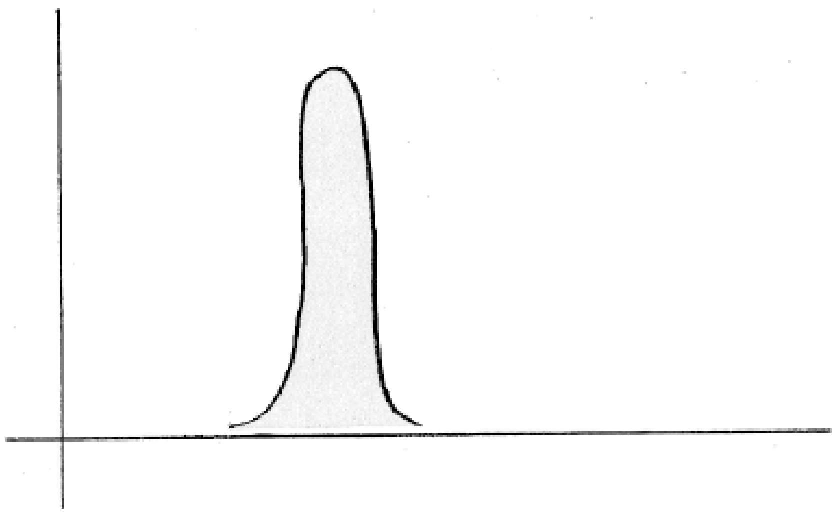
Interpolating functions



DISPLACEMENT INTERPOLATION

Part. 1 Optimal Transport

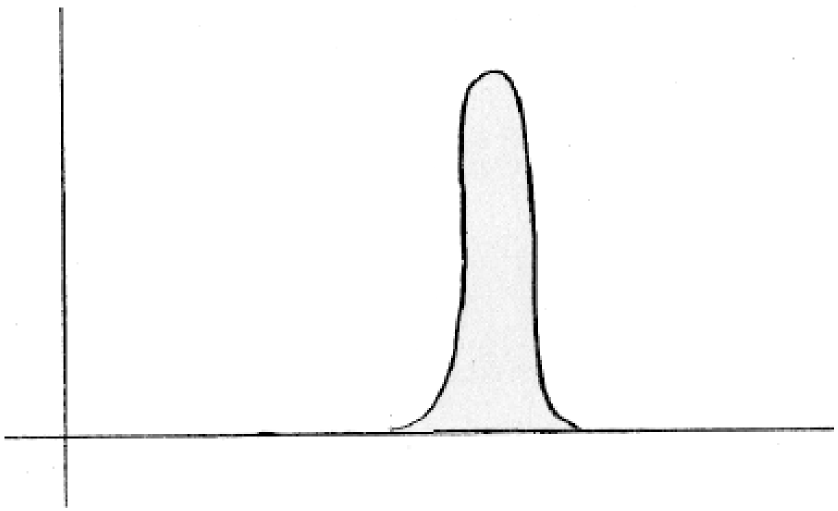
Interpolating functions



DISPLACEMENT INTERPOLATION

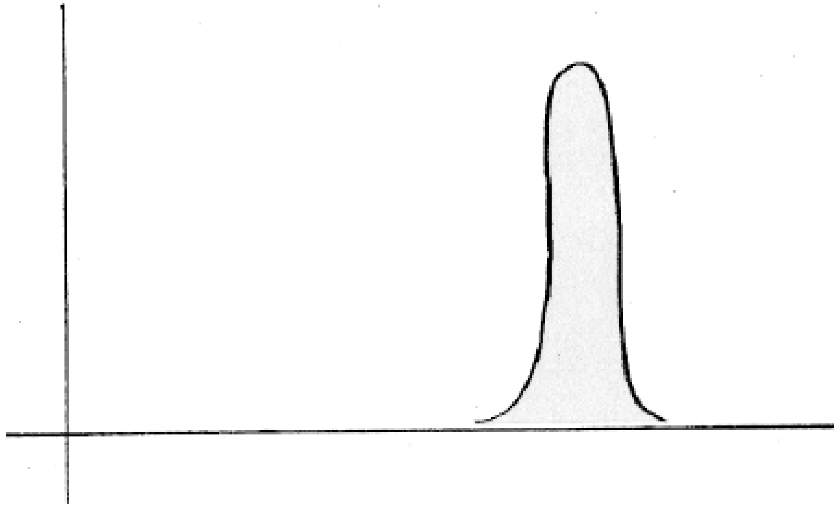
Part. 1 Optimal Transport

Interpolating functions



DISPLACEMENT INTERPOLATION

Part. 1 Optimal Transport
Interpolating functions



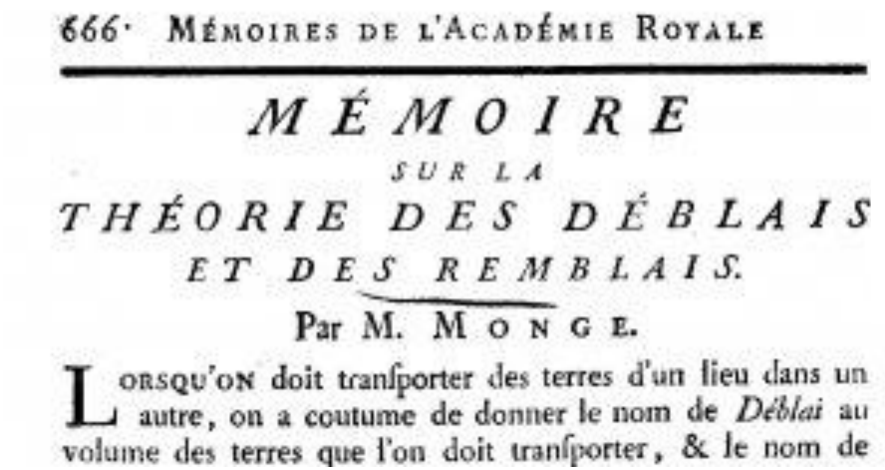
DISPLACEMENT INTERPOLATION

Part. 1 Optimal Transport
Interpolating functions

DISPLACEMENT INTERPOLATION

Part. 1 Optimal Transport

Gaspard Monge - 1784

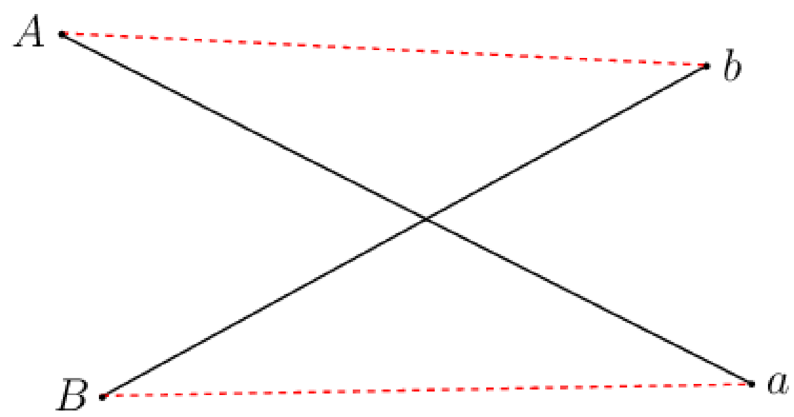


666· MÉMOIRES DE L'ACADÉMIE ROYALE

MÉMOIRE
SUR LA
THÉORIE DES DÉBLAIS
ET DES REMBLAIS.

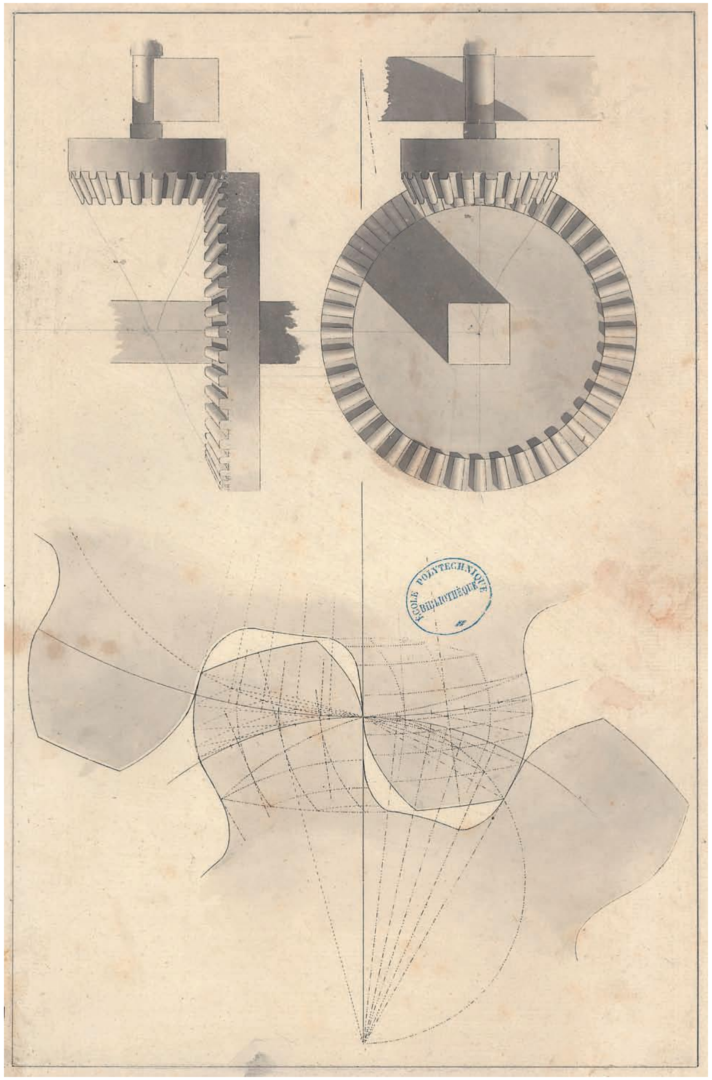
Par M. MONGE.

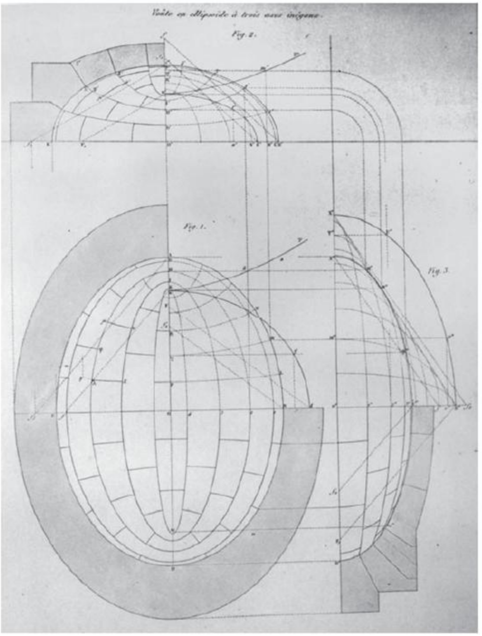
LORSQU'ON doit tranſporter des terres d'un lieu dans un autre, on a coutume de donner le nom de *Déblai* au volume des terres que l'on doit tranſporter, & le nom de



Part. 1 Optimal Transport

Gaspard Monge – geometry and light





Part. 1 Optimal Transport

Monge-Brenier-Villani, the french connection

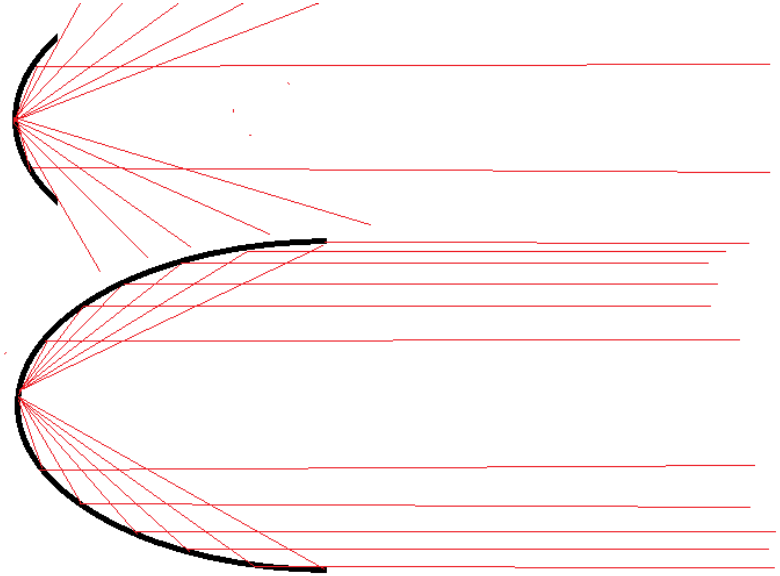
Cédric Villani
Optimal Transport Old & New
Topics on Optimal Transport

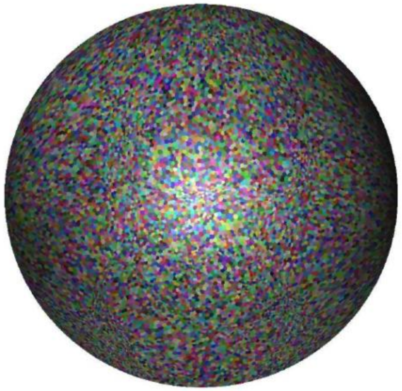
Yann Brenier
The polar factorization theorem
(Brenier Transport)

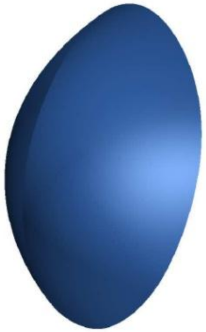
Part. 1 Optimal Transport

Optimal transport
geometry and light

[Caffarelli, Kochengin, and Oliker 1999]

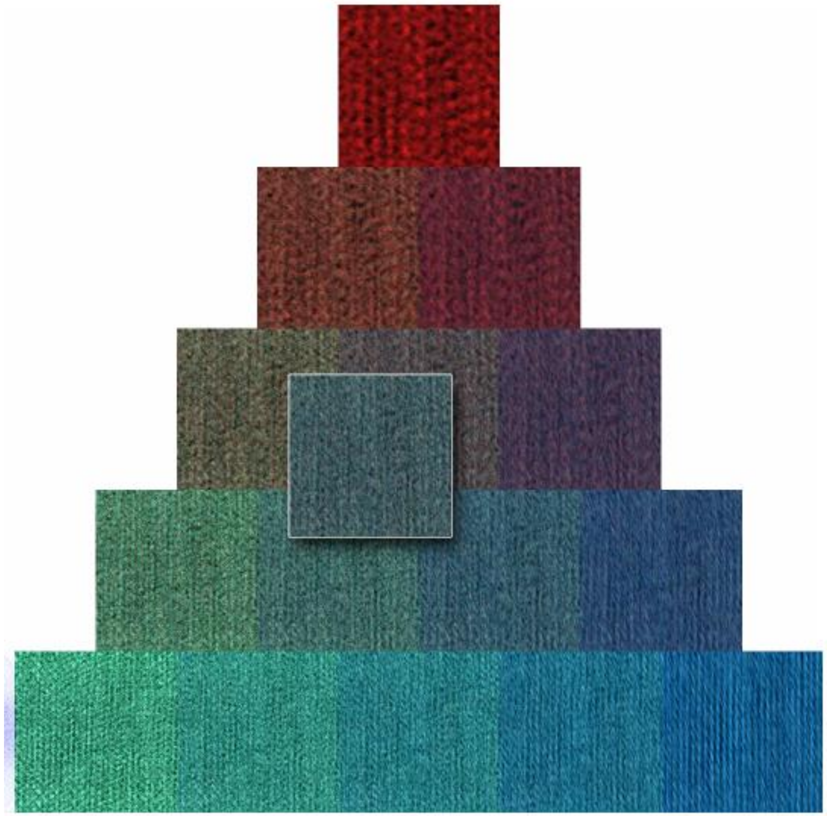






[Castro, Merigot, Thibert 2014]

Part. 1 Optimal Transport – Image Processing



Barycenters / mixing textures

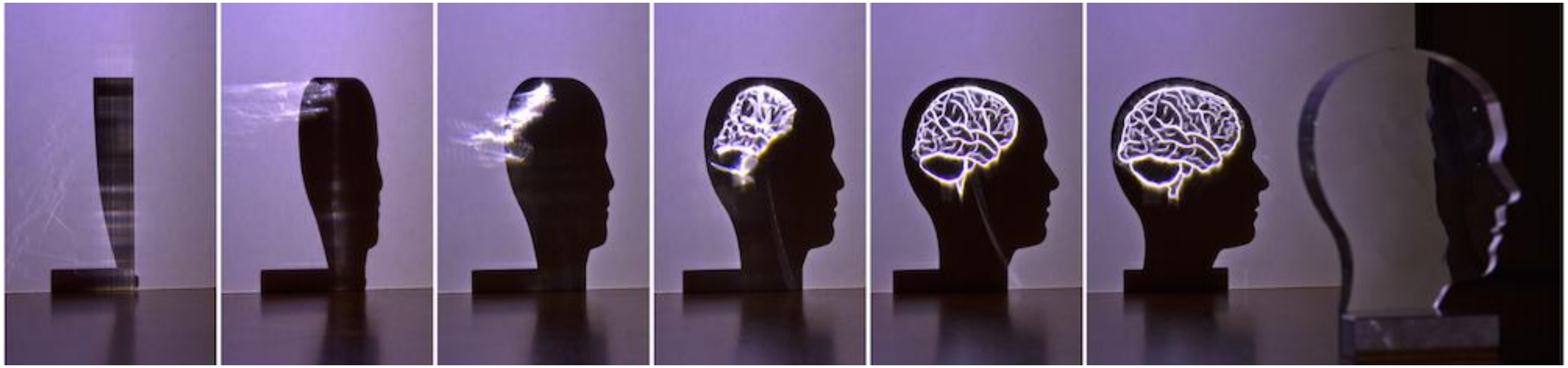
[Nicolas Bonneel, Julien Rabin, Gabriel Peyŕe, Hanspeter Pfister]

Video-style transfer,
A.I., “data sciences”

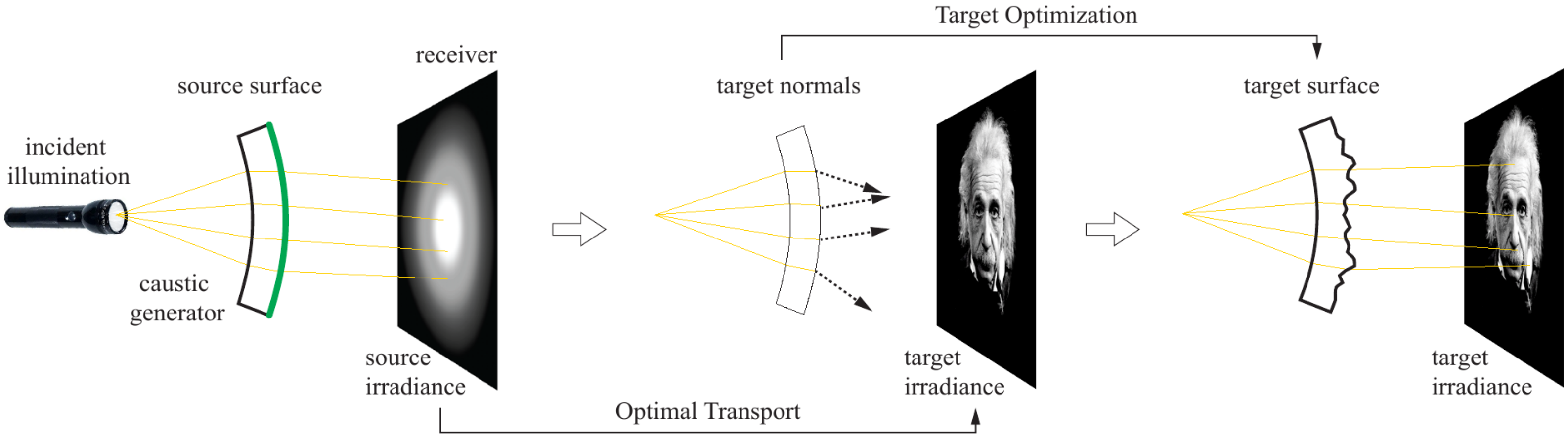
[Nicolas Bonneel, Kalyan Sunkavalli, Sylvain Paris, Hanspeter Pfister]
[Marco Cuturi, Gabriel Peyré]

Part. 1 Optimal Transport

Optimal transport - geometry and light



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

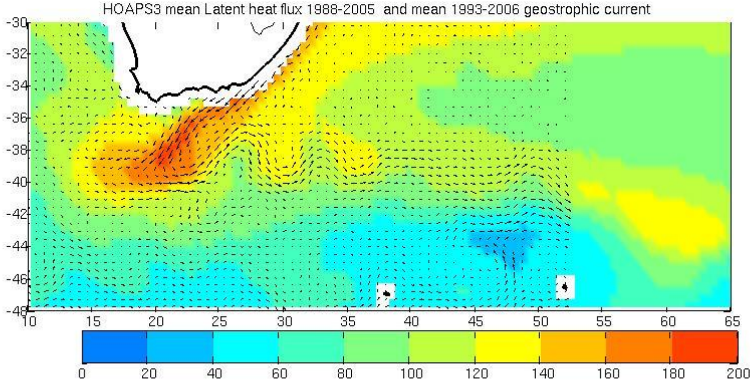


Part. 1. Motivations

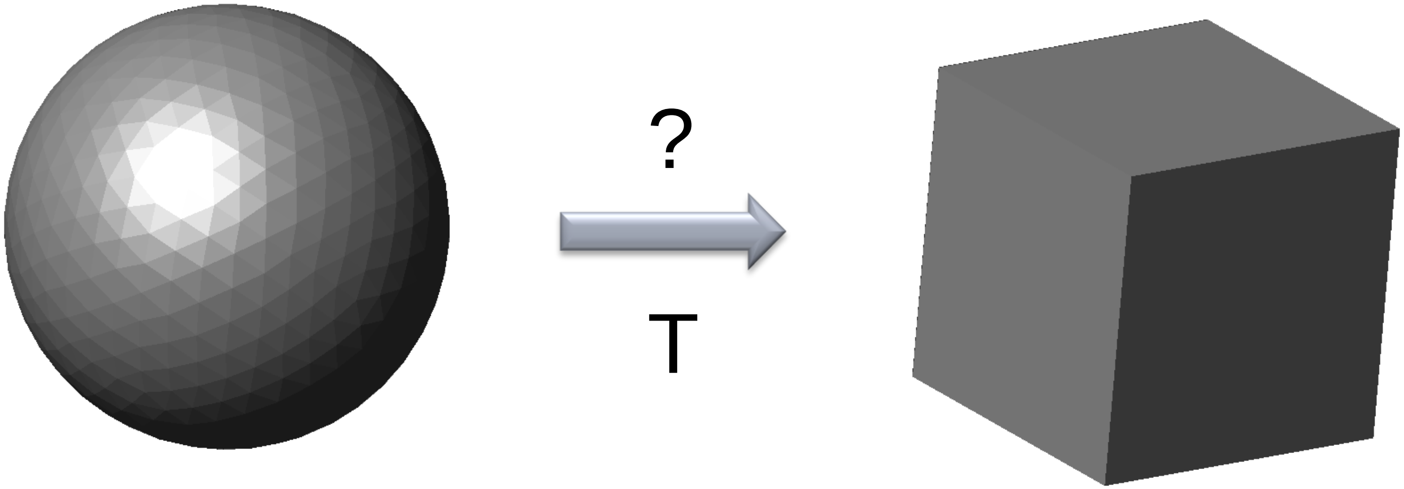
Discretization of functionals involving the Monge-Ampère operator,
Benamou, Carlier, Mérigot, Oudet
arXiv:1408.4536

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

Geostrophic current

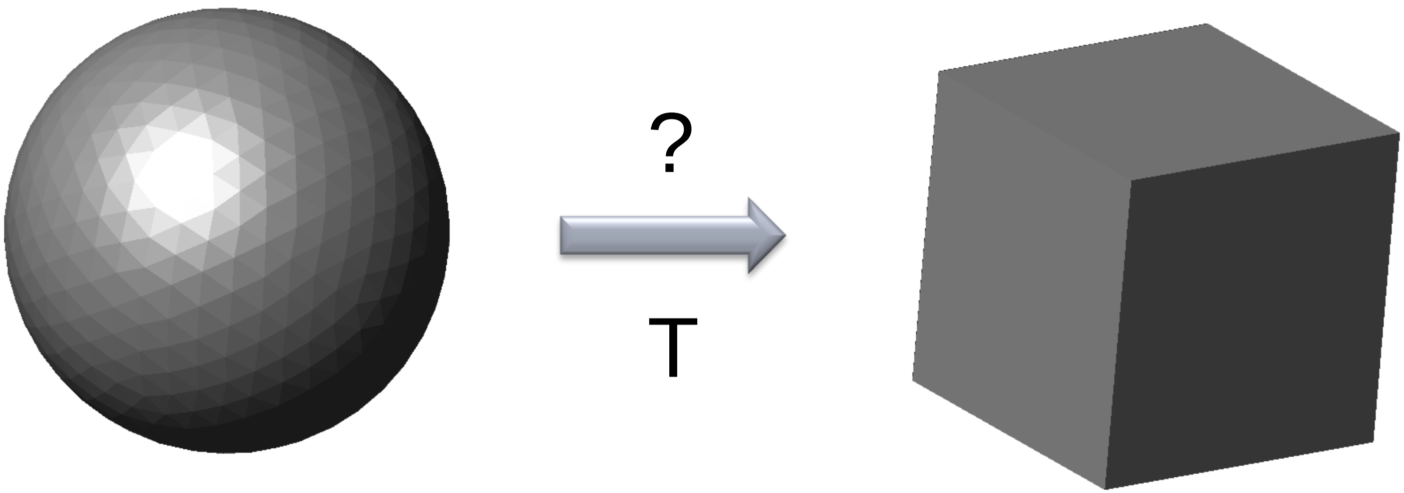


Part. 1 Optimal Transport



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

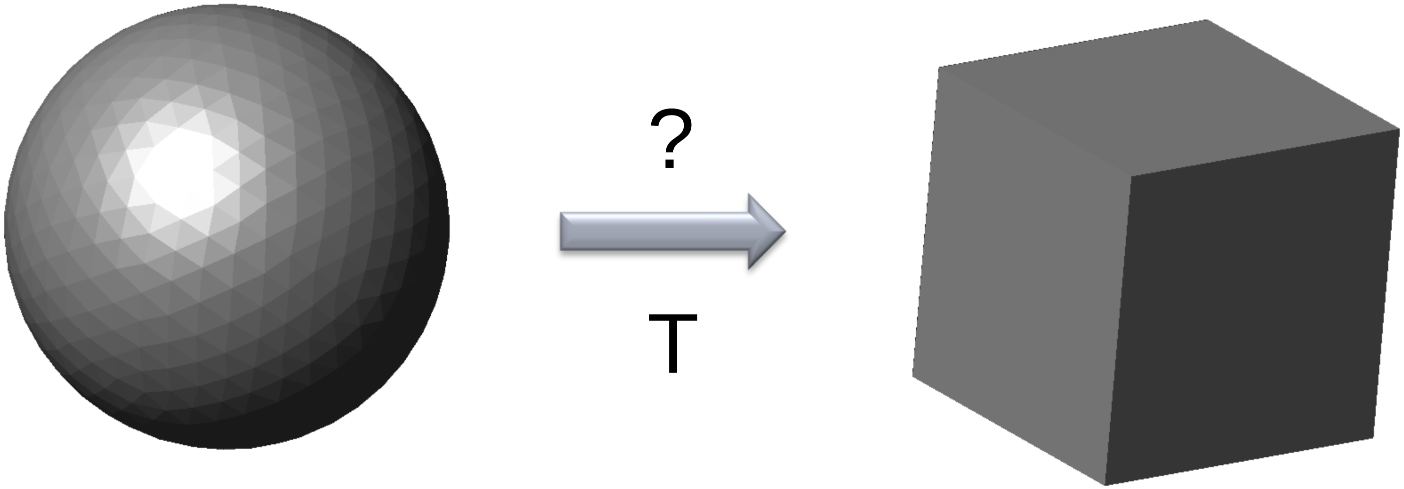
Part. 1 Optimal Transport



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

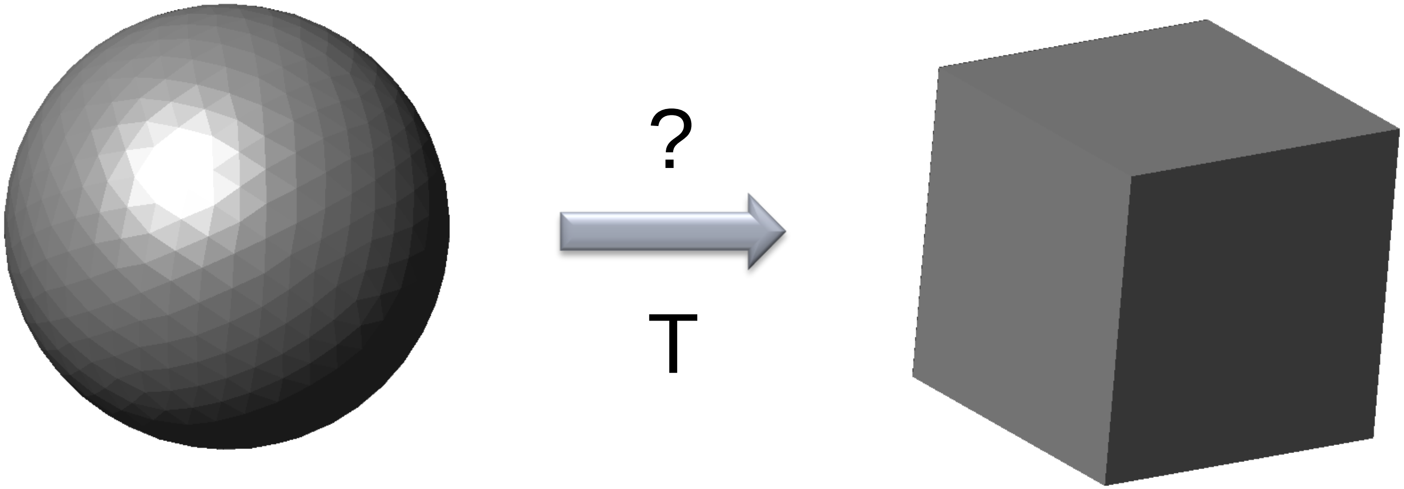
Part. 1 Optimal Transport



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

Part. 1 Optimal Transport

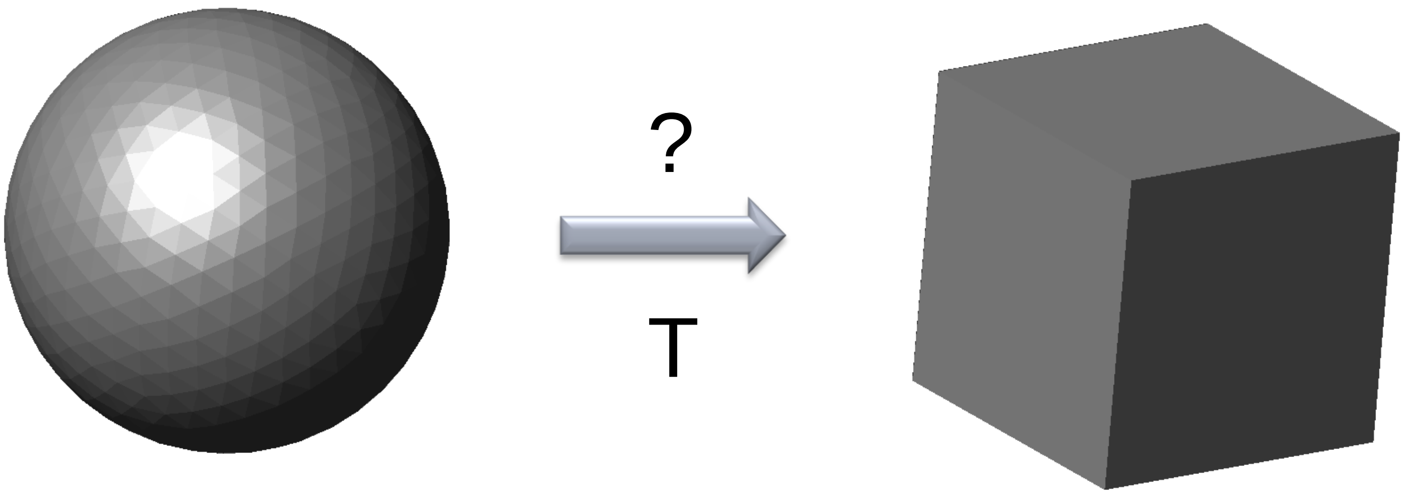
Part. 1 Optimal Transport



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 **<u>preserving mass</u>** and **<u>minimizing the effort</u>** ?

"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”

Part. 1 Optimal Transport

OT=

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New ways of simulating physics with a computer

Part. 1 Optimal Transport

OT=

"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

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”*

Fast Fourier Transform

Fast OT algo. ???

New ways of simulating physics with a computer

2

Optimal Transport

an elementary introduction

Part. 2 Optimal Transport – Monge's problem

(X;μ)

(Y;ν)

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

Part. 2 Optimal Transport – Monge's problem

(X;μ)

(Y;ν)

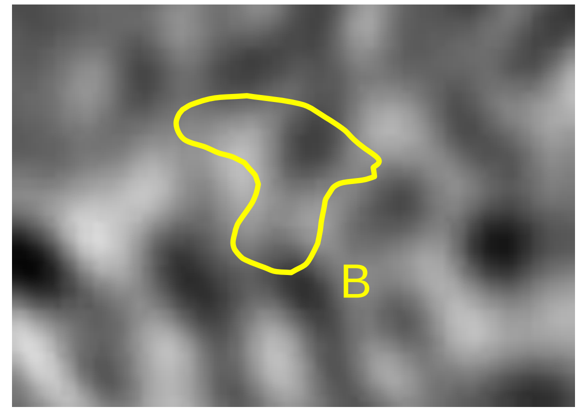
A map T is a ***transport map*** between μ and ν if

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

(Borel subset = subset that can be measured)

Part. 2 Optimal Transport – Monge's problem

(X;μ)



(Y;ν)

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

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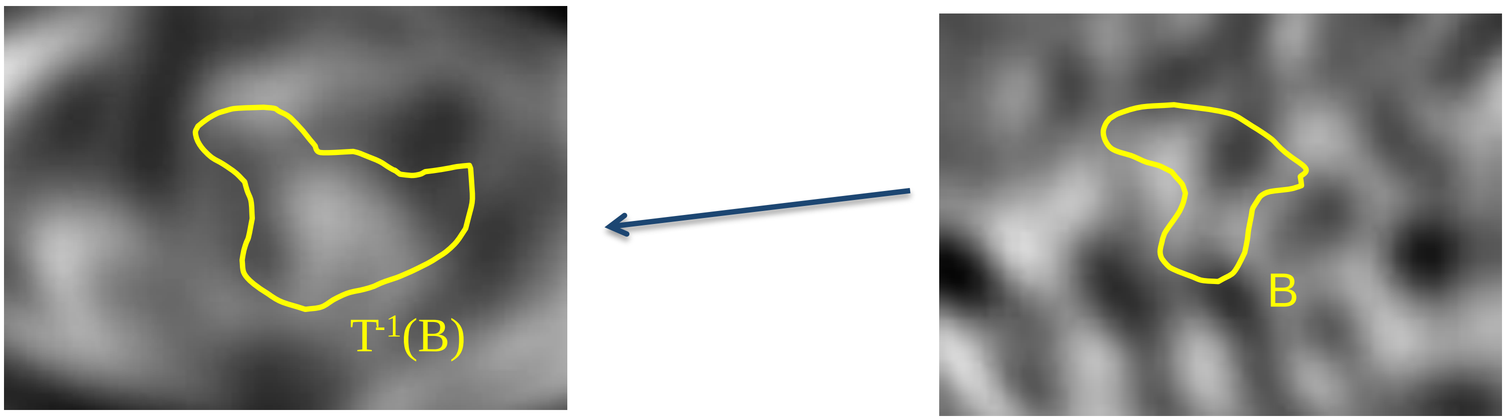
Part. 2 Optimal Transport – Monge's problem



$(X;\mu)$ $(Y;\nu)$

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

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

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

Notation: if T is a ***transport map*** between μ and ν then one writes $\nu = T\#\mu$ (ν is the ***pushforward*** of μ)

Part. 2 Optimal Transport – Monge's problem

(X;μ)

(Y;v)

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

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

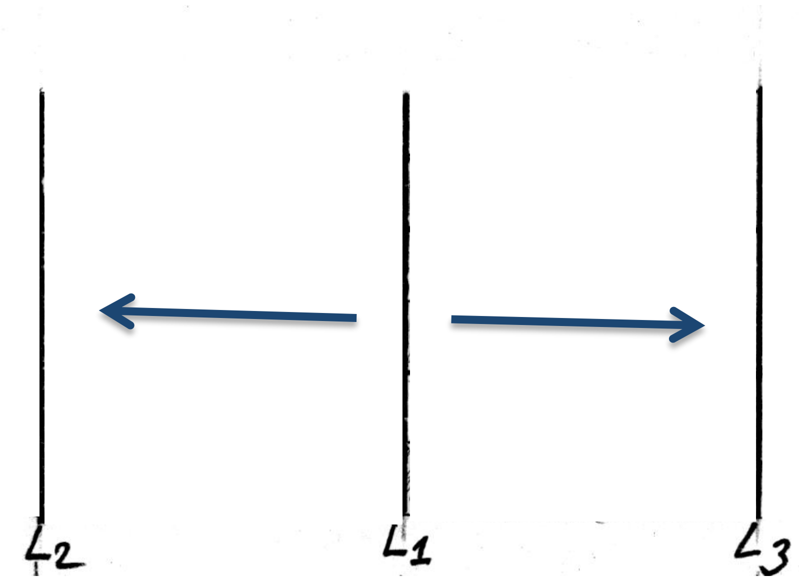
Find a transport map T that minimizes $C(T) = \int_X \| x - T(x) \|^2 d\mu(x)$

- 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

Monge's problem:

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

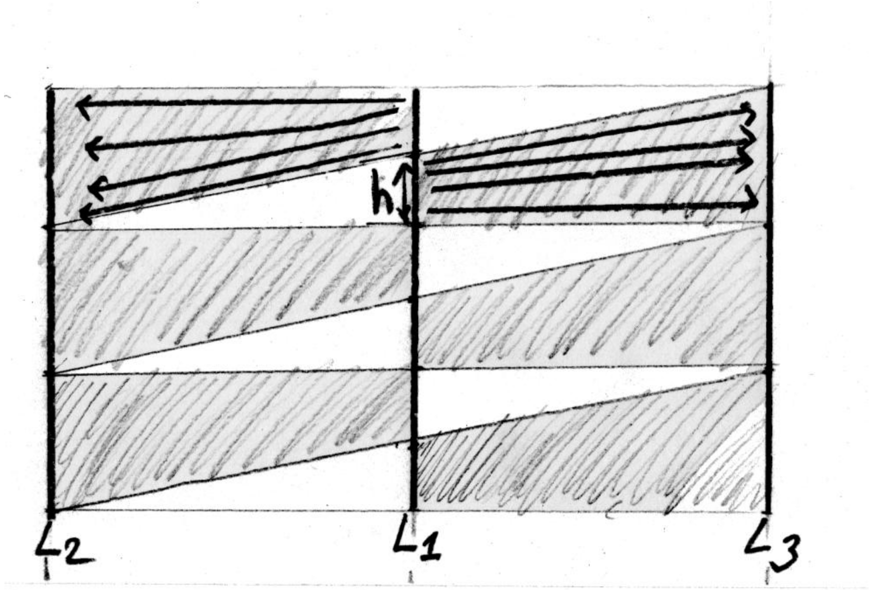


Transport from a measure concentrated on L_1 onto another one concentrated on L_2 and L_3

Part. 2 Optimal Transport – Monge's problem

Monge's problem:

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



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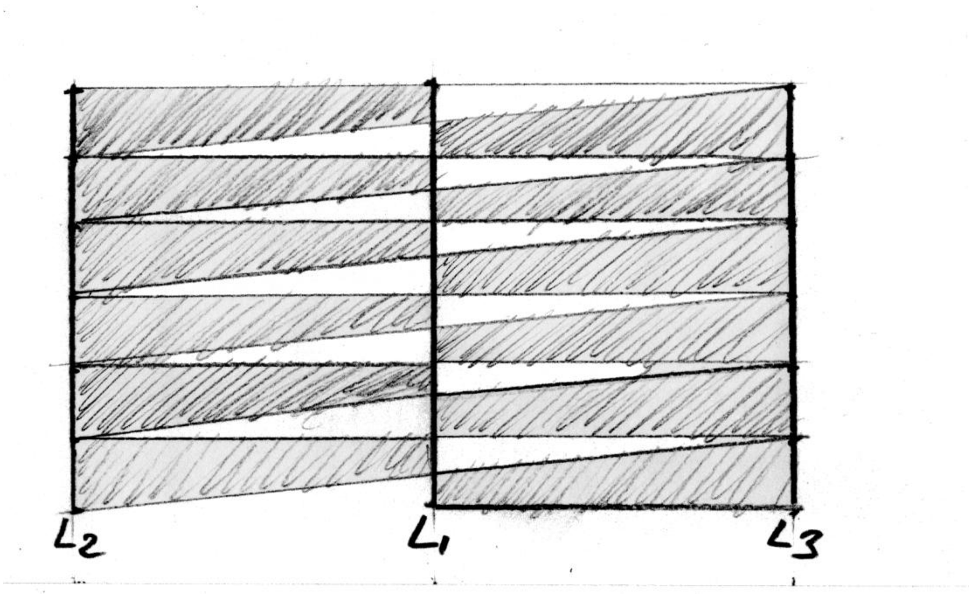
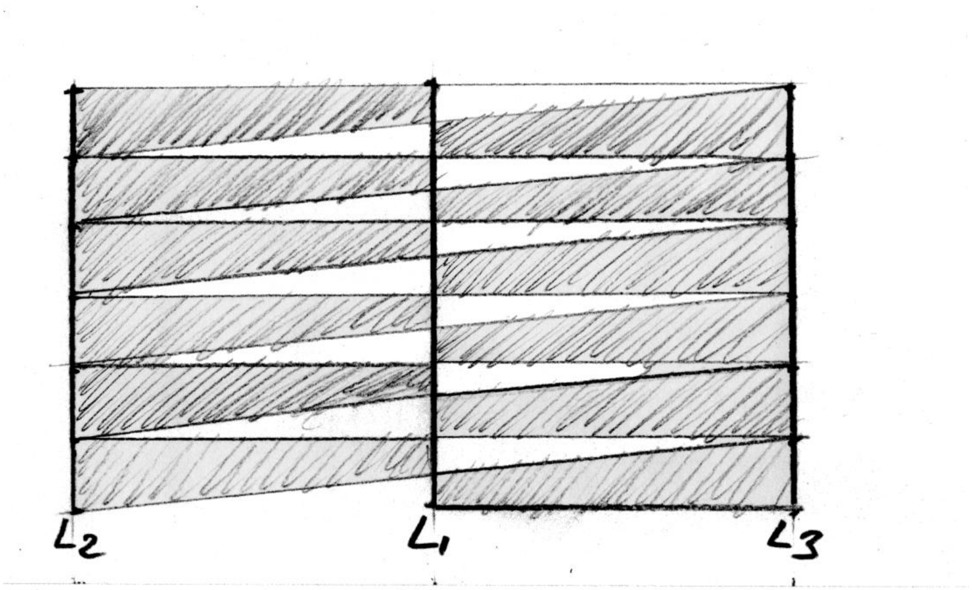


Transport from a measure concentrated on L_1 onto another one concentrated on L_2 and L_3

Part. 2 Optimal Transport – Monge's problem

Monge's problem:

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



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

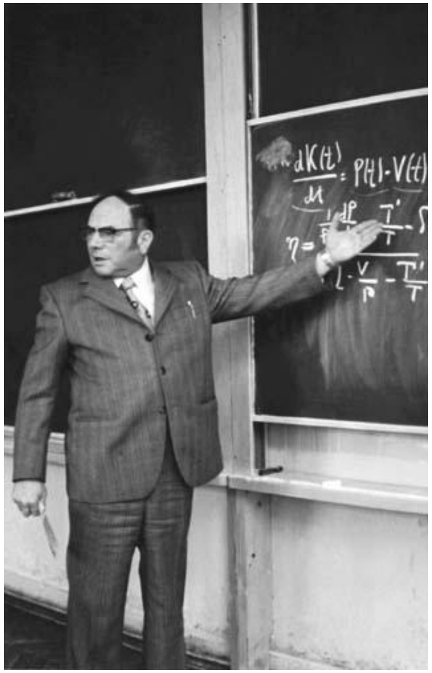
The infimum is never realized by a map, need for a relaxation

Part. 2 Optimal Transport – Kantorovich

Monge's problem:

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

***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

Monge's problem:

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

Kantorovich's problem:

Find a measure γ defined on X x 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 $\iint_{X \times Y} \| x - y \|^2 \, d\gamma(x,y)$

"γ(x,y)" :
How much sand goes from x to y

Part. 2 Optimal Transport – Kantorovich

Monge's problem:

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

Kantorovich's problem:

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

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

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

Everything that is transported **from x** sums to "$\mu(x)$"

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

Part. 2 Optimal Transport – Kantorovich

Monge's problem:

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

Kantorovich's problem:

Find a measure γ defined on X x Y

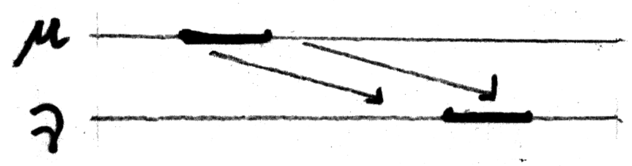
such that $\int_{x \text{ in } X} d\gamma(x,y) = d\nu(y)$

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

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

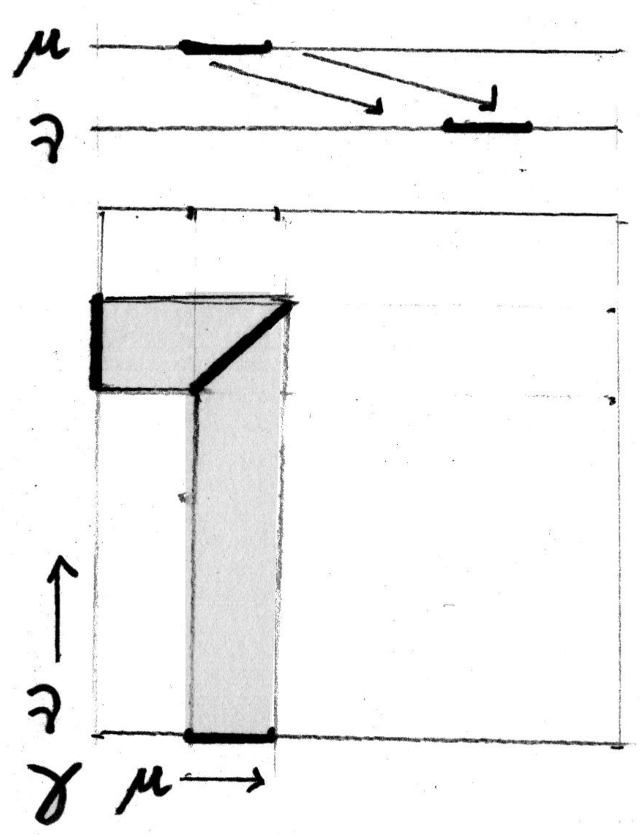
that minimizes $\iint_{X \times Y} \| x - y \|^2 \, d\gamma(x,y)$

Part. 2 Optimal Transport – Kantorovich



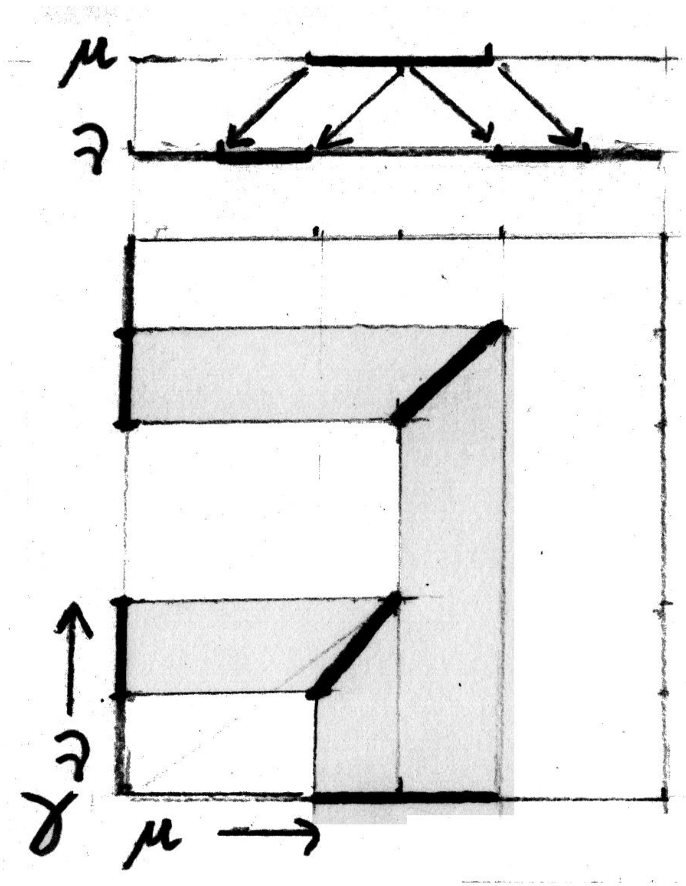
Transport plan – example 1/4 : translation of a segment

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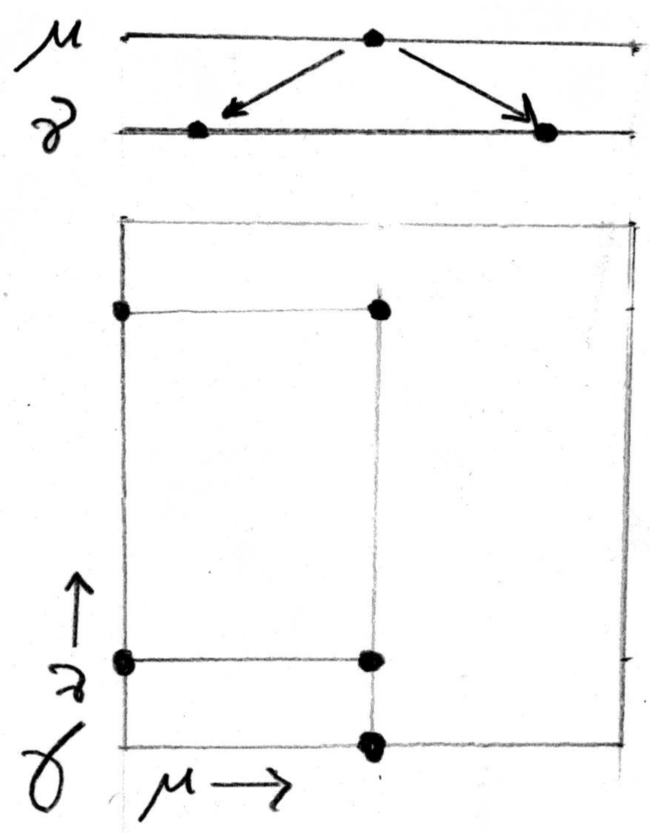
With this observation, for transport plans of the form $\gamma = (Id \times T)\sharp\mu$, (K) becomes

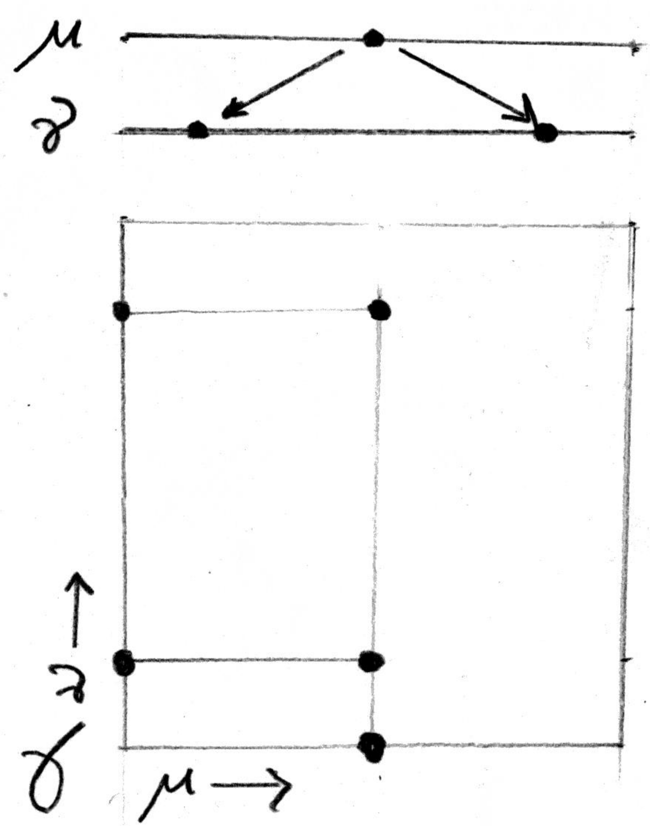
$$\min \left\{ \int_{\Omega \times \Omega} c(x, y) d\left((Id \times T)\sharp\mu\right) \right\} \quad = \quad \min \left\{ \int_{\Omega} c(x, T(x)) d\mu \right)$$

Part. 2 Optimal Transport – Kantorovich



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

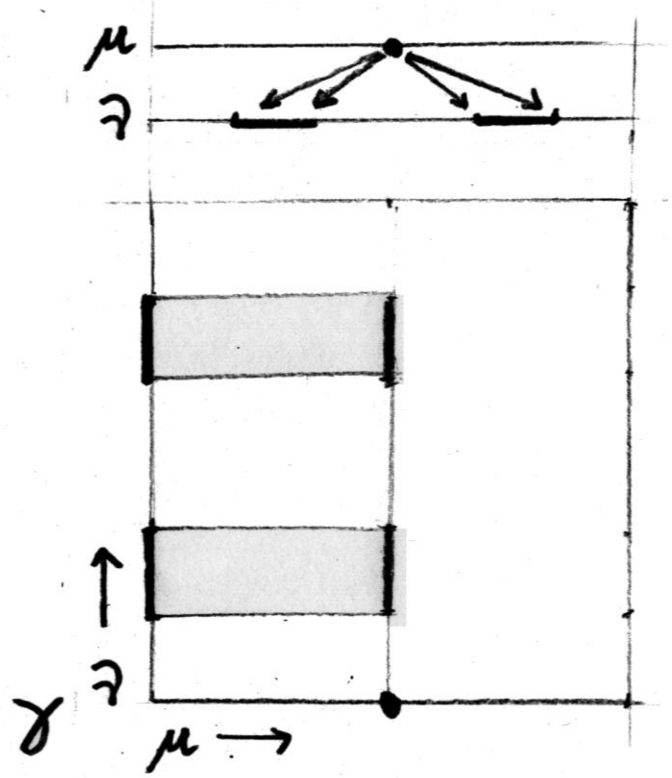
Part. 2 Optimal Transport – Kantorovich



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

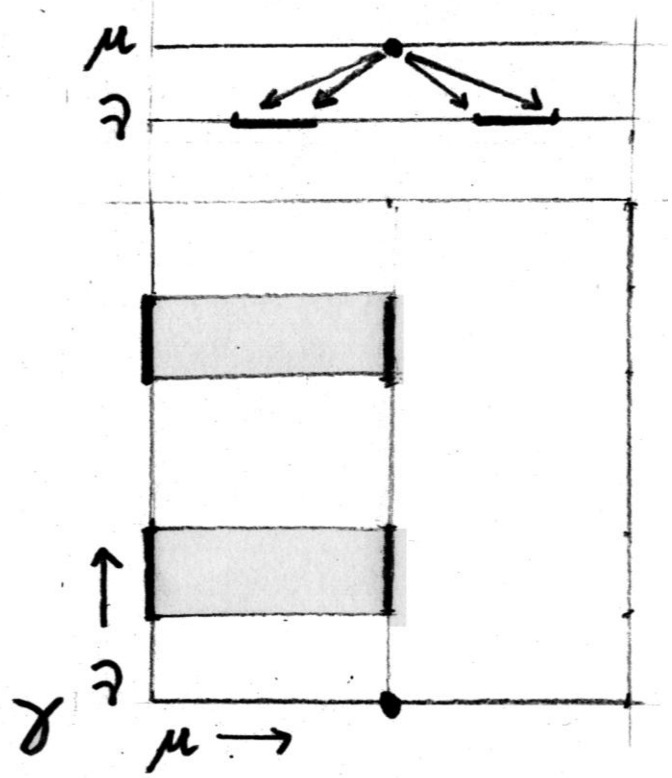
(No transport map)

Part. 2 Optimal Transport – Kantorovich



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

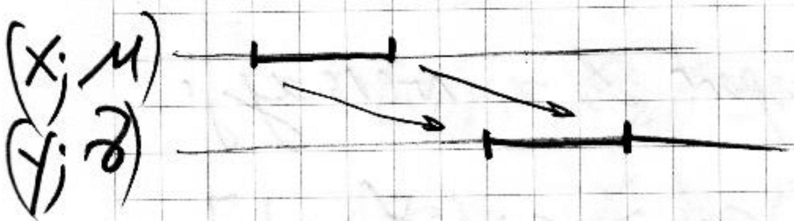
Part. 2 Optimal Transport – Kantorovich

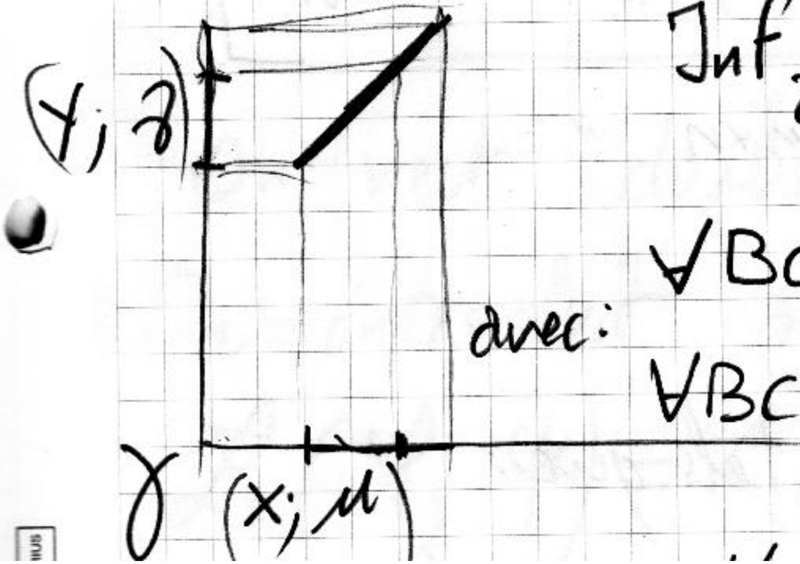


Transport plan – example 4/4 : splitting a Dirac into two segments

(No transport map)

Part. 2 Optimal Transport – Duality





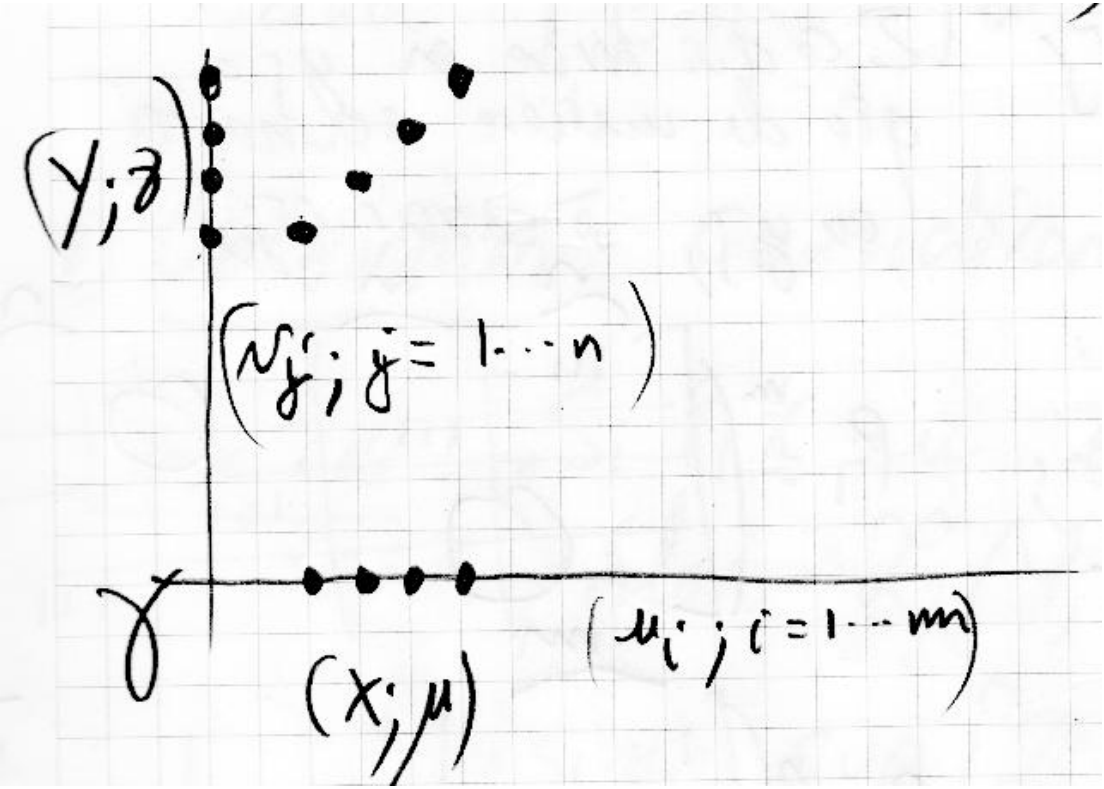
$$\mathrm{Inf}_{\gamma} \int_{X\times Y} c(x,y)\, d\gamma$$

avec:

$$\forall B \subset X, \int_B d\mu = \int_{B\times Y} d\gamma \quad (P_1 \# \gamma = \mu)$$

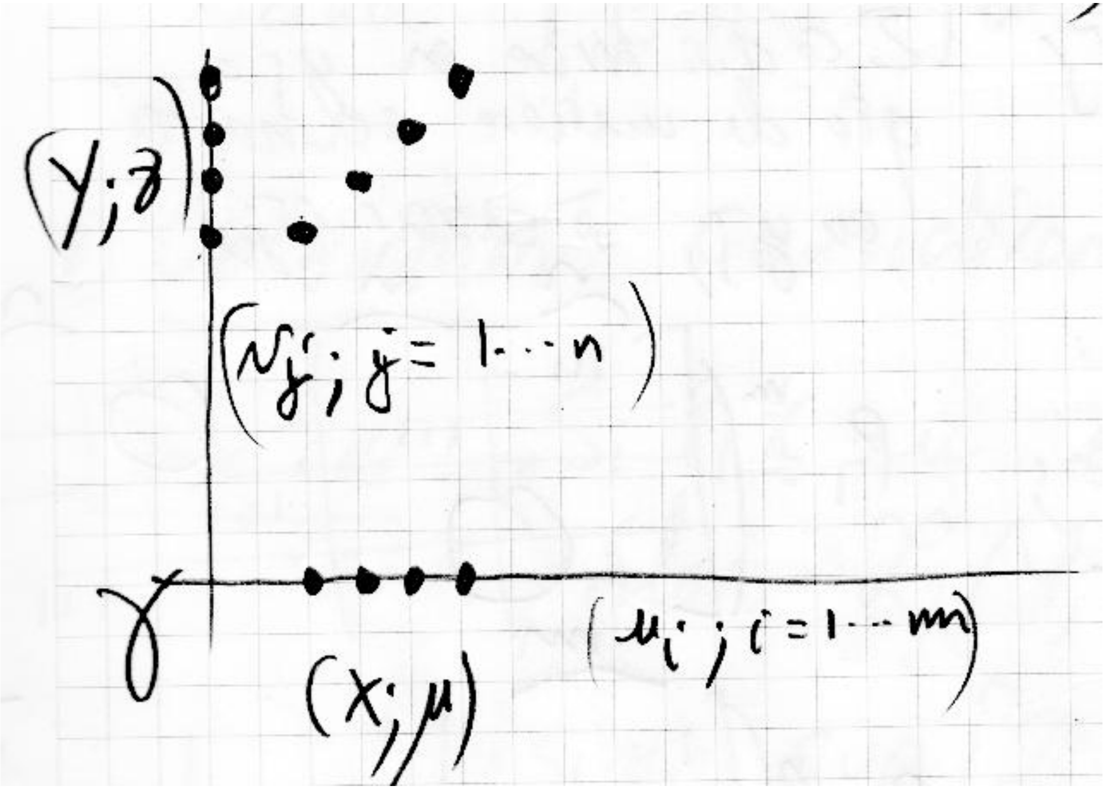
$$\forall B \subset Y, \int_B d\nu = \int_{X\times B} d\gamma \quad (P_1 \# \gamma = \nu)$$

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

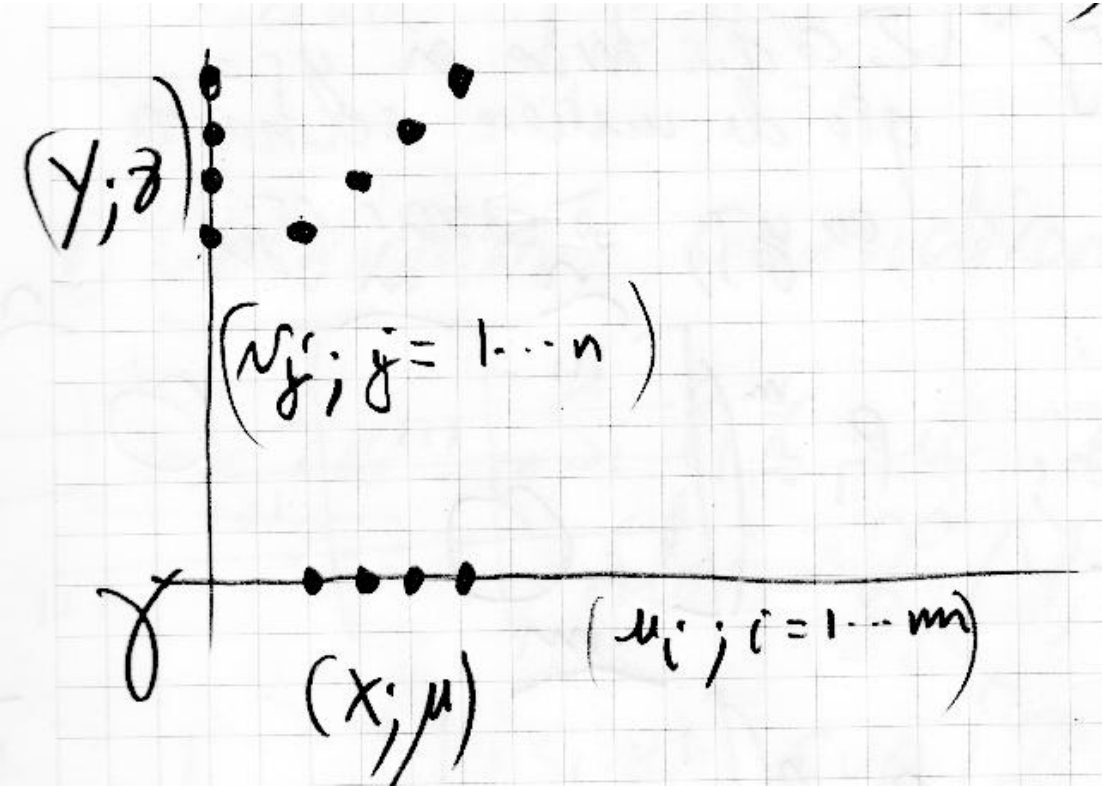


(DMK):

Min $\langle c, \gamma \rangle$

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

Part. 2 Optimal Transport – Duality



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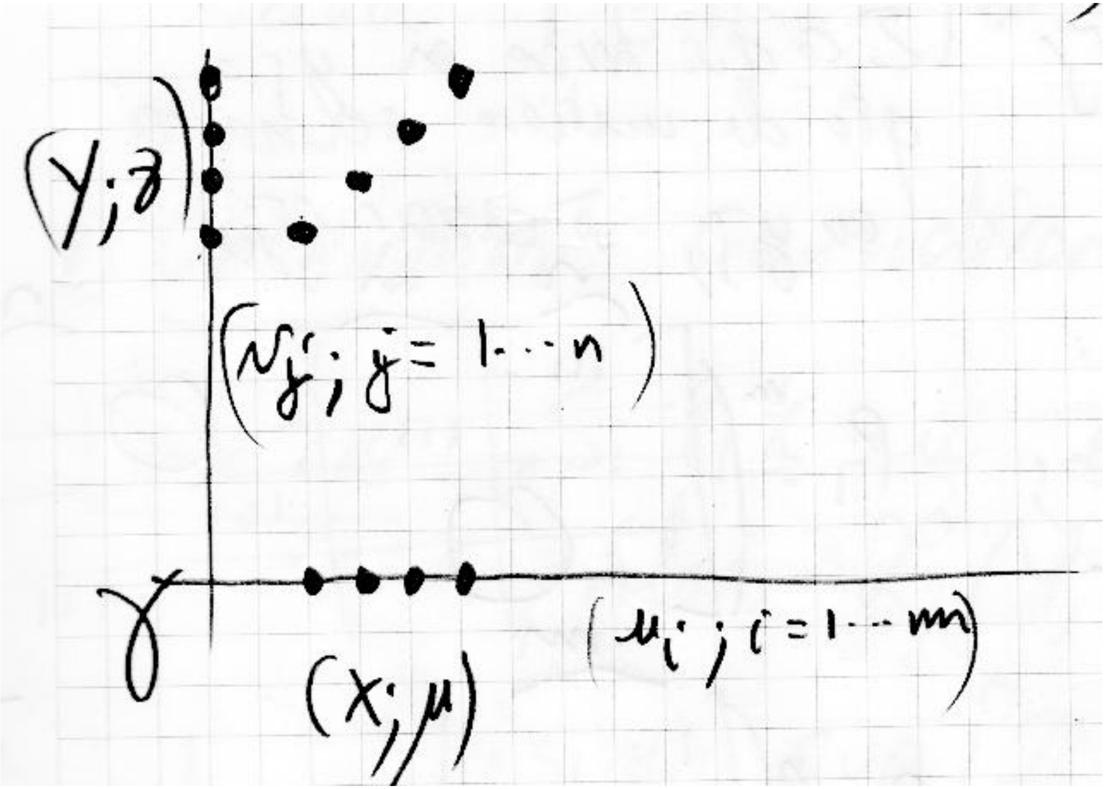
$$s.t. \begin{cases} P_1 \gamma = u \\ P_2 \gamma = v \\ \gamma \geq 0 \end{cases}$$

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

Part. 2 Optimal Transport – Duality



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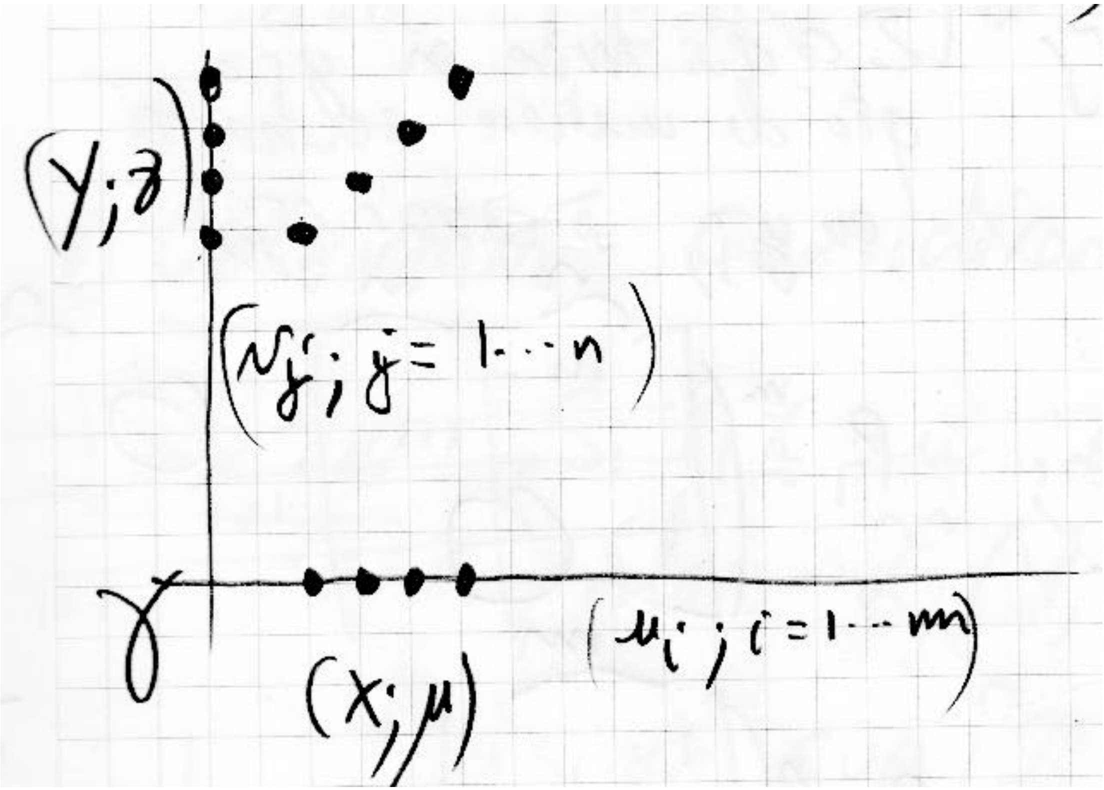
$$s.t. \begin{cases} P_1 \gamma = u \\ P_2 \gamma = v \\ \gamma \geq 0 \end{cases}$$

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

Part. 2 Optimal Transport – Duality



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

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

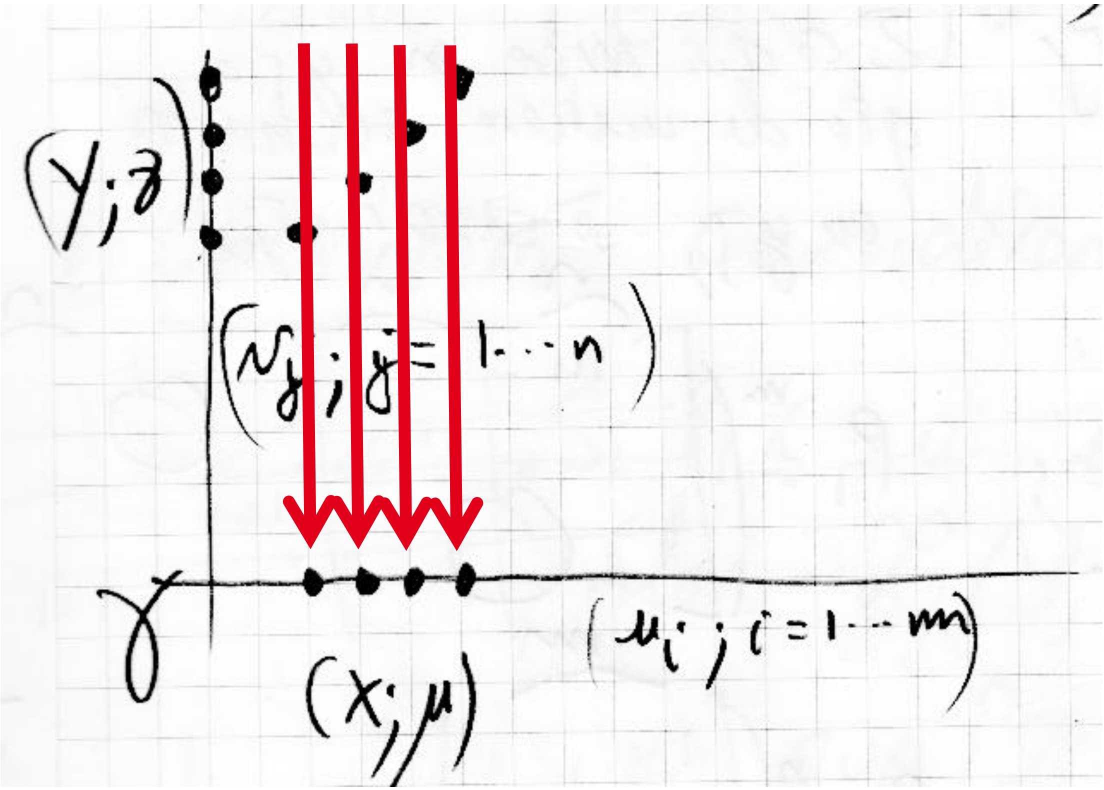
Part. 2 Optimal Transport – Duality

(DMK):

Min $\langle c, \gamma \rangle$

mn X m

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



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

$c \in \mathrm{IR}^{mn}$ $\qquad$ $\gamma \in \mathrm{IR}^{mn}$

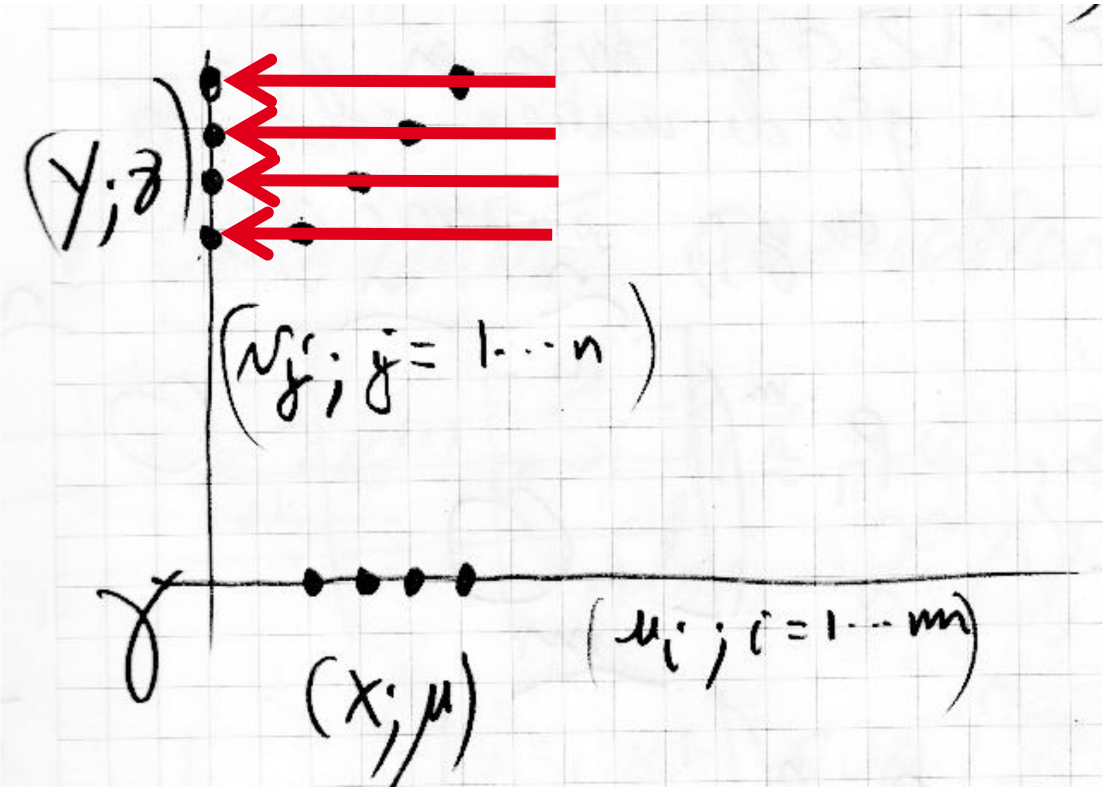
$c_{ij} = \| x_i - y_j \|^2$

Part. 2 Optimal Transport – Duality

(DMK):

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

$$\text{s.t.} \quad \begin{cases} P_1 \, \gamma = u & (P_1: mn \times m) \\ \color{red}{P_2} \, \gamma = v & (\color{red}{P_2: mn \times n}) \\ \gamma \geq 0 \end{cases}$$



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

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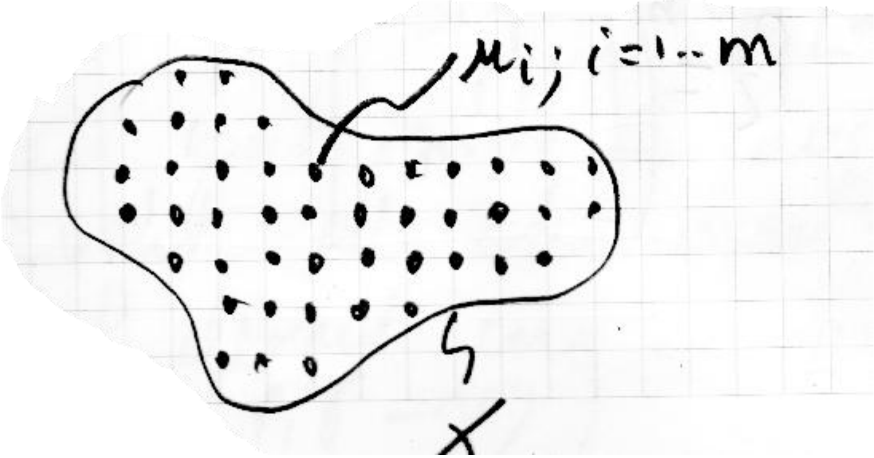
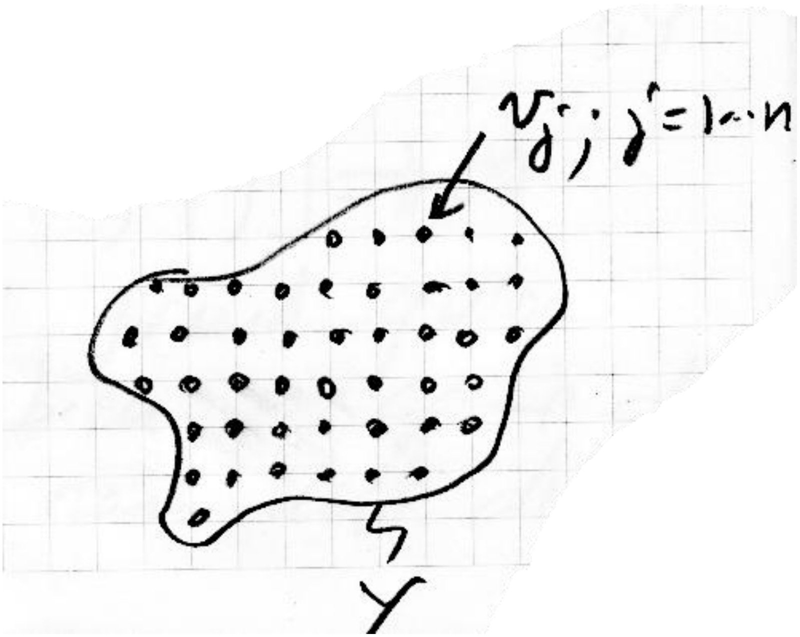
Part. 2 Optimal Transport – Duality





(DMK):

Min $\langle c, \gamma \rangle$

s.t.

$$\left\{\begin{array}{ll} \text{mn X m} \rightarrow & P_1 \gamma = u \\ \text{mn X n} \rightarrow & P_2 \gamma = v \\ & \gamma \geq 0 \end{array}\right.$$

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

Part. 2 Optimal Transport – Duality

(DMK):

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):

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

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

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

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$= +\infty$ otherwise

Part. 2 Optimal Transport – Duality

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

$= +\infty$ otherwise

Consider now: $\operatorname{Inf}_{\gamma \geq 0} \left[\operatorname{Sup}_{\substack{\varphi \in \mathbb{R}^m \\ \psi \in \mathbb{R}^n}} [\ \mathcal{L}(\varphi,\psi)\ ] \right]$

Part. 2 Optimal Transport – Duality

(DMK):

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

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

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

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Consider now: $\displaystyle \operatorname*{Inf}_{\gamma \geq 0} \Big[\operatorname*{Sup}_{\substack{\varphi \in \mathbb{R}^m \\ \psi \in \mathbb{R}^n}} [\, \mathcal{L}(\varphi,\psi) \,] \Big] = \operatorname*{Inf}_{\substack{\gamma \geq 0 \\ P_1 \gamma = u \\ P_2 \gamma = v}} [\, \langle c, \gamma \rangle \,]$

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

$= +\infty$ otherwise

Consider now: $\inf_{\gamma \geq 0} \Big[\sup_{\substack{\varphi \in IR^m \\ \psi \in IR^n}} [\mathcal{L}(\varphi,\psi)] \Big] = \inf_{\substack{\gamma \geq 0 \\ P_1 \gamma = u \\ P_2 \gamma = v}} [\langle c, \gamma \rangle]$ **(DMK)**

Part. 2 Optimal Transport – Duality

(DMK):

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

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

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

Part. 2 Optimal Transport – Duality

(DMK):

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

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

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):

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

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

Exchange Inf Sup

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

Expand/Reorder/Collect

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

Part. 2 Optimal Transport – Duality

(DMK):

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

$$\operatorname*{Inf}_{\gamma \geq 0} \Big[\operatorname*{Sup}_{\varphi \in IR^m, \ \psi \in IR^n} [\ \langle c, \gamma \rangle - \langle \varphi, P_1 \gamma - u \rangle - \langle \psi, P_2 \gamma - v \rangle \ ] \Big]$$

Exchange Inf Sup

$$\operatorname*{Sup}_{\varphi \in IR^m, \ \psi \in IR^n} \Big[\operatorname*{Inf}_{\gamma \geq 0} [\ \langle c, \gamma \rangle - \langle \varphi, P_1 \gamma - u \rangle - \langle \psi, P_2 \gamma - v \rangle \ ] \Big]$$

Expand/Reorder/Collect

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

Interpret

Part. 2 Optimal Transport – Duality

(DMK):

Min $\langle c, \gamma \rangle$

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

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

Interpret

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

Part. 2 Optimal Transport – Duality

(DMK):

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

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

Interpret

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

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

Part. 2 Optimal Transport – Kantorovich dual

Kantorovich's problem:

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

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

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 $X \times Y$

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, $\varphi(x) + \psi(y) \leq \frac{1}{2}\| x - y \|^2$

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Part. 2 Optimal Transport – Kantorovich dual

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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 $X \times Y$

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

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, $\varphi(x) + \psi(y) \leq \frac{1}{2}\| x - y \|^2$

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, $\varphi^c(y) = \inf_{x \in X} \frac{1}{2}\| x - y \|^2 - \varphi(y)$

Part. 2 Optimal Transport – c-conjugate functions

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Find two functions φ in $L^1(\mu)$ and ψ in $L^1(\nu)$
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For all y, $\varphi^c(y) = \inf_{x \text{ in } X} ½\| x - y \|^2 - \varphi(y)$

- 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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What about our initial problem ?

Part. 2 Optimal Transport – c-subdifferential

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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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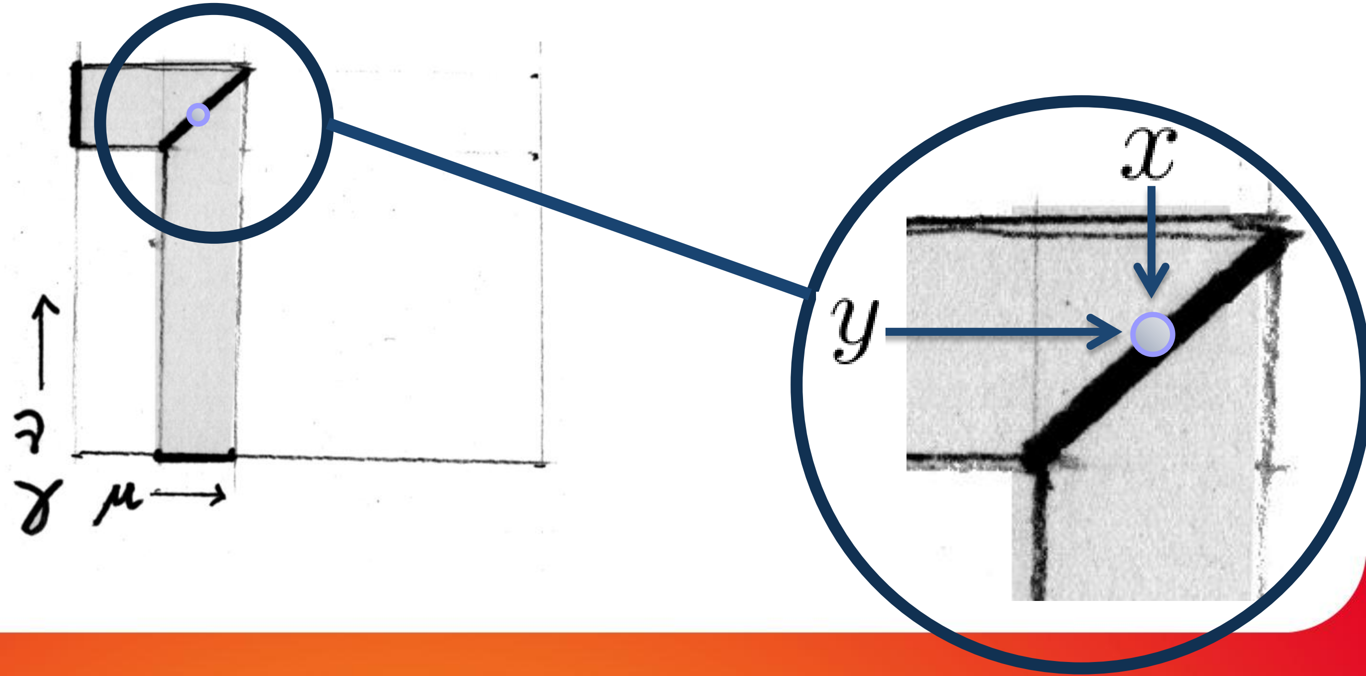

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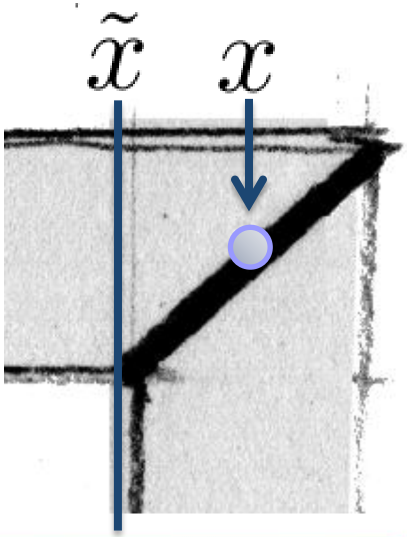

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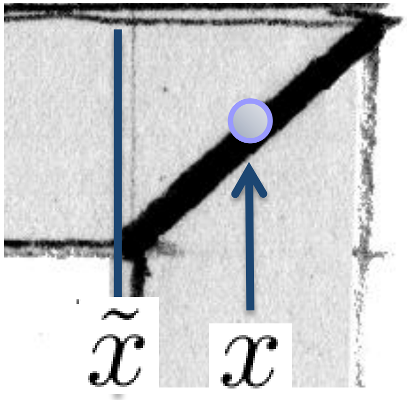

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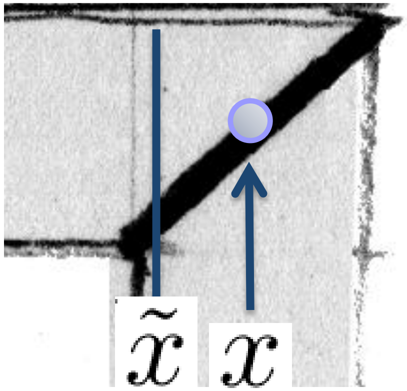

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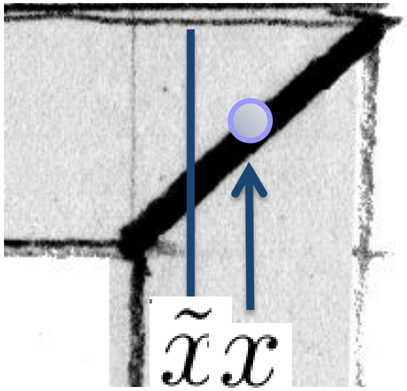

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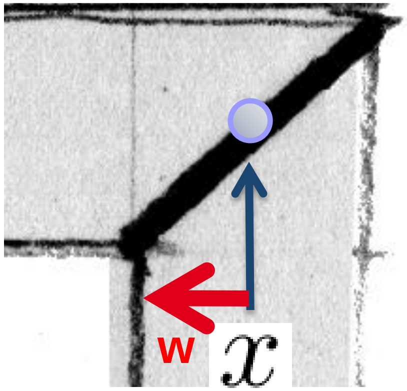
Thus we have $\nabla \psi(x) \cdot w \leq \nabla_x c(x,y) \cdot w$



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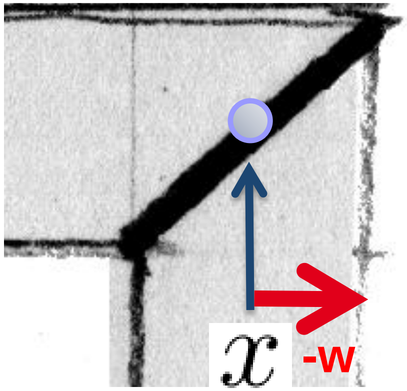
Thus we have $\nabla \psi(x) \cdot w \le \nabla_x c(x,y) \cdot w$
The same derivation can be done with $-w$ instead of w, and one gets:
$\forall w, \nabla \psi(x) \cdot w = \nabla_x c(x,y) \cdot w$, thus $\forall (x,y) \in \partial_c \psi, \nabla \psi(x) - \nabla_x c(x,y) = 0$.



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 $T(x) = x - \nabla\psi(x) = \nabla(\|x\|^2/2 - \psi(x))$.

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Part. 2 Optimal Transport – convexity

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grad $\overline{\psi}(x)$ with $\overline{\psi}(x)$:= (½ x^2- $\psi(x)$)

$\overline{\psi}$ is convex

Part. 2 Optimal Transport – convexity

<u>Dual formulation of Kantorovich's problem:</u>

Find a c-concave function ψ

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grad $\bar{\psi}$(x) with $\bar{\psi}$(x) := (½ x^2- ψ(x))

$\bar{\psi}$ 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)
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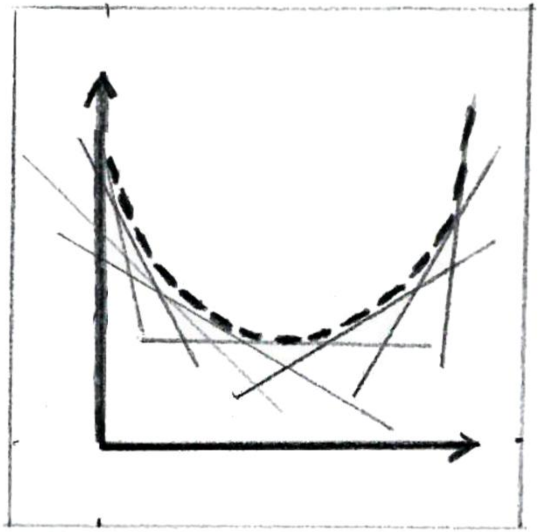

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Part. 2 Optimal Transport – no collision

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

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

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$\downarrow$

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:

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

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

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:

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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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for all borel set A, $\int_A d\mu = \int_{T(A)} (|JT|)\, dv = \int_{T(A)} (H\ \overline{\psi}\ )\, dv$

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

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When μ and ν have a density u and v, $\boxed{(H\,\overline{\psi}(x)).\ v\big(\text{grad}\,\overline{\psi}(x)\big) = u(x)}$ *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 $(H\,\overline{\psi}(x)).\, v\left(\text{grad}\,\overline{\psi}(x)\right) = u(x)$ *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 $(H\,\overline{\psi}(x)).\, \nu\big(\mathrm{grad}\,\overline{\psi}(x)\big) = u(x)$ *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:***
$T(x) = \mathrm{grad}\,\overline{\psi}(x)$

3

Semi-Discrete Optimal Transport

Part. 3 Optimal Transport – how to program ?

(X;μ)

(Y;ν)

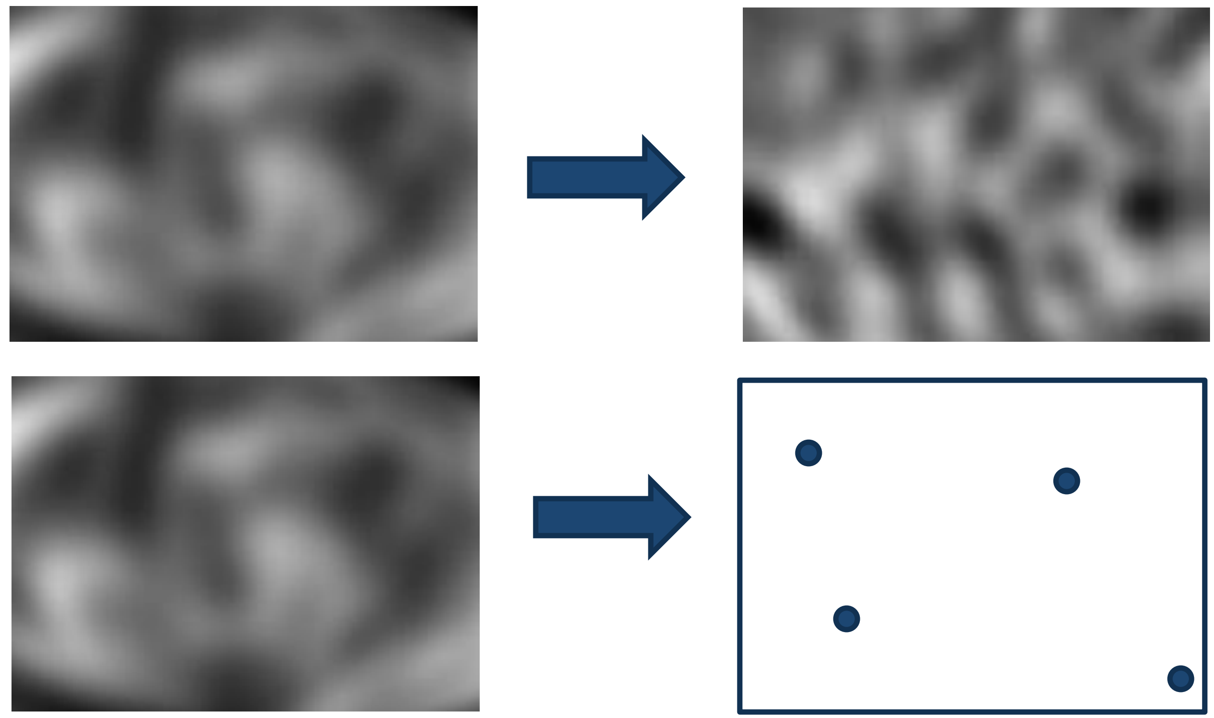
Continuous

Part. 3 Optimal Transport – how to program ?

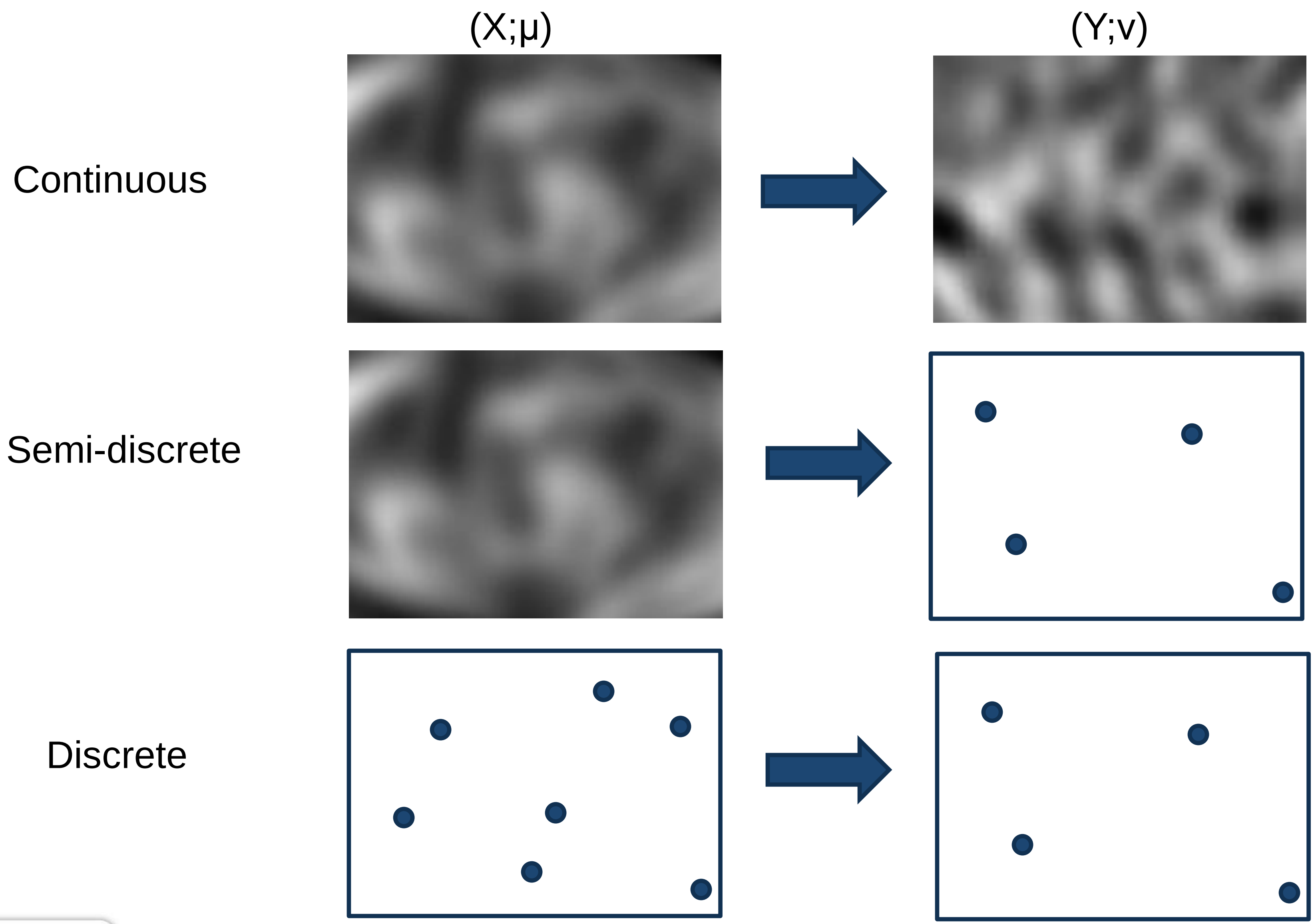
(X;μ) (Y;ν)

Continuous

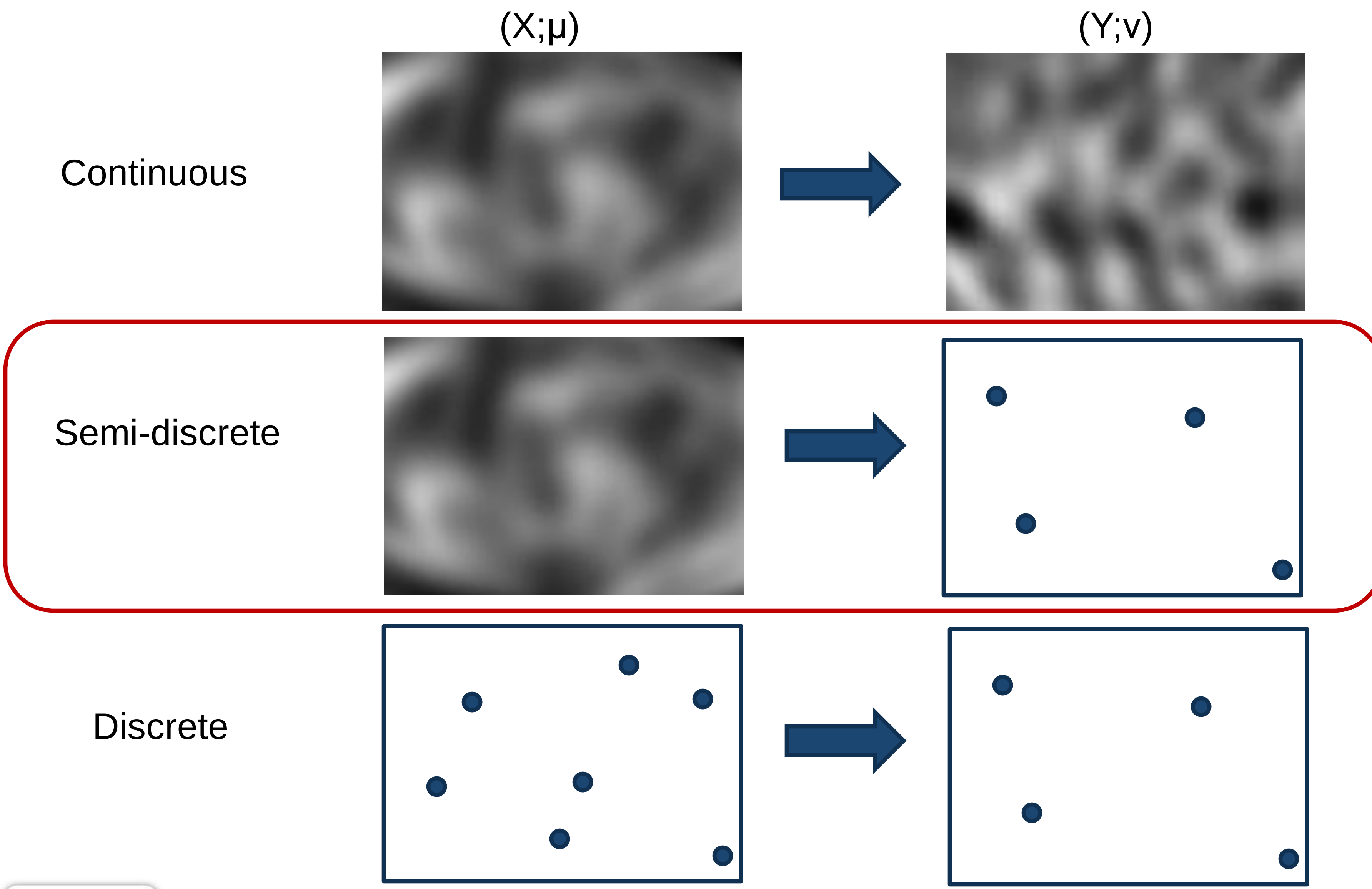
Semi-discrete



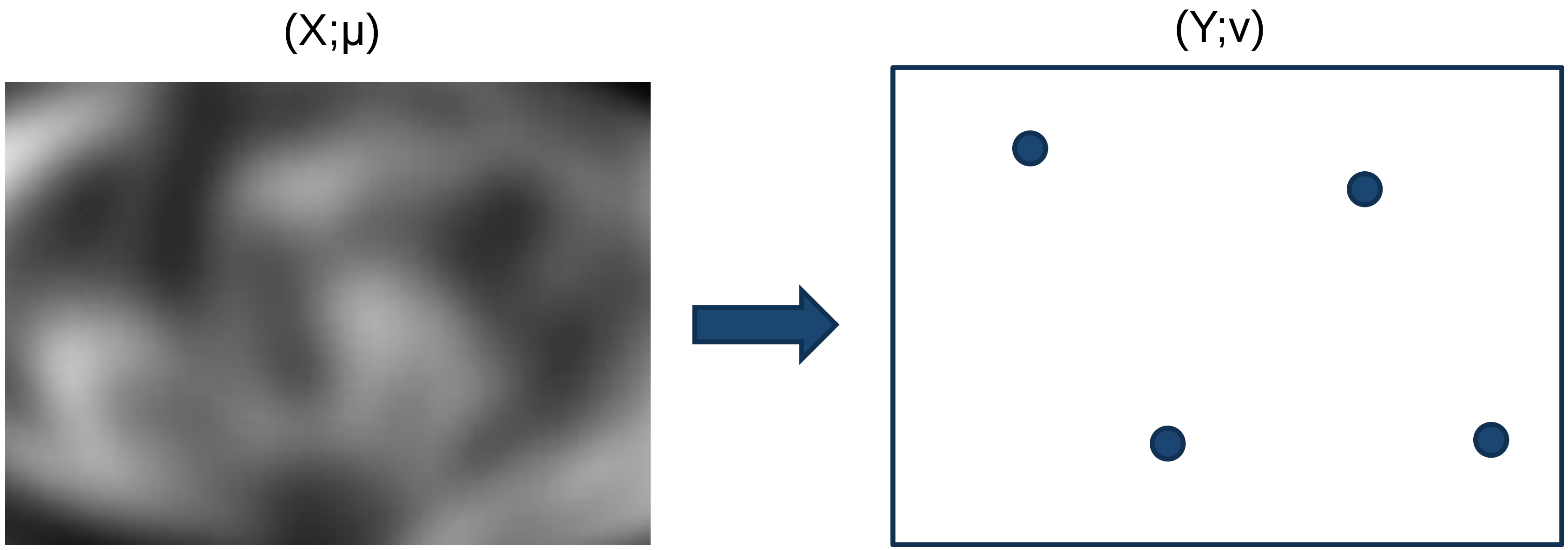
Part. 3 Optimal Transport – how to program ?



Part. 3 Optimal Transport – how to program ?

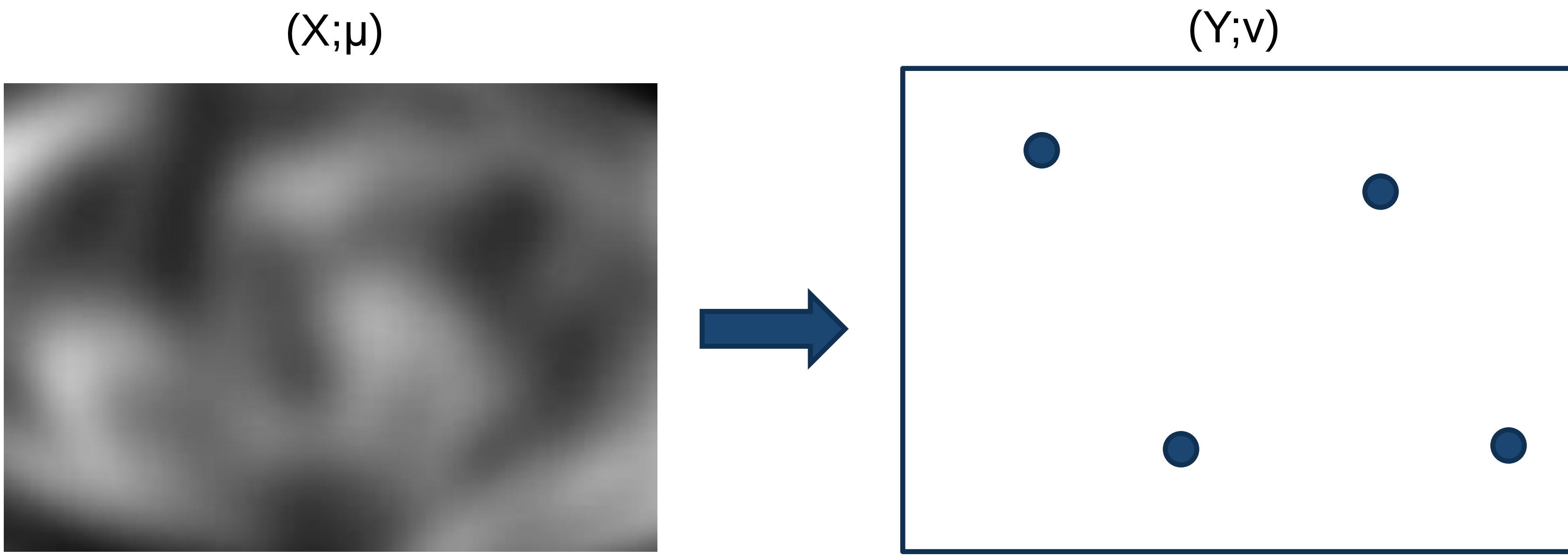


Part. 3 Optimal Transport – semi-discrete



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

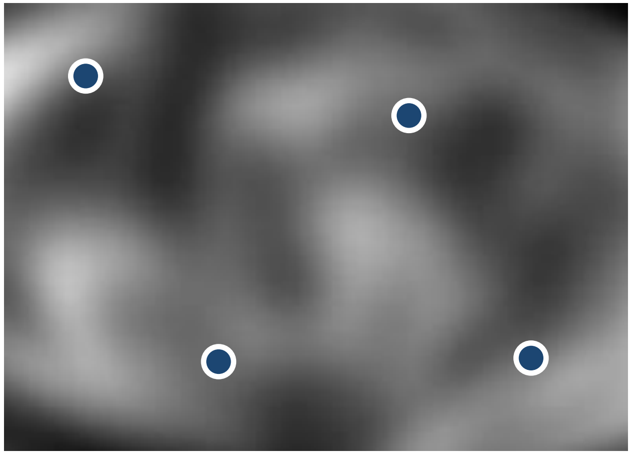
Part. 3 Optimal Transport – semi-discrete



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

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

Part. 3 Optimal Transport – semi-discrete



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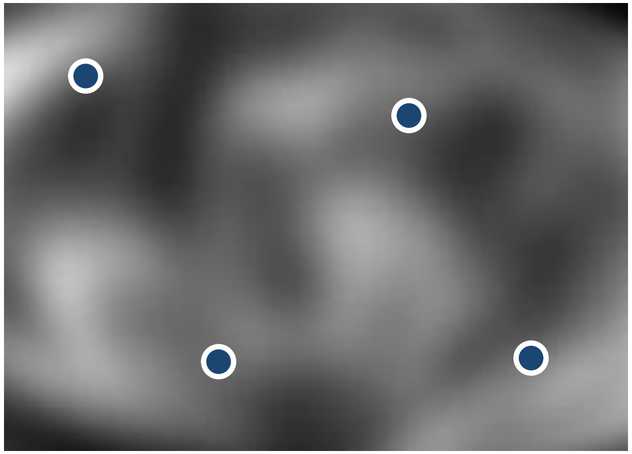
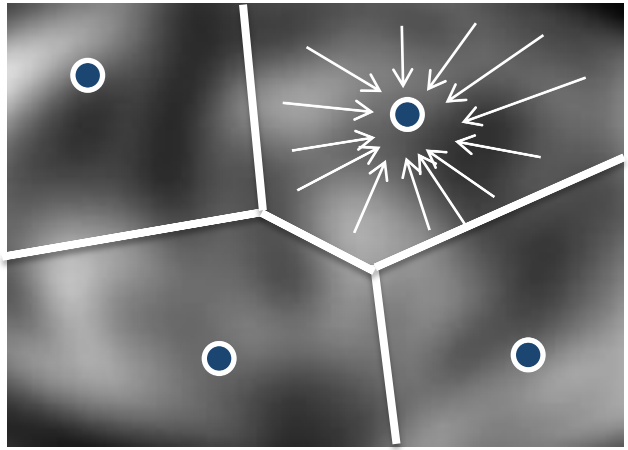


(DMK) $\sup_{\psi \in \Psi^c} \int_X \psi^c(x)d\mu + \int_Y \psi(y)dv$

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

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

Part. 3 Optimal Transport – semi-discrete



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

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

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

Part. 3 Optimal Transport – semi-discrete

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

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

Part. 3 Optimal Transport – semi-discrete

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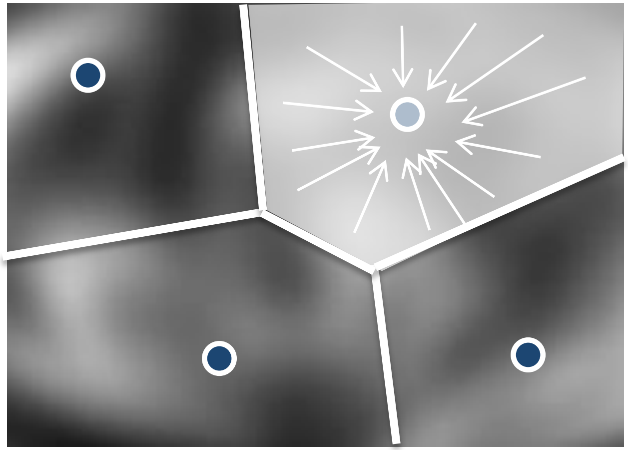
Laguerre diagram of the y_j's
(with the L_2 cost $\| x - y \|^2$ used here, Power diagram)



Part. 3 Optimal Transport – semi-discrete

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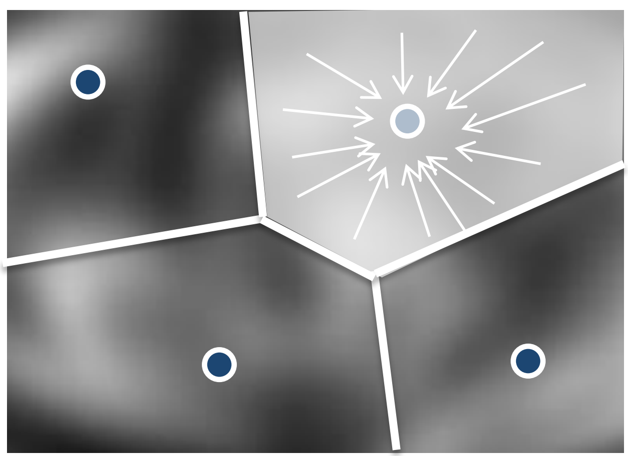
Weight of y_j in the power diagram



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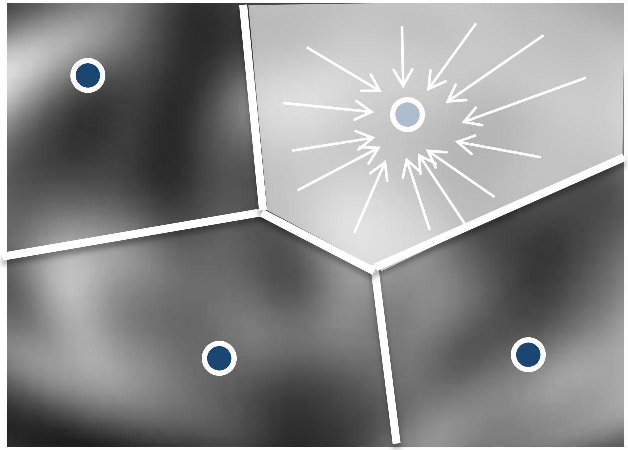

ψ is determined by the
weight vector $[\psi(y_1)\ \psi(y_2)\ \dots\ \psi(y_m)]$

Part. 3 Power Diagrams

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

Part. 3 Power Diagrams

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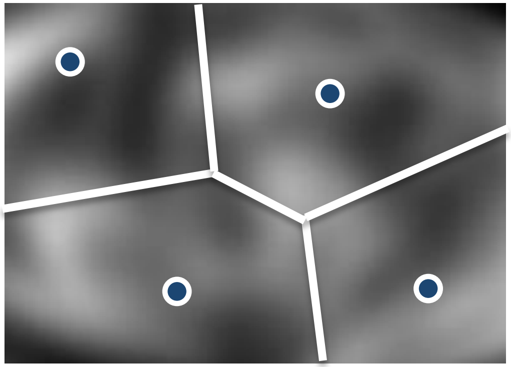
Power diagram: $Pow(x_i) = \{ x \mid d^2(x,x_i) - \psi_i < d^2(x,x_j) - \psi_j \}$

Part. 3 Power Diagrams

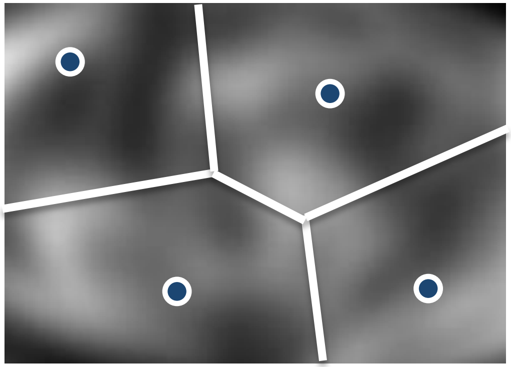
Part. 3 Optimal Transport



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 $W = [\psi(y_1)\ \psi(y_2)\ \ldots\ \psi(y_m)]$ such that the map T_S^W is the unique optimal transport map between μ and $\nu = \sum v_j\, \delta(y_j)$

Part. 3 Optimal Transport



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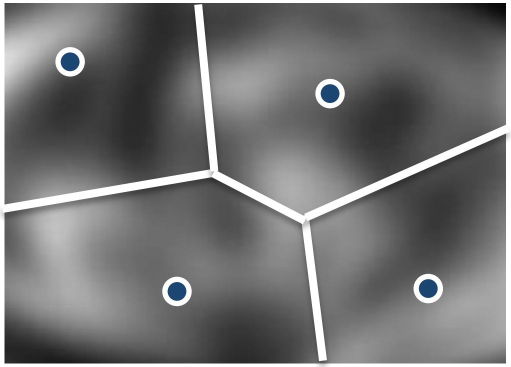
Proof: $G(\psi) = \sum_j \int_{\mathrm{Lag}\ \psi(yj)} \| x - y_j \|^2 - \psi(y_j)\, d\mu \ + \ \sum_j \psi(y_j)\, v_j$

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 $$f_T(W) = \int \Big(\| x - T(x) \|^2 - \psi\big(T(X)\big) \Big)\, d\mu(x)$$

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

Part. 3 Optimal Transport – the AHA paper

<u>Idea of the proof</u>

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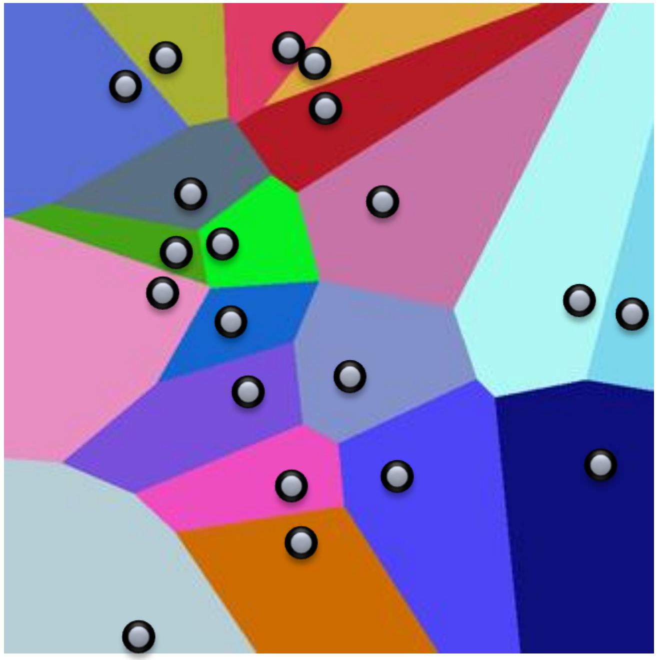

T : an arbitrary but fixed assignment.

Part. 3 Optimal Transport – the AHA paper

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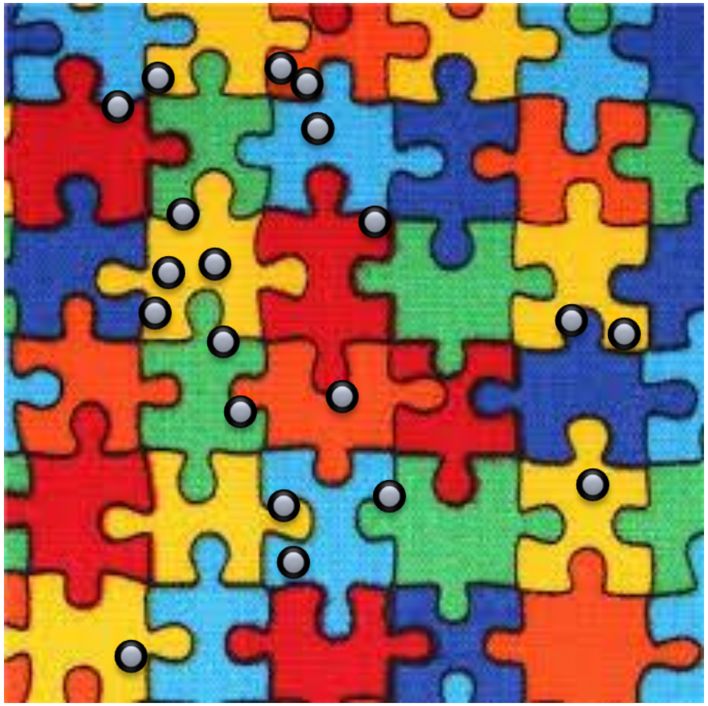

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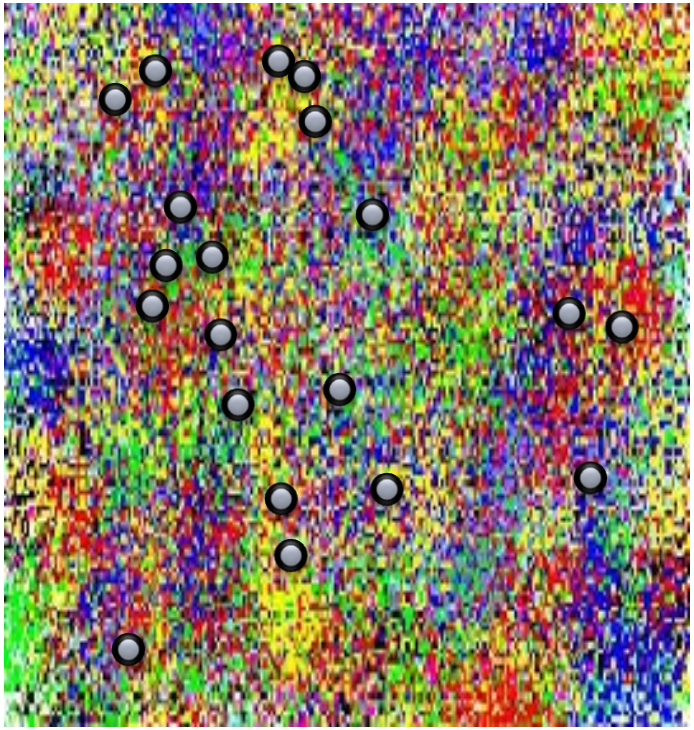

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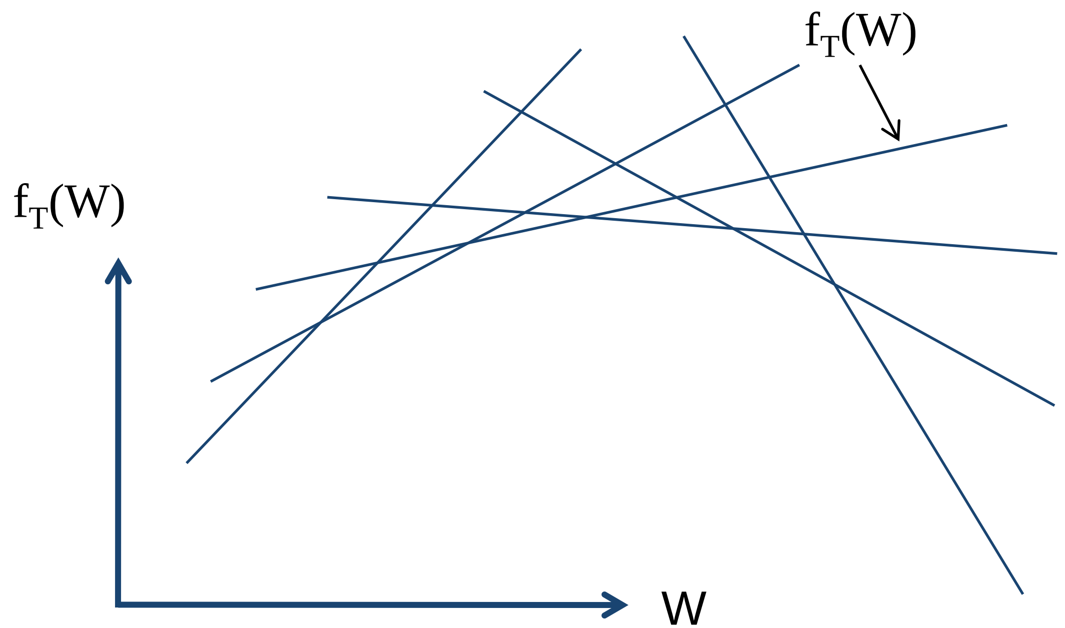

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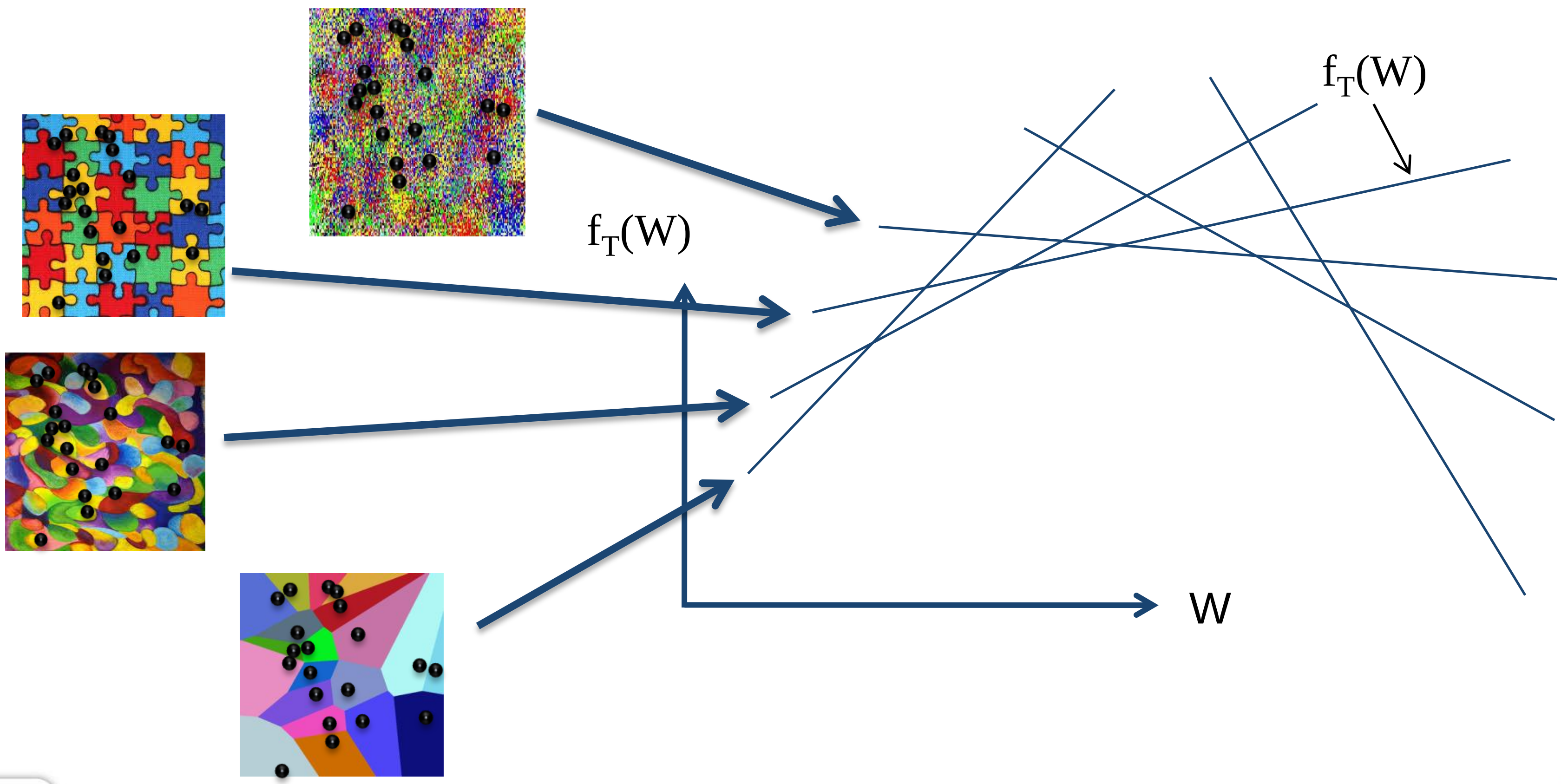

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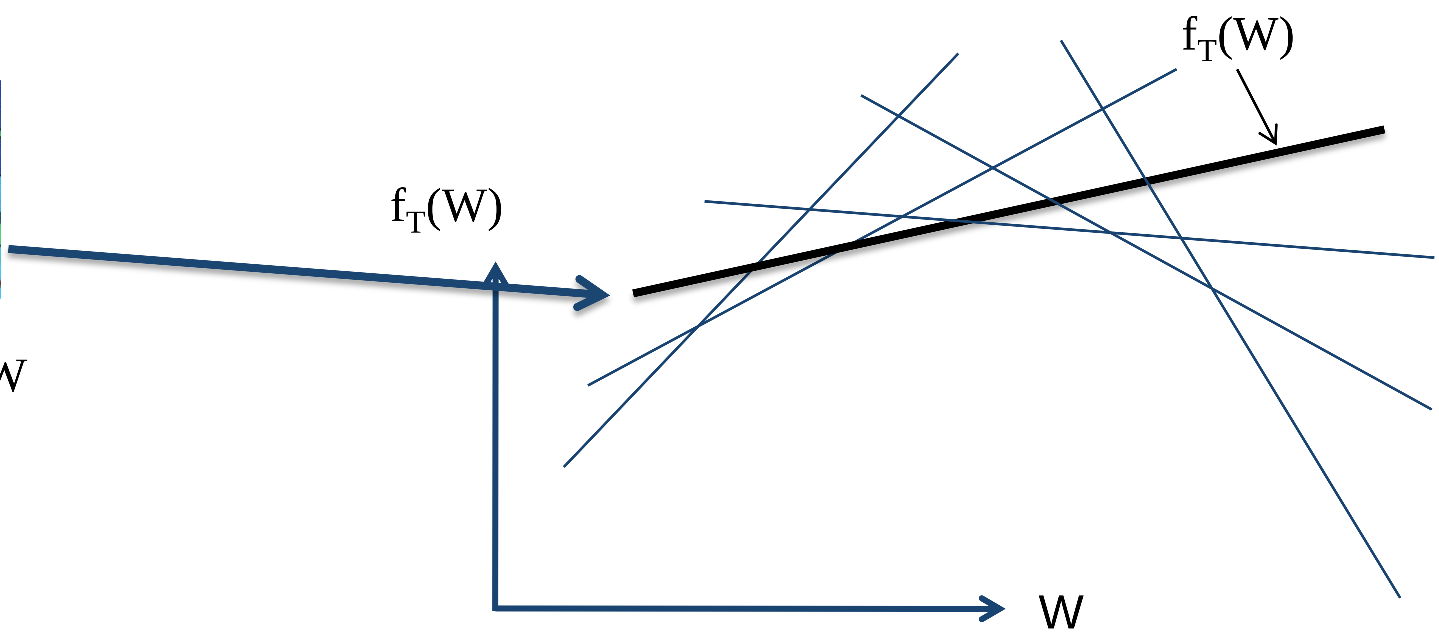
Fixed T



$f_T(W)$ is linear in W

Part. 3 Optimal Transport – the AHA paper

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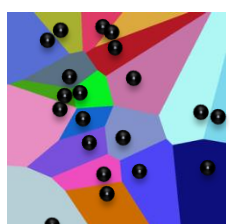
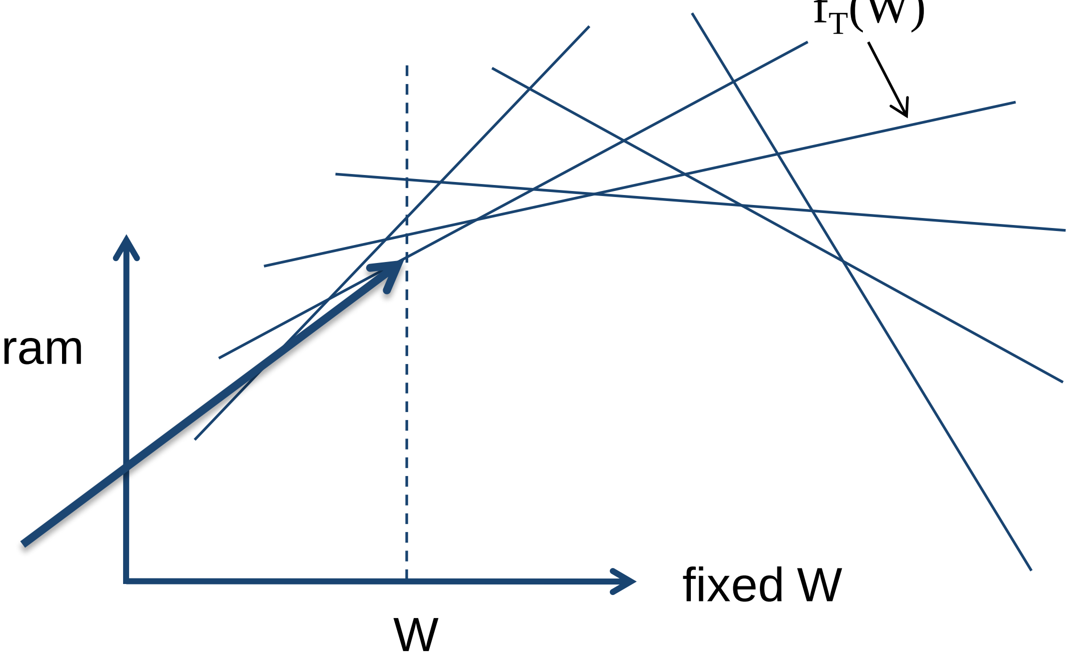
Consider the function $f_T(W) = \int \left(\| x - T(x) \|^2 - \psi(T(X)) \right) d\mu(x)$

$f_T(W)$ is linear in W

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





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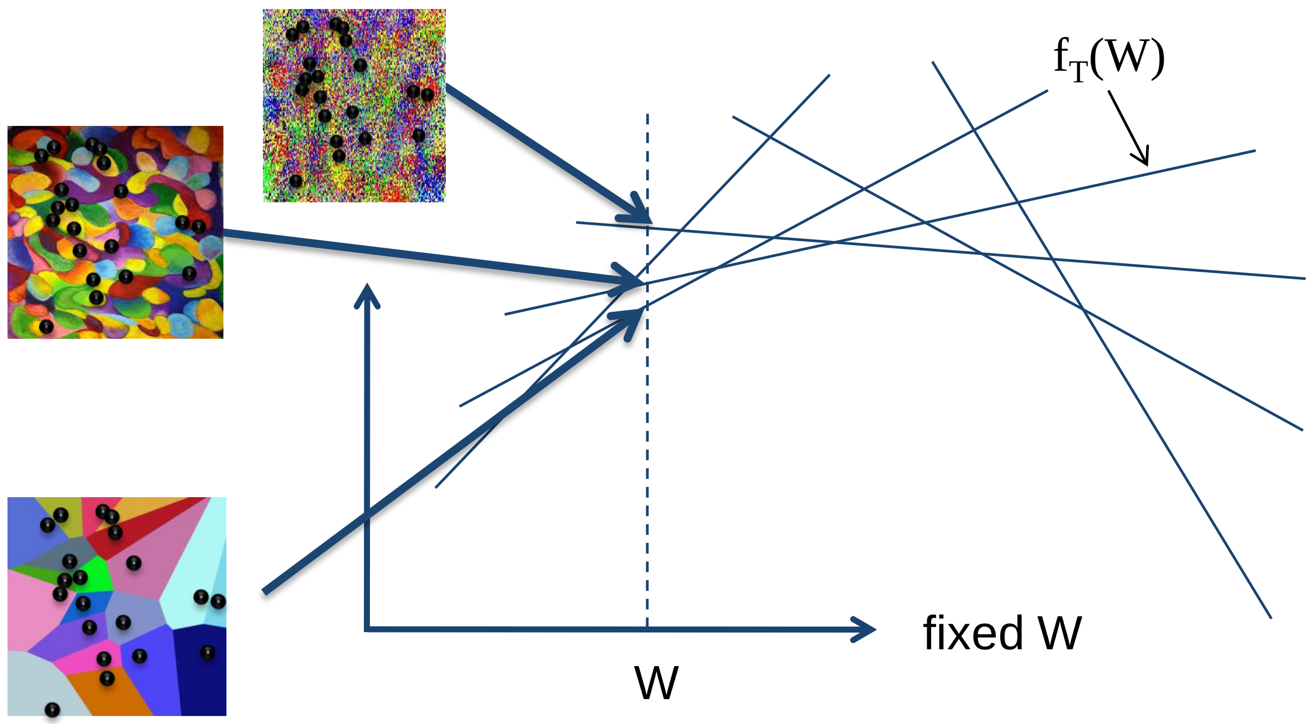
$f_T(W)$ is linear in W

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



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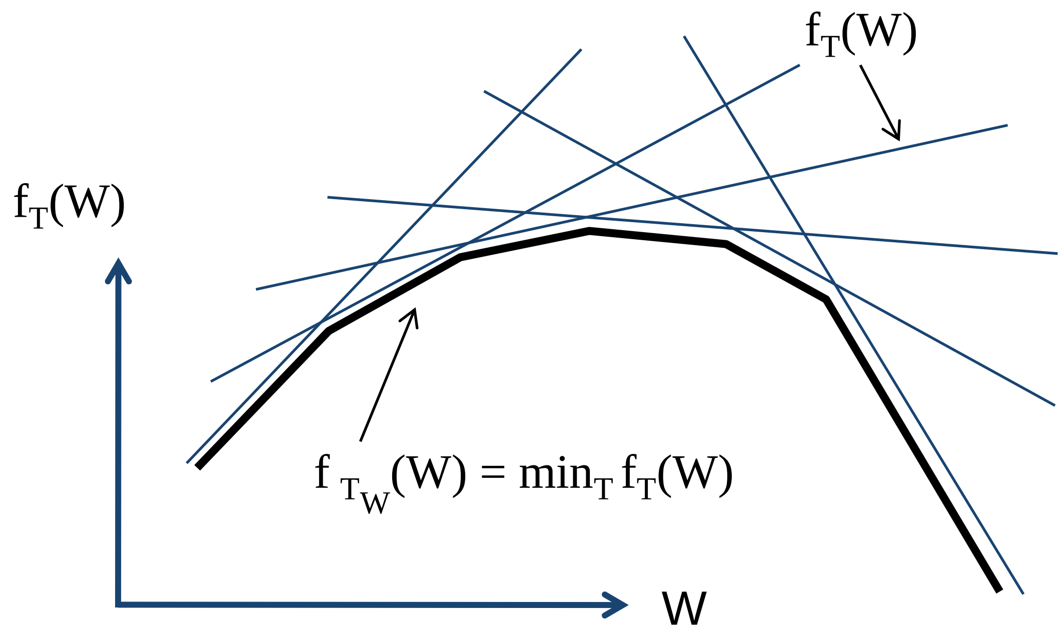
$f_T(W)$ is linear in W

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

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



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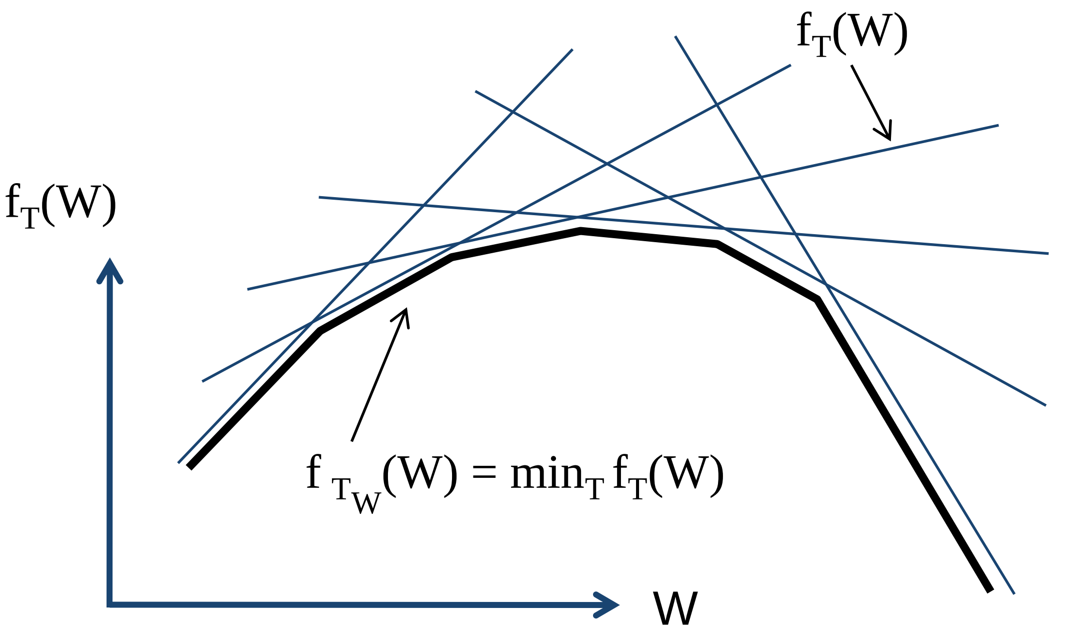

Consider $g(W) = f_{T_W}(W) + \sum v_j \psi_j$

Part. 3 Optimal Transport – the AHA paper

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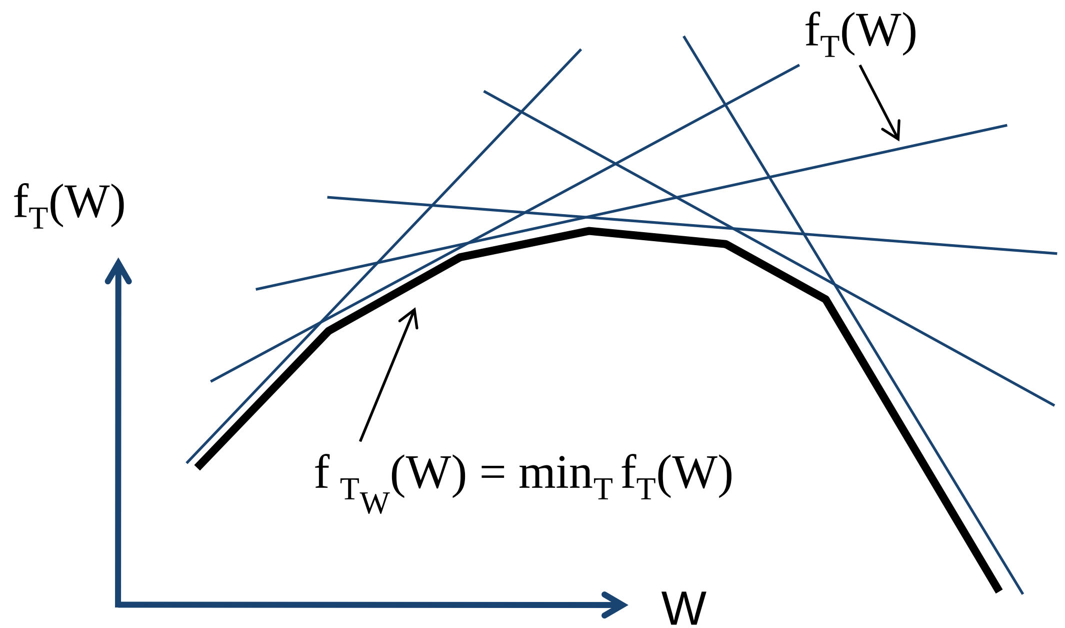
Consider the function $f_T(W) = \int \left(\| x - T(x) \|^2 - \psi(T(X)) \right) d\mu(x)$



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

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

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

Part. 3 Optimal Transport – the algorithm

Semi-discrete OT Summary:

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

Part. 3 Optimal Transport – the algorithm

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$$G(\psi) = g(W) = \sum_j \int_{Lag^\psi(y_j)} \| x - y_j \|^2 - \psi(y_j)\, d\mu + \sum_j \psi(y_j)\, \nu_j$$ is concave

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

<u>Semi-discrete OT Summary:</u>

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$$\partial G / \partial \psi_j = \underbrace{v_j}_{\text{Desired mass at } y_j} - \underbrace{\int_{Lag(yj)} d\mu(x)}_{\text{Mass transported to } y_j} \quad (= 0 \text{ at the maximum})$$

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

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

$$\partial^2 G / \partial \Psi_i \Psi_j = - \partial / \partial \Psi_j \int_{Lag(yj)} d\mu(x)$$

Part. 3 Optimal Transport – the Hessian

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

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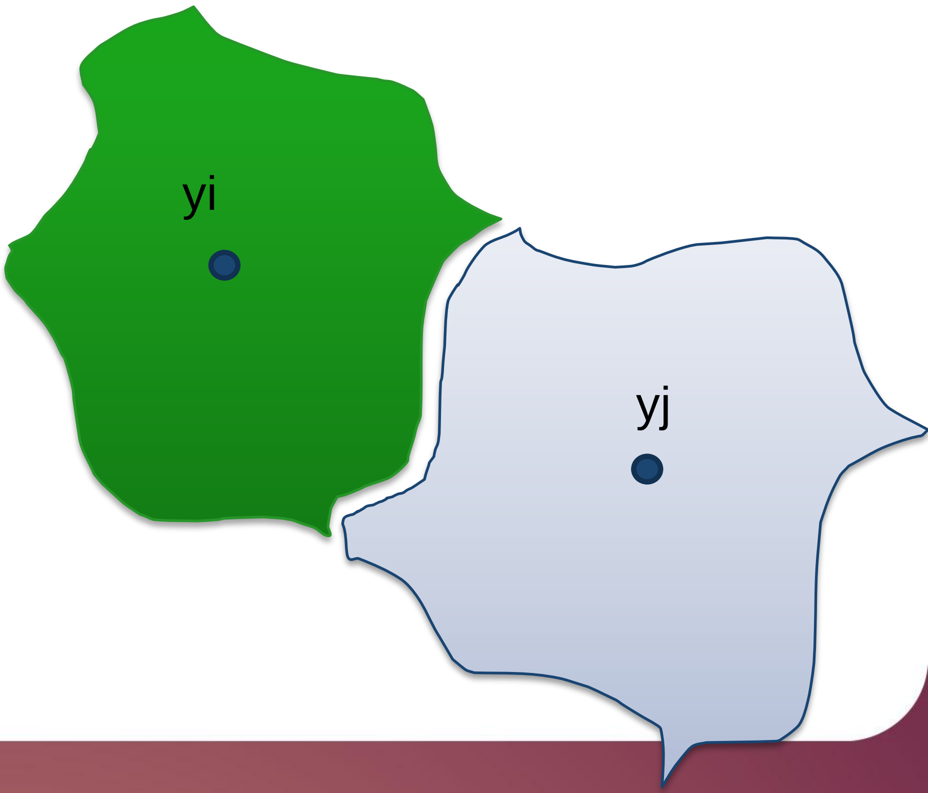
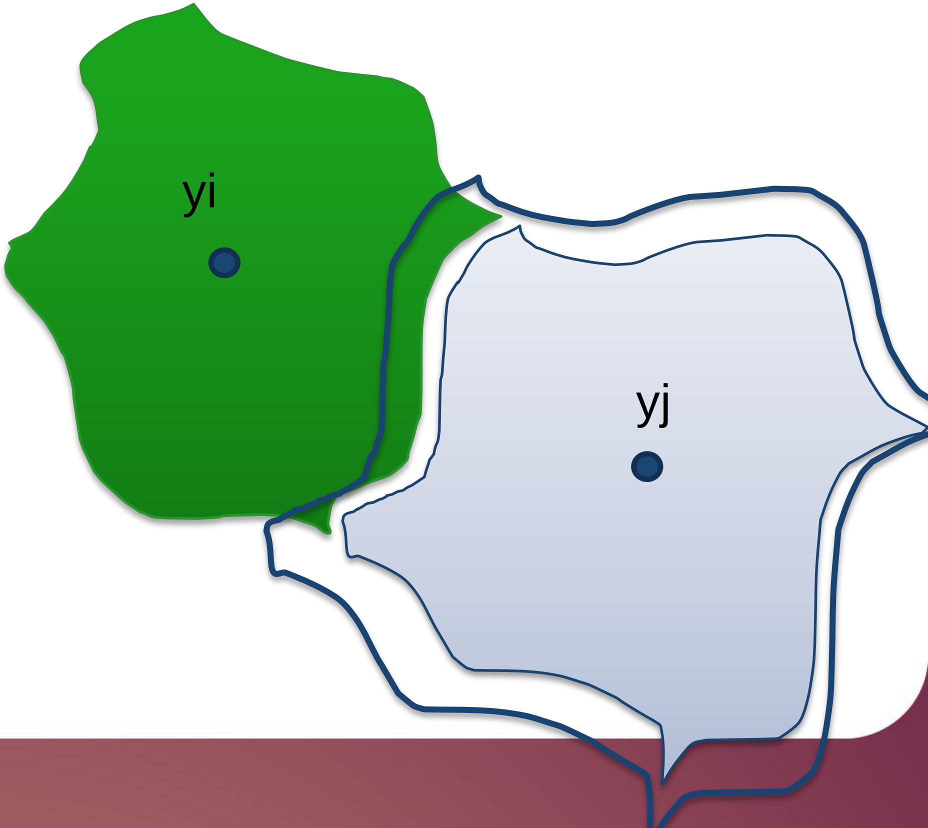


Part. 3 Optimal Transport – the Hessian

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

$$\partial^2 G / \partial \psi_i \psi_j = - \partial / \partial \psi_j \int_{Lag(yj)} d\mu(x)$$

$$\psi_j \leftarrow \psi_j + \delta\psi_j$$



Part. 3 Optimal Transport – the Hessian

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

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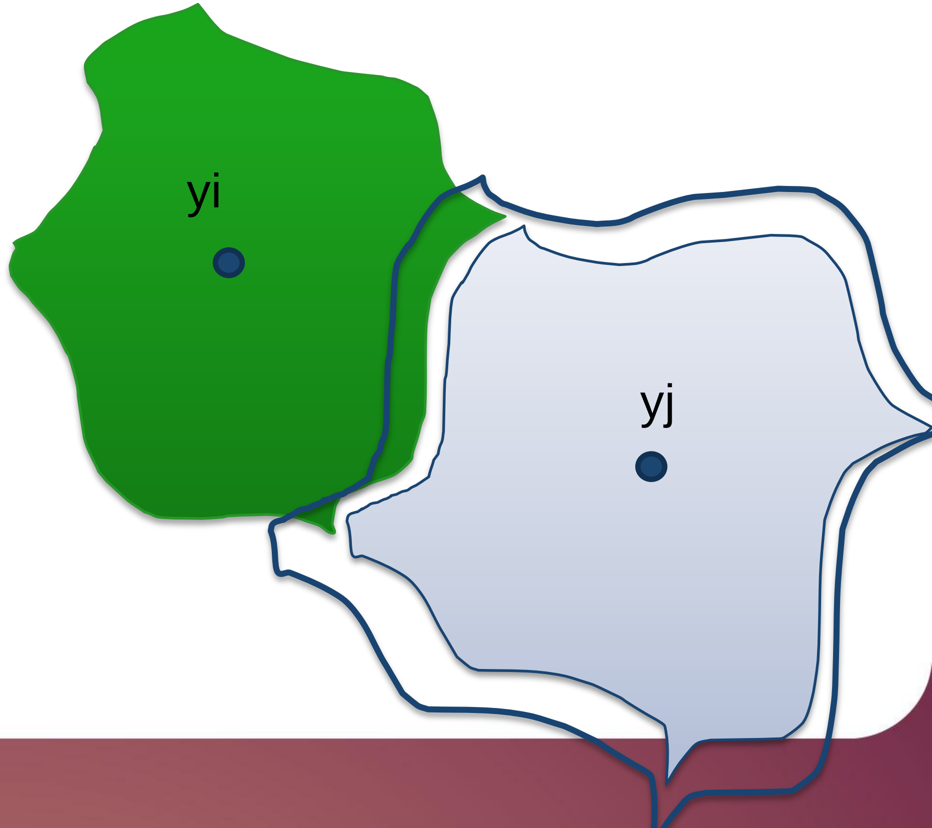
$$\Psi_j \leftarrow \Psi_j + \delta\Psi_j$$

Reynold's thm:

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

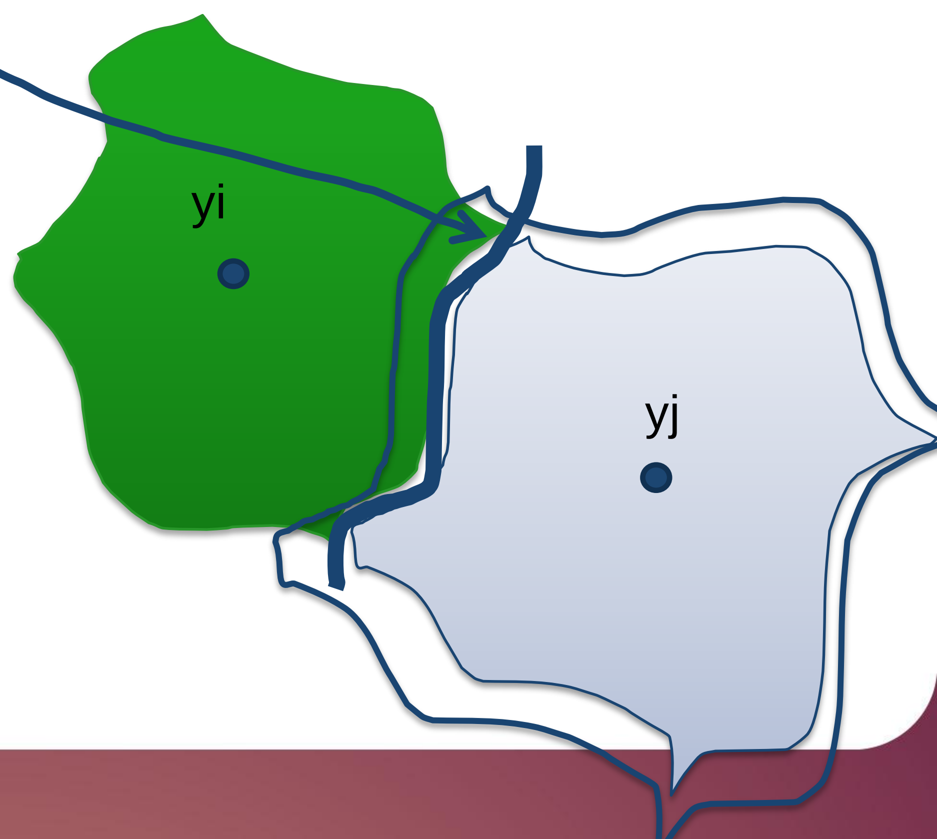


Part. 3 Optimal Transport – the Hessian

Reynold's thm:

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

$f_{ij}(x) = 0$



Part. 3 Optimal Transport – the Hessian

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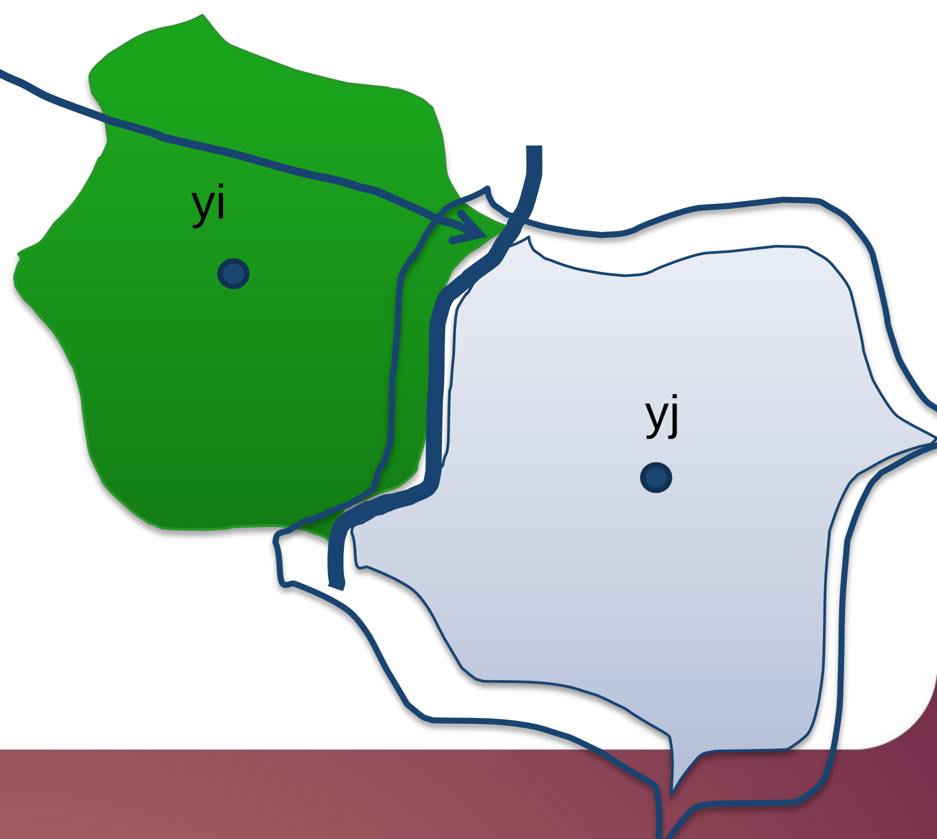
$f_{ij}(x) = 0$

$c(x,y_i) - c(x,y_j) + \psi_j - \psi_i = 0$



Part. 3 the Hessian

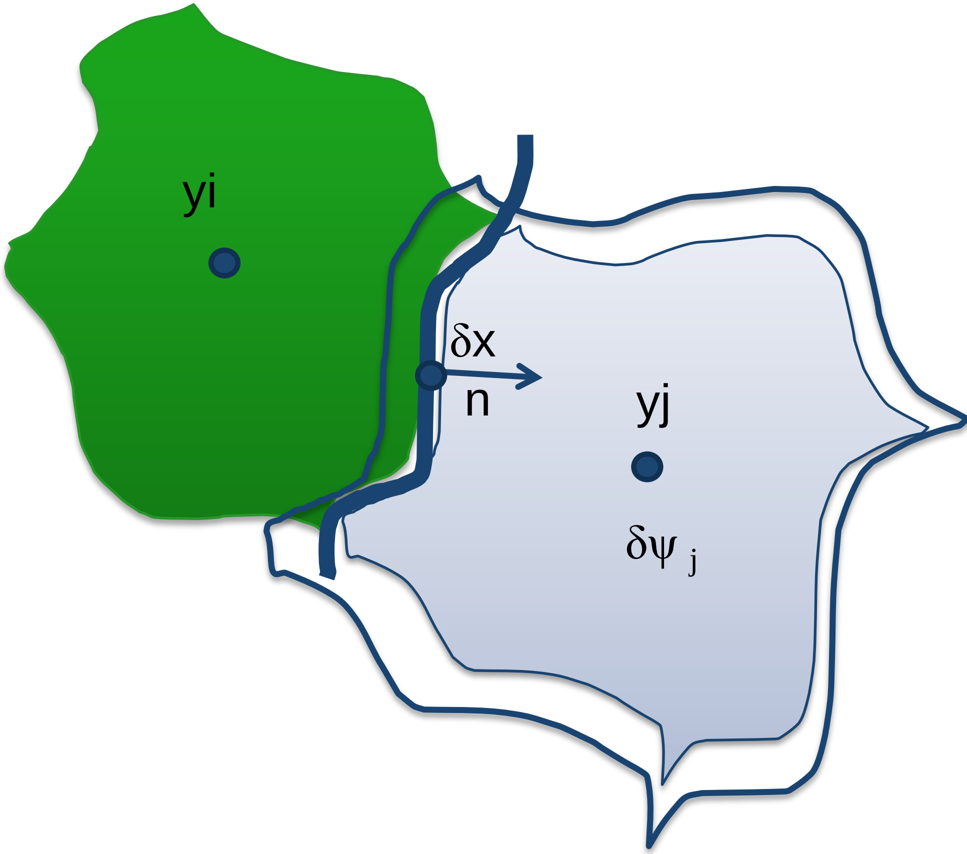
Reynold's thm:

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

$f_{ij}(x) = 0$

$c(x,y_i) - c(x,y_j) + \psi_j - \psi_i = 0$

$df_{ij} = \mathrm{grad}_x(c(x,y_i) - c(x,y_j))dx + d\psi_j$



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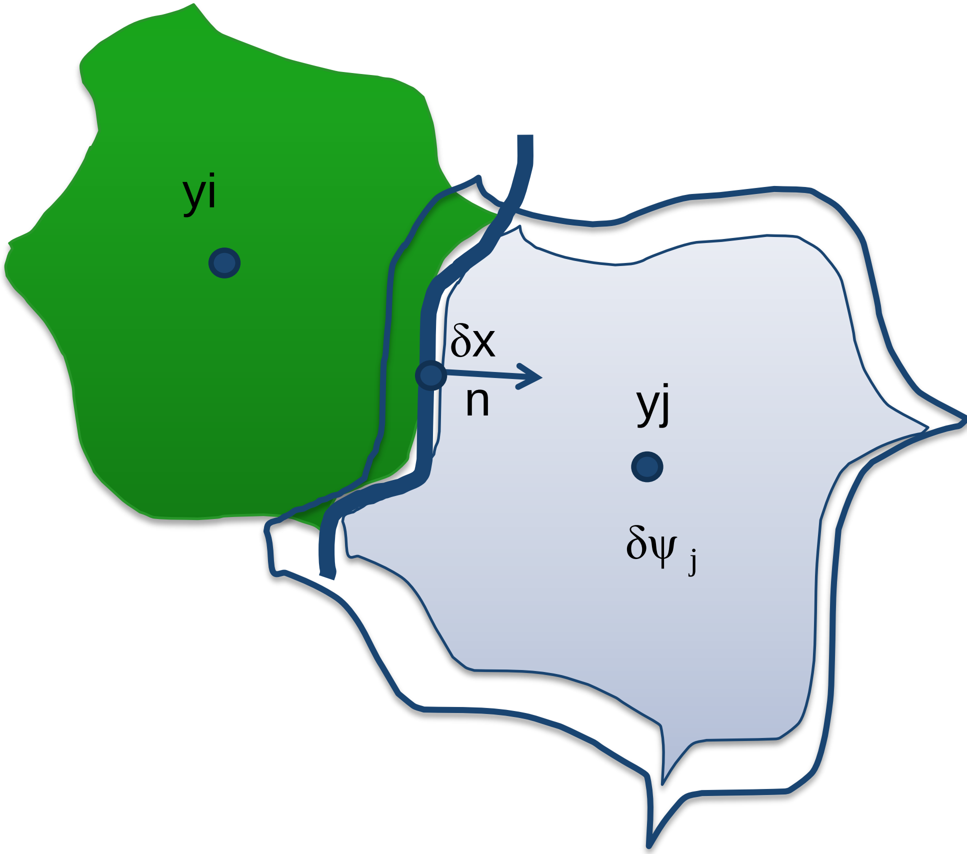
$\delta x = \delta h \, n = \delta h \, grad_x f_{ij}(x) / || grad_x f_{ij}(x)||$



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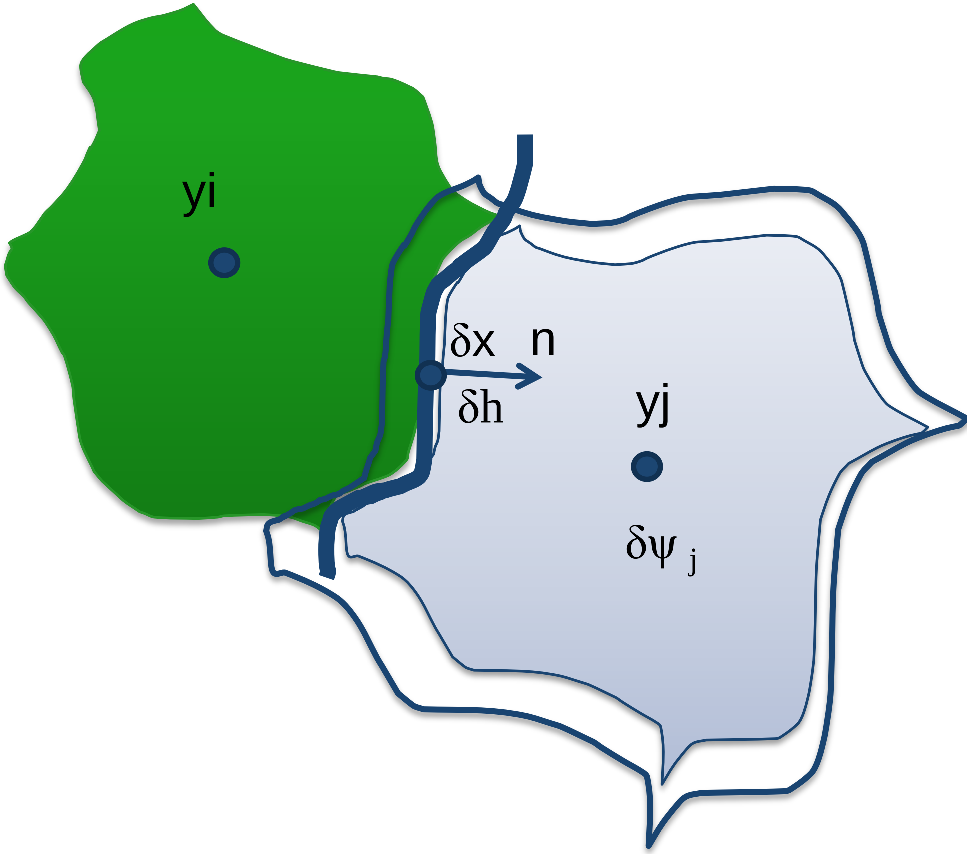

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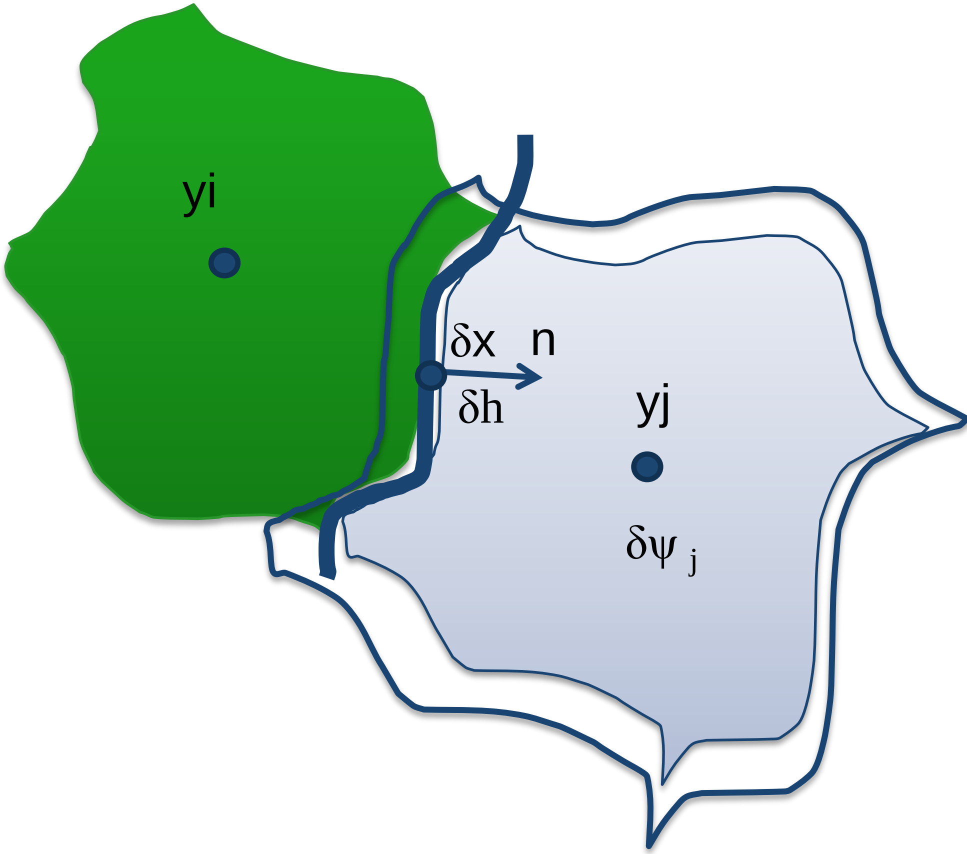

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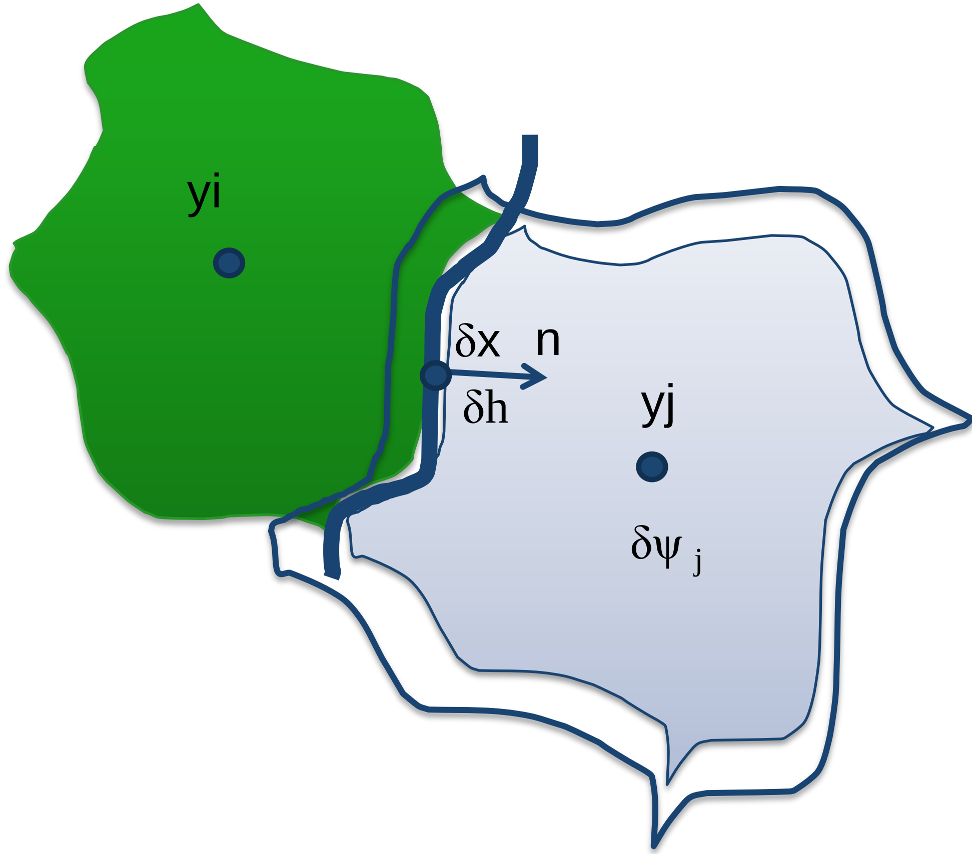
Part. 3 the Hessian



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

Part. 3 the Hessian

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

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

Part. 3 the Hessian

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

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

Part. 3 the Hessian

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

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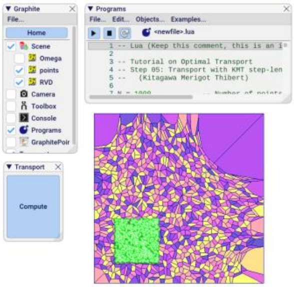
IP_1 FEM Laplacian (not a big surprise)

Part. 3 Optimal Transport
Let’s program it !

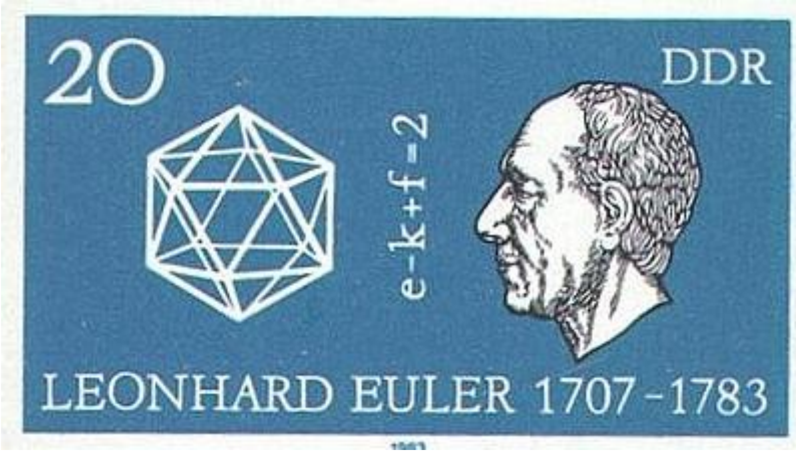
Hierarchical algorithm [Mérigot]
Geometry, 3D [**L**], [**L**, Schwindt]
Damped Newton algorithm, [Kitagawa, Mérigot, Thibert]



4

Optimal Transport

applications in computational physics



Euler

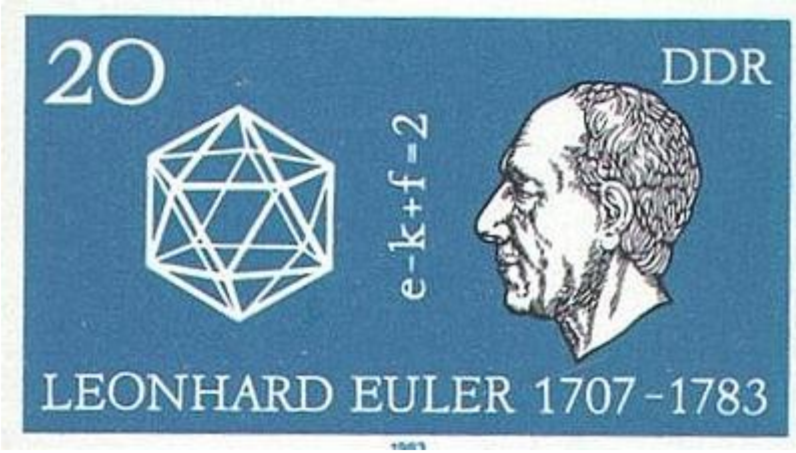
Hamilton,
Legendre,
Maupertuis

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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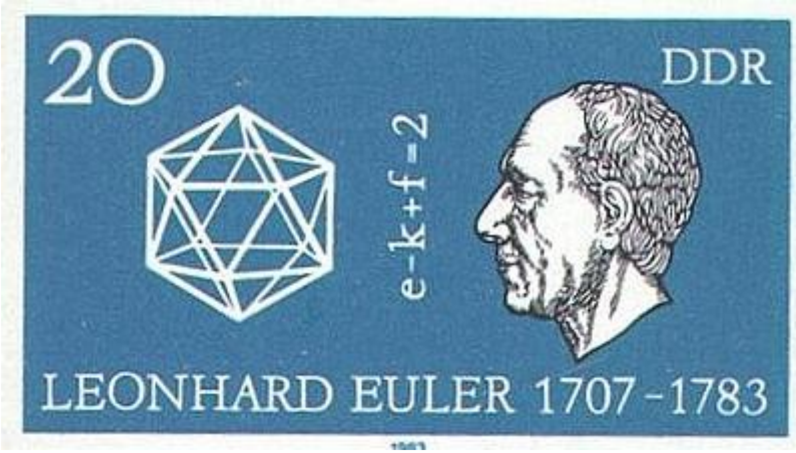

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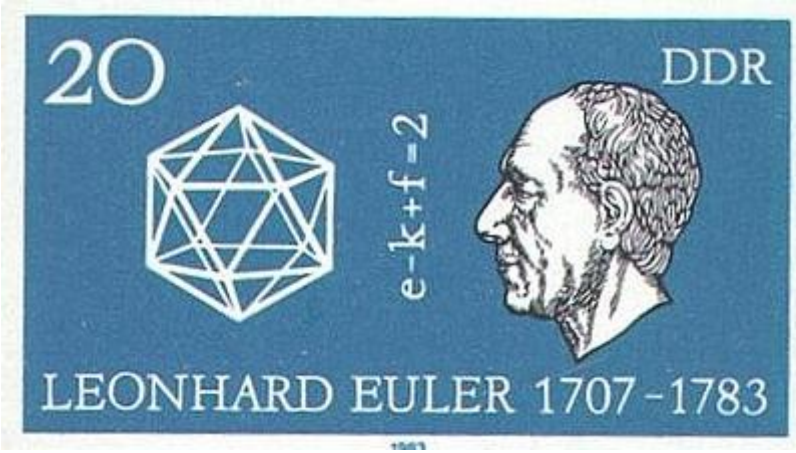

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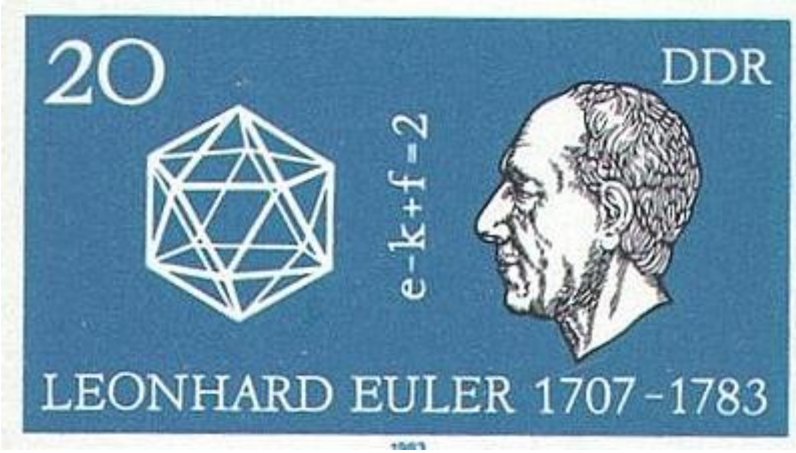

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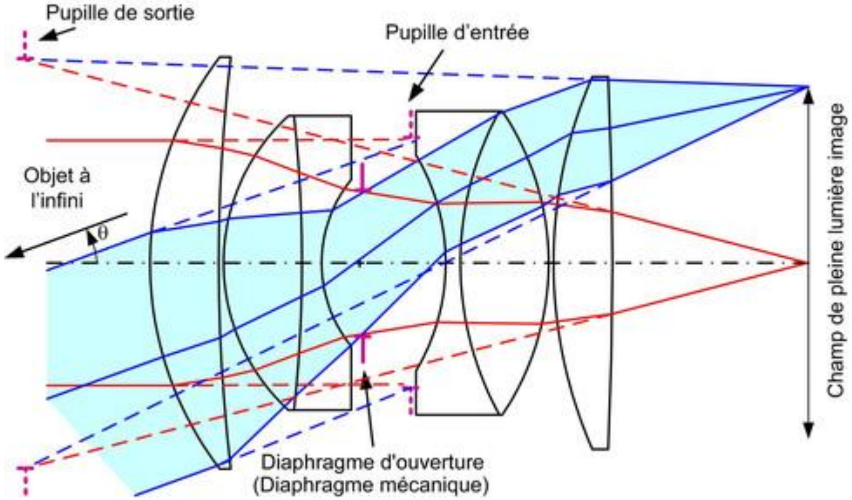
The Least Action Principle

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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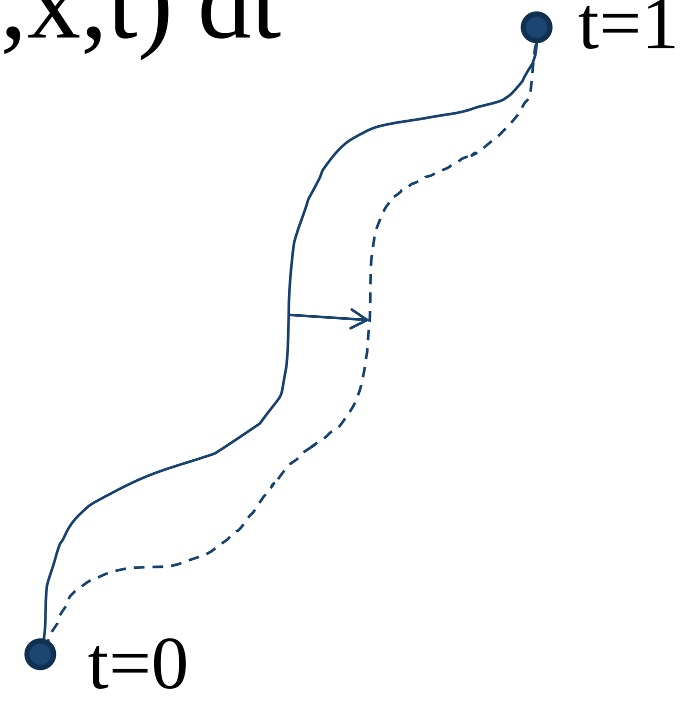

Theorem 1: (Lagrange equation):

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

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:

$$\dot{x}\frac{\partial L}{\partial \dot{x}} - L = cte$$

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Preservation of **energy**

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

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Preserved quantities

"Integrals of Motion"

Noether's theorem

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Free particle:

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

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Expression of the Lagrangian:

$$L = ½\, m\, v^2$$

Axiom 3:
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<u>Free particle:</u>

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

Expression of the Lagrangian:

$$L = \frac{1}{2} m v^2$$

Expression of the Energy:

$$E = \frac{1}{2} m v^2$$

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Expression of the Energy:

$$E = ½\, m\, v^2$$

Particle in a field:

Expression of the Lagrangian:

$$L = ½\, m\, v^2 - U(x)$$

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Expression of the Lagrangian:

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

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Particle in a field:

Expression of the Lagrangian:

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

Expression of the Energy:

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

Theorem 4:

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

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

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. Lorentz change of frame

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

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

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

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

Theorem 5:

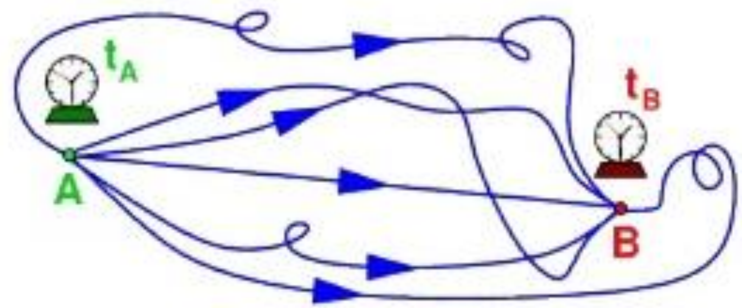
$$E = \tfrac{1}{2} \gamma m v^2 + mc^2$$

The Least Action Principle

(quantum physics setting – just for fun…)

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

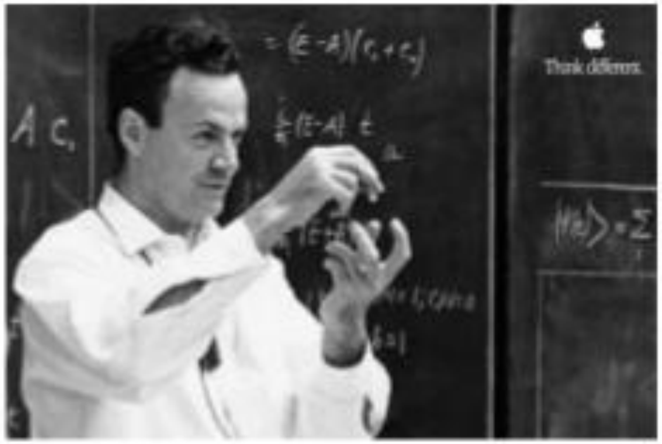
$$P(B,A)=|K(2,1)|^2$$



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

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

?

T

ρ_2

Fluids – Benamou Brenier

ρ_1

$$\xrightarrow[T]{?}$$

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

Fluids – Benamou Brenier

ρ_1

$\xrightarrow[T]{?}$

ρ_2

Minimize

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

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

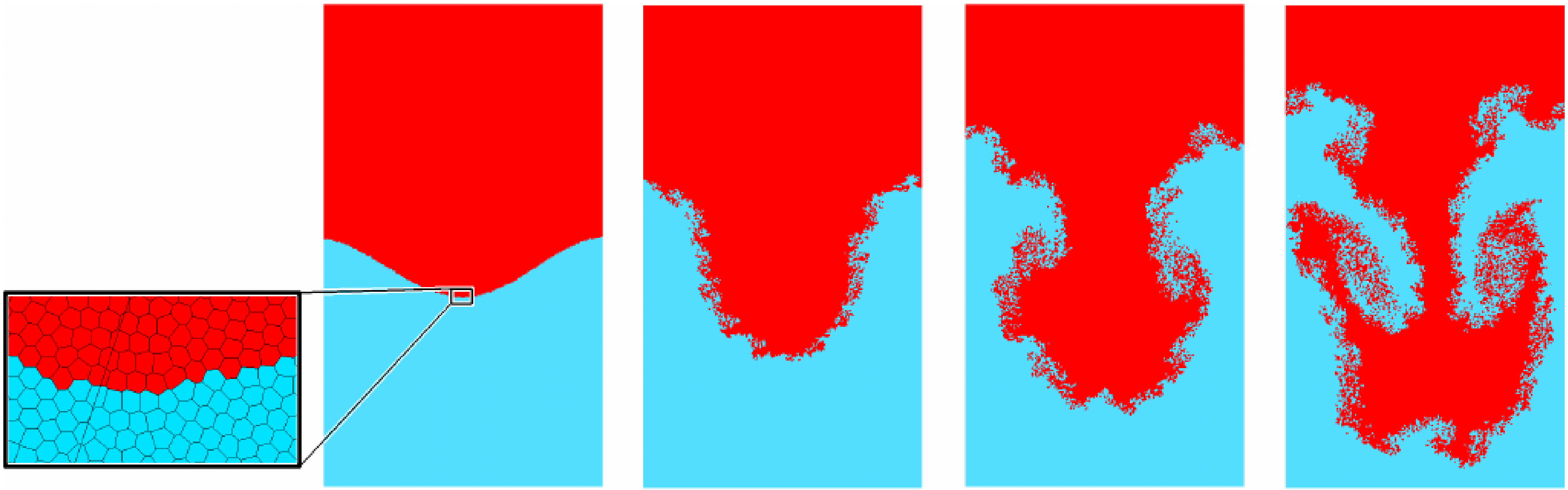
$\Leftrightarrow$

Minimize C(T) =

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

s.t. T is measure-preserving

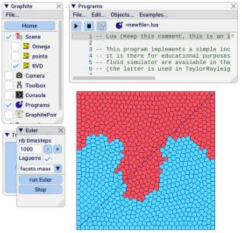
Part. 4 Optimal Transport – Fluids



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

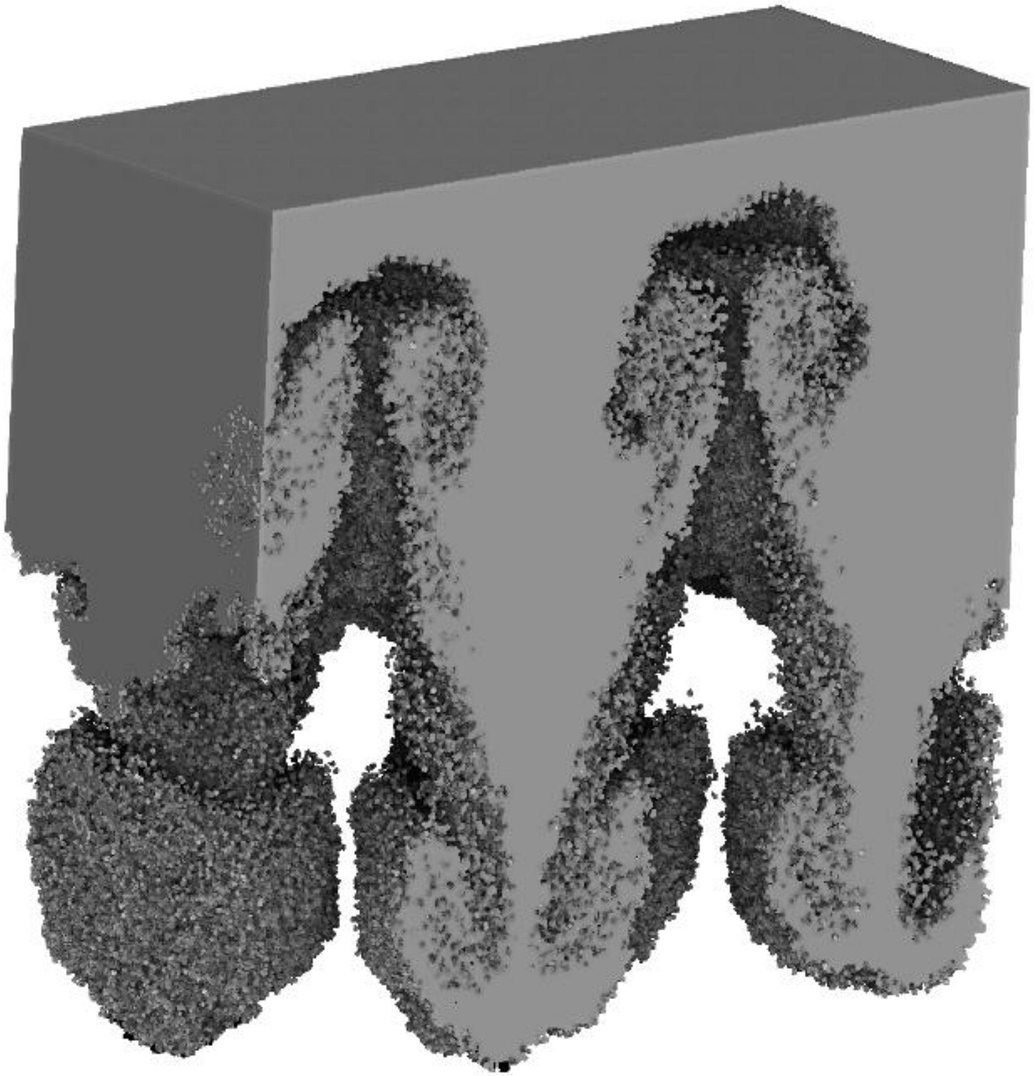
Part. 4 Optimal Transport – Fluids

Let's code it !



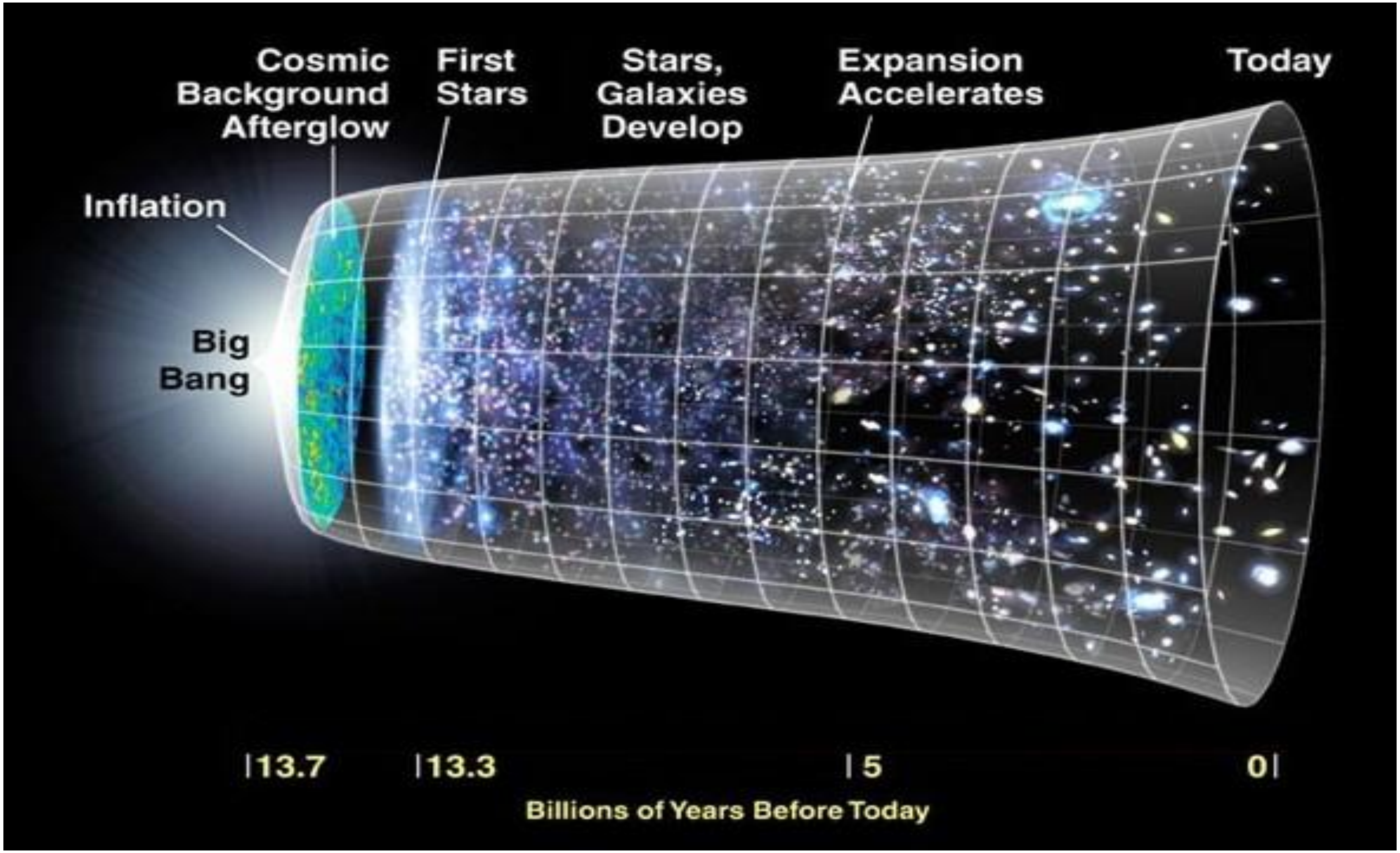
Part. 4 Optimal Transport – Fluids

Part. 4 Optimal Transport – Fluids



Part. 4 Optimal Transport – Fluids

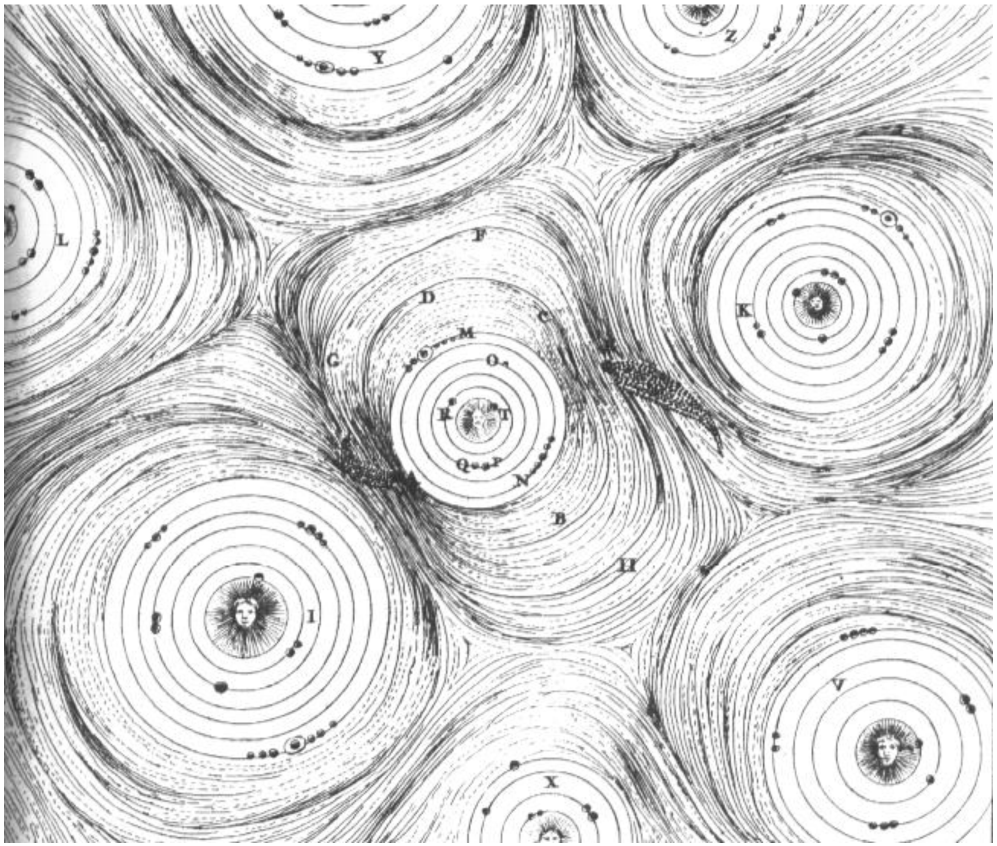
Part. 4 To infinity and beyond…

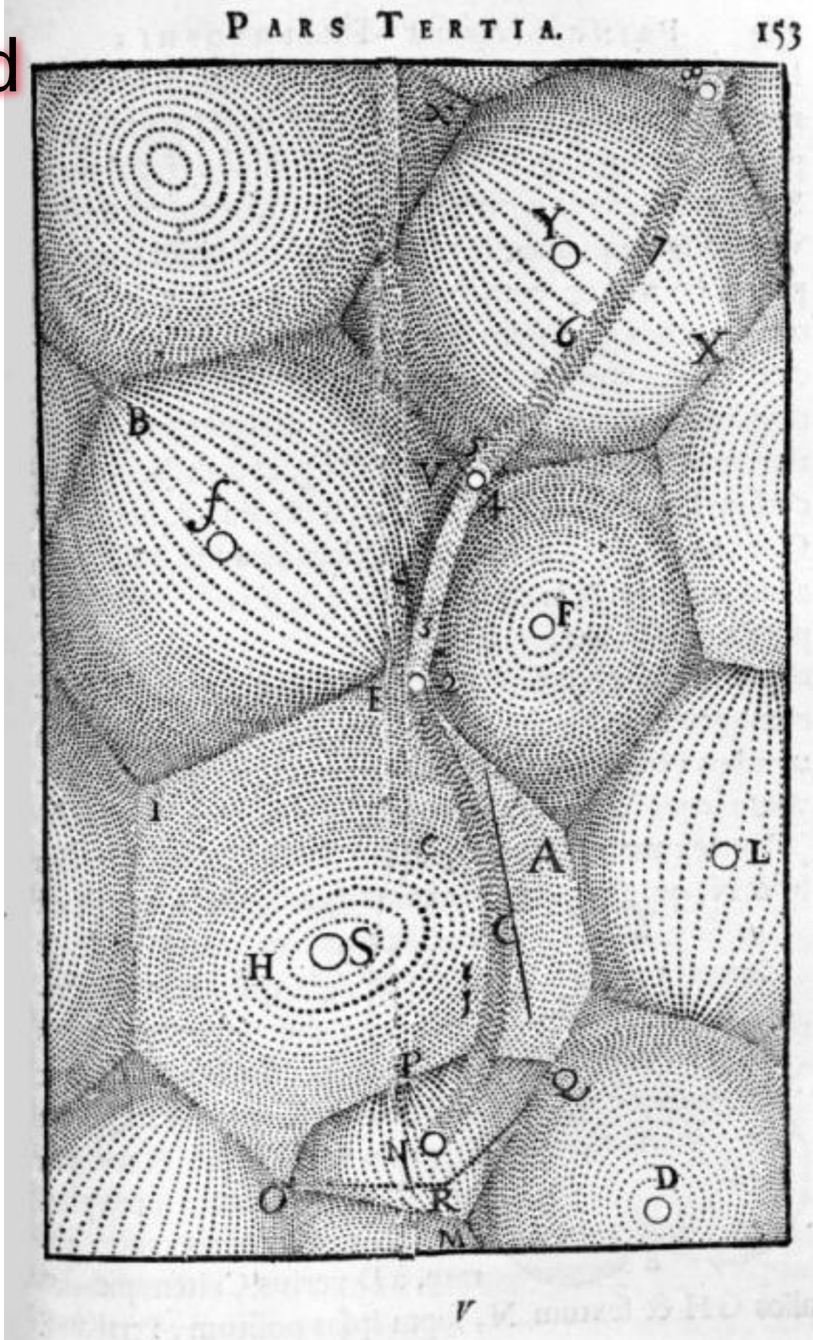


Part. 4 To infinity and beyond

Vortices in “ether” ?

René Descartes - 1663

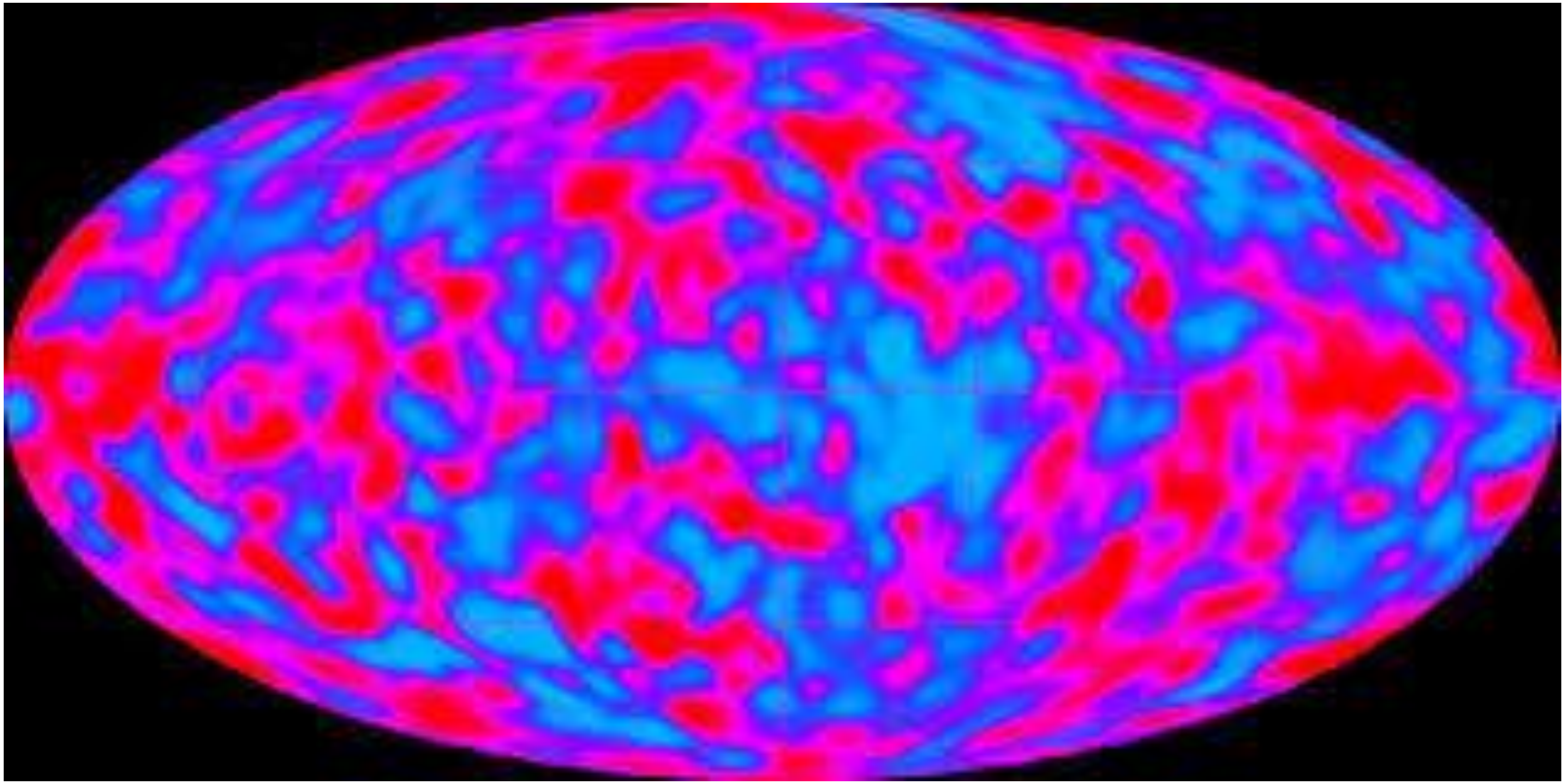




Part. 4 To infinity and beyond…

COBE 1992

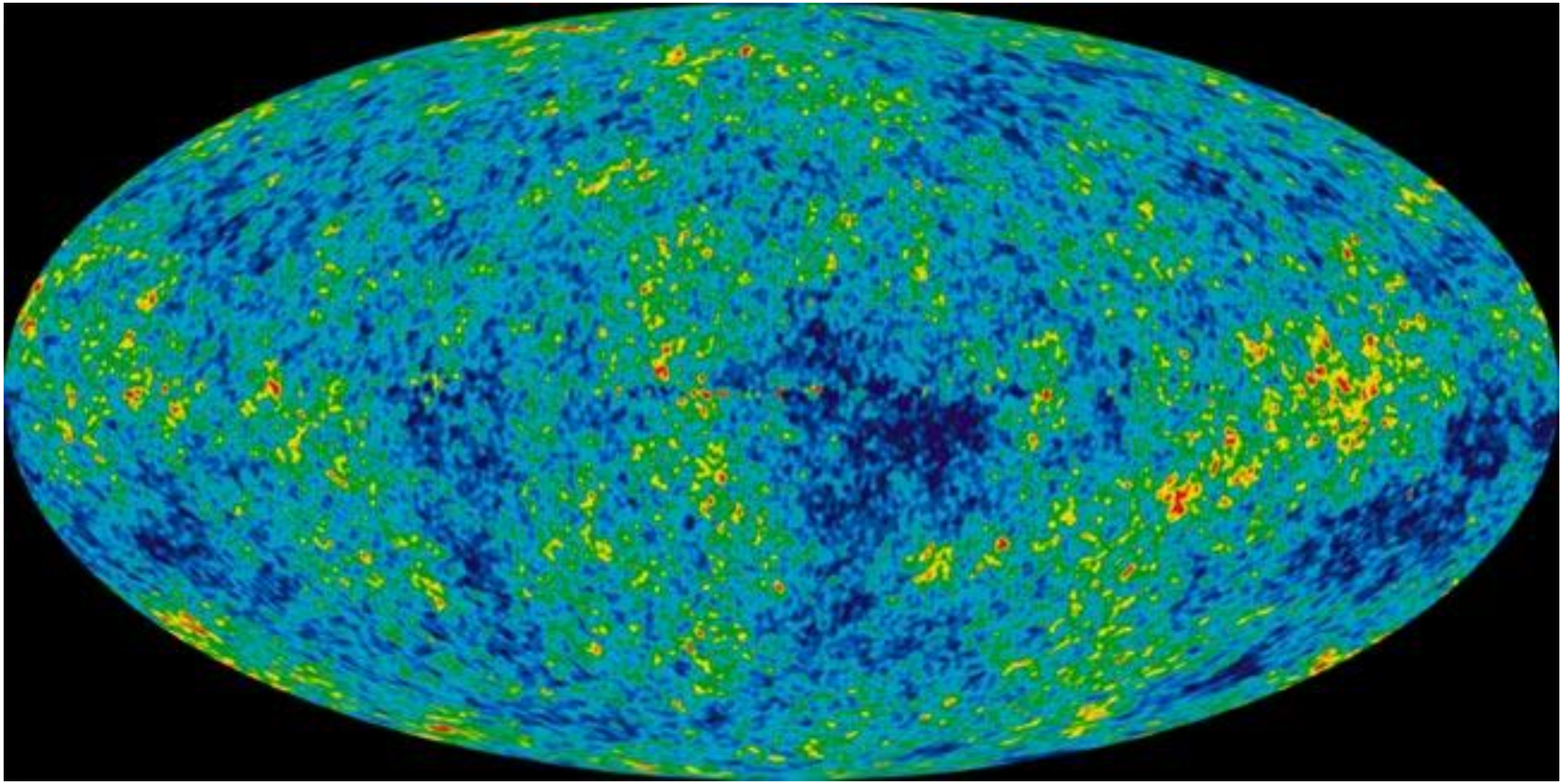
The Data: #1: the Cosmic Microwave Background



Part. 4 To infinity and beyond…

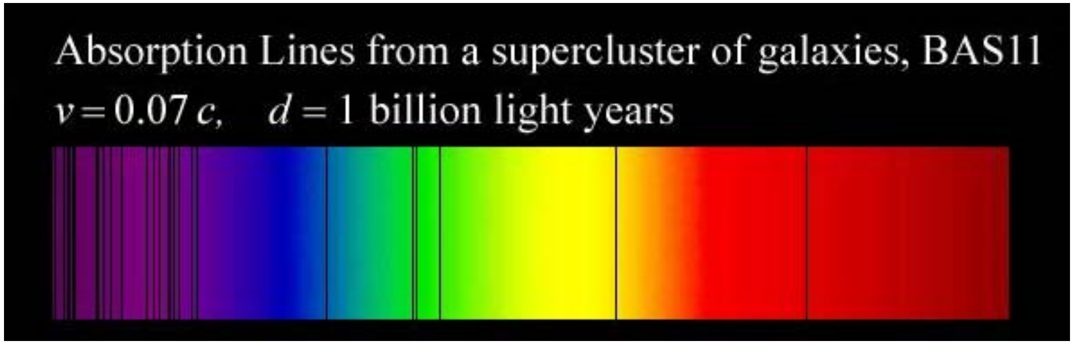
WMAP 2003
2006
2008
2010

The Data: #1 the Cosmic Microwave Background



Part. 4 To infinity and beyond…

The Data: #2 redshift acquisition surveys



Part. 4 To infinity and beyond…

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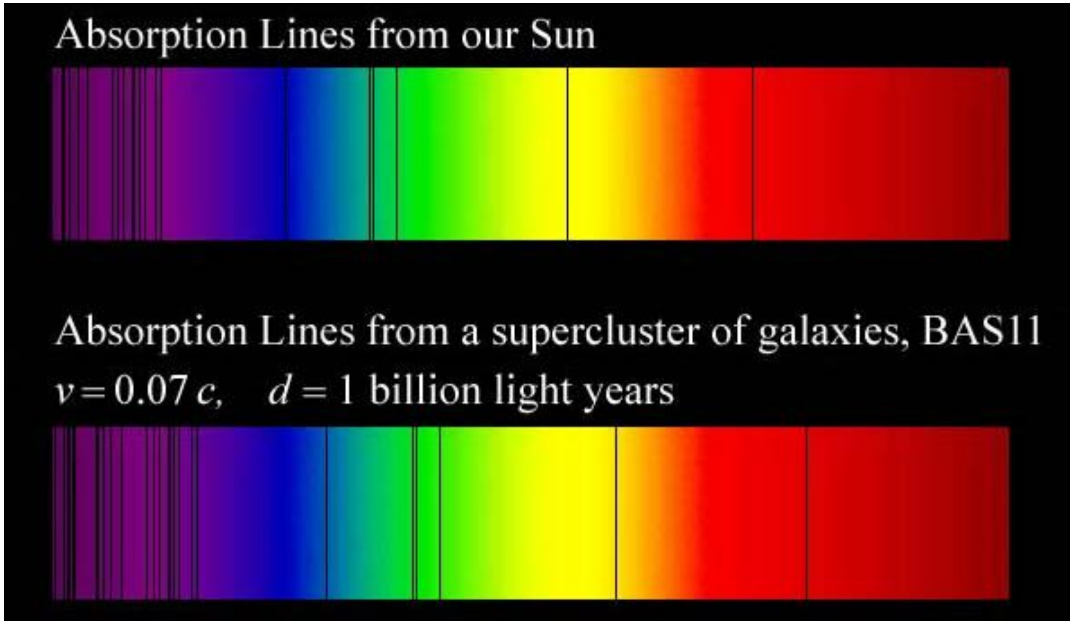
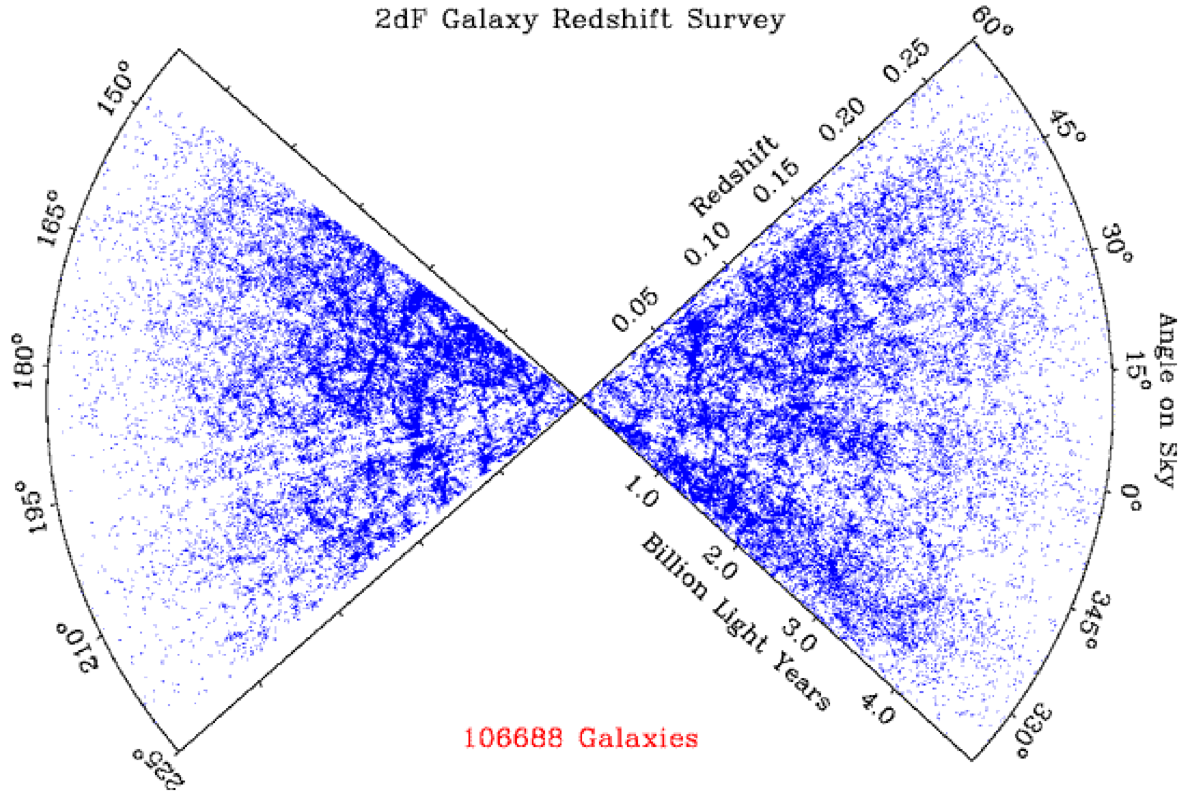


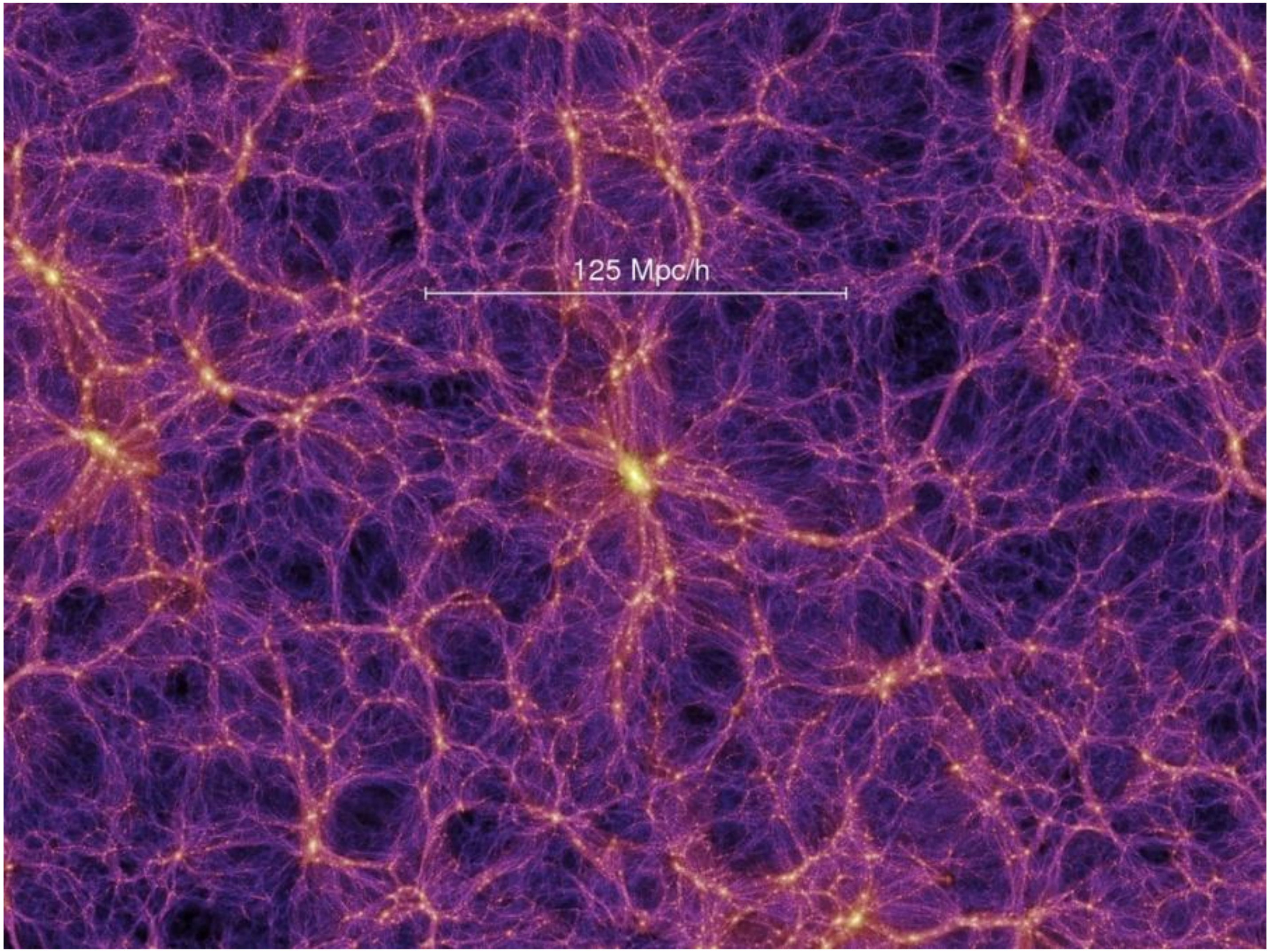
Part. 4 To infinity and beyond…

The Data: #2 redshift acquisition surveys



Part. 4 To infinity and beyond…

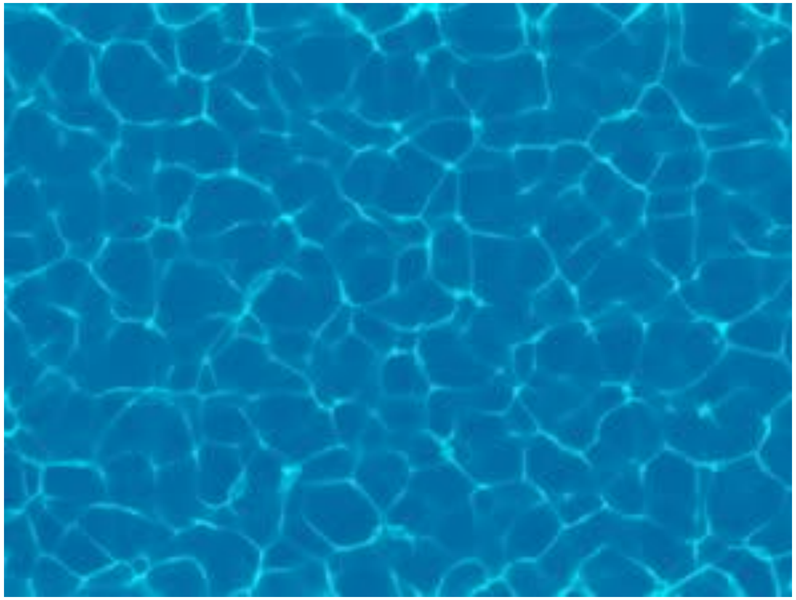
pc/h : parsec (= 3.2 années lumières)



The millenium simulation project, Max Planck Institute fur Astrophysik

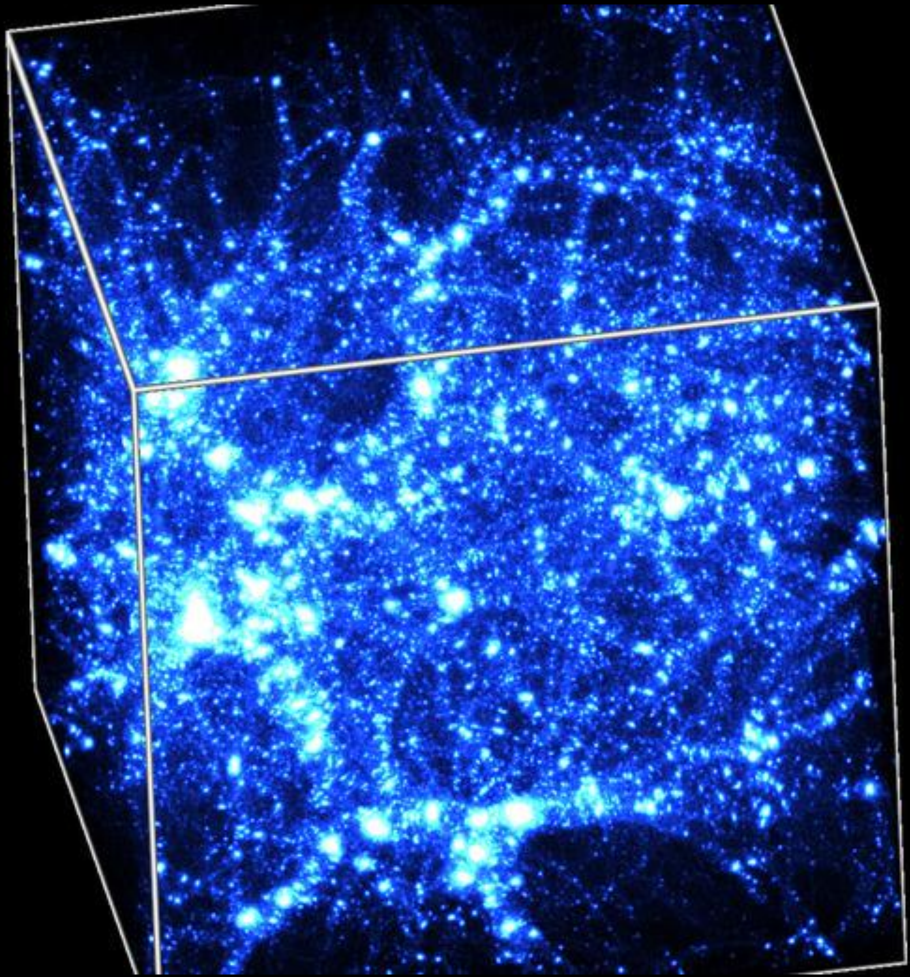
Part. 4 To infinity and beyond…

The universal swimming pool



Early Universe Reconstruction

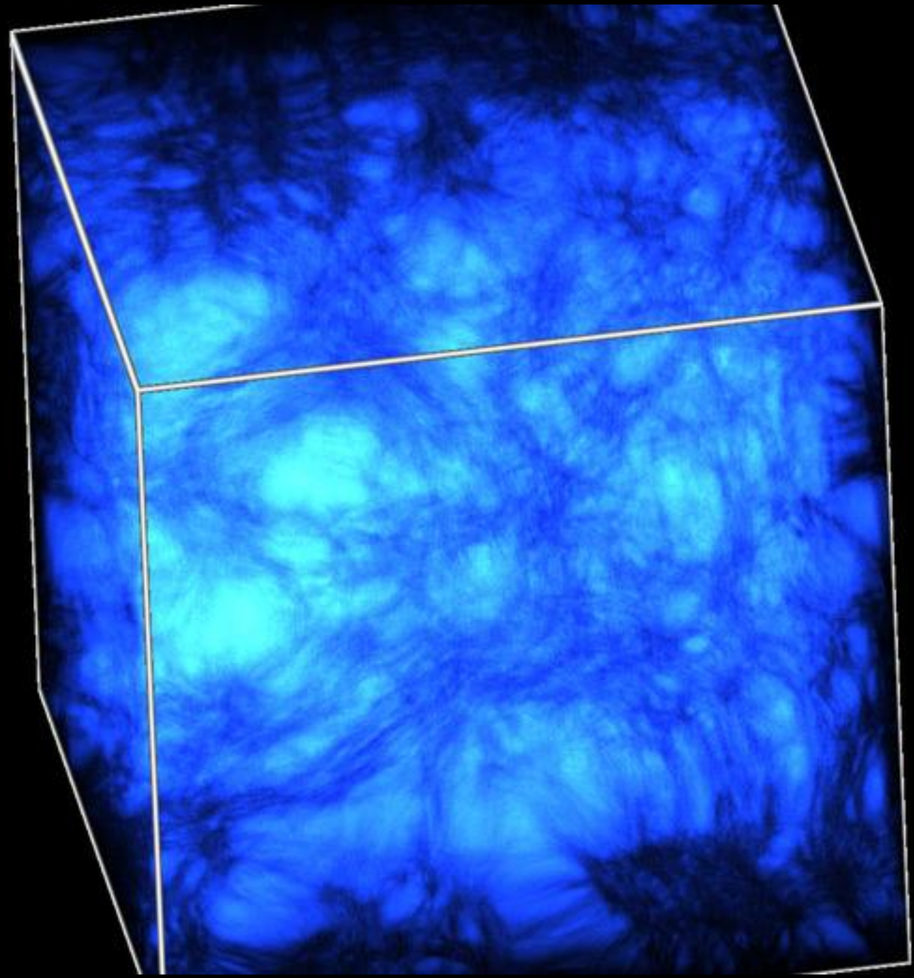
Time = Now



Coop. with MOKAPLAN & Institut d'Astrophysique de Paris & Observatoire de Paris

Early Universe Reconstruction

. . . . .



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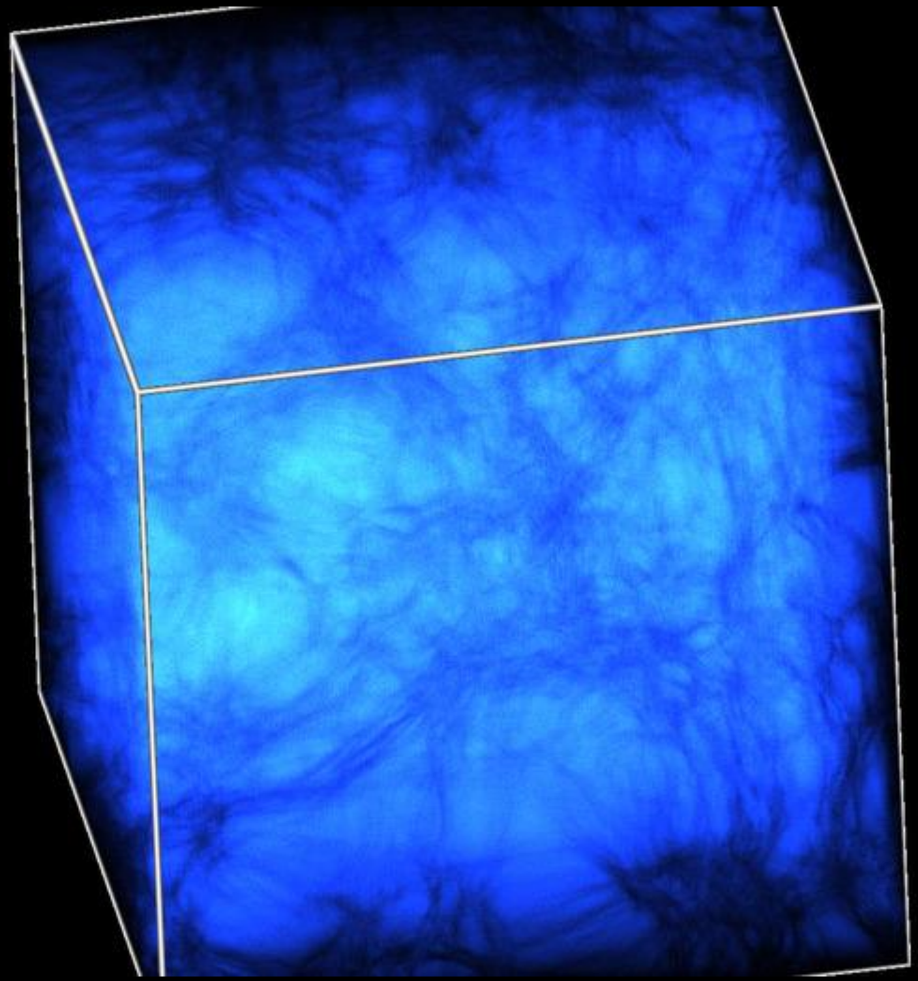
Early Universe Reconstruction

Time = BigBang
(- 13.7 billion Y)



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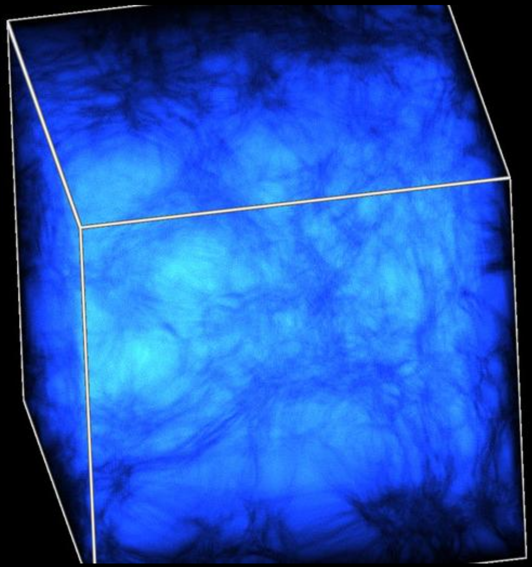
Early Universe Reconstruction

"Time-warped" map of the universe



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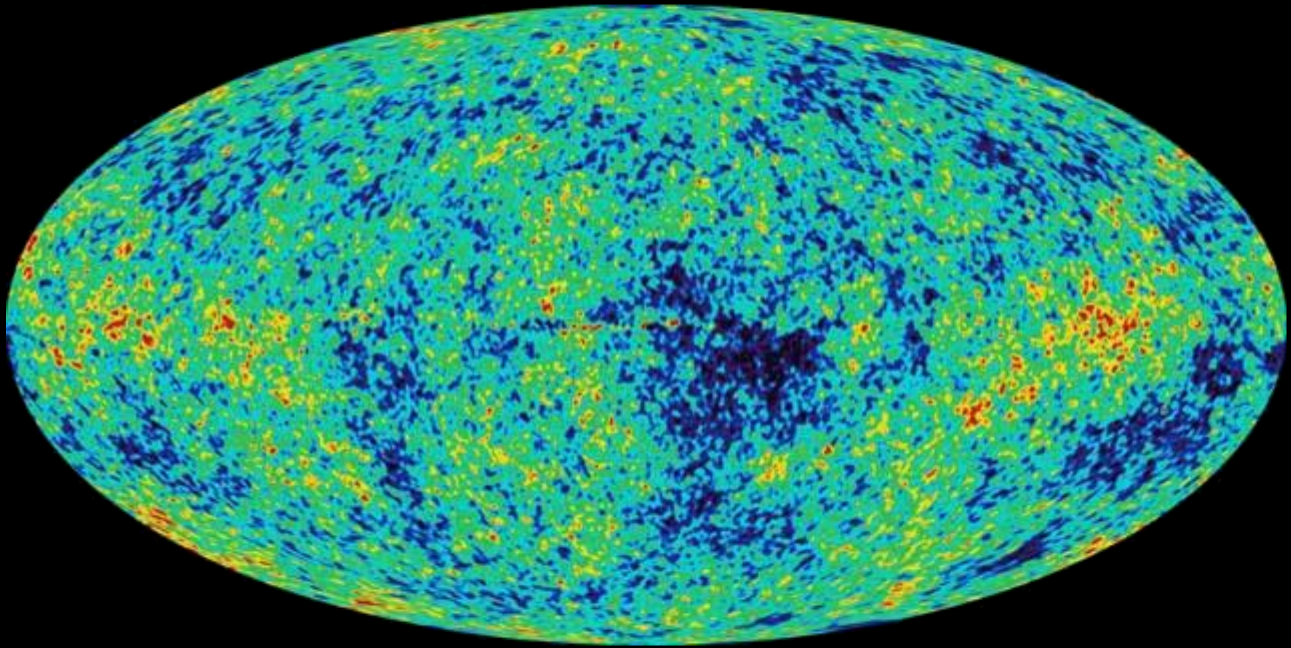
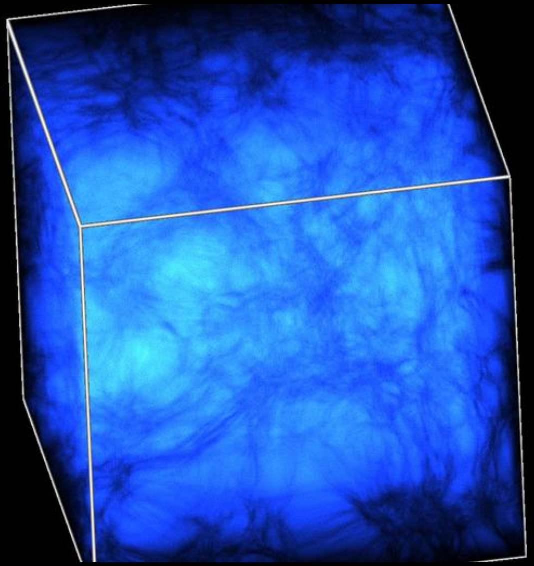
Early Universe Reconstruction



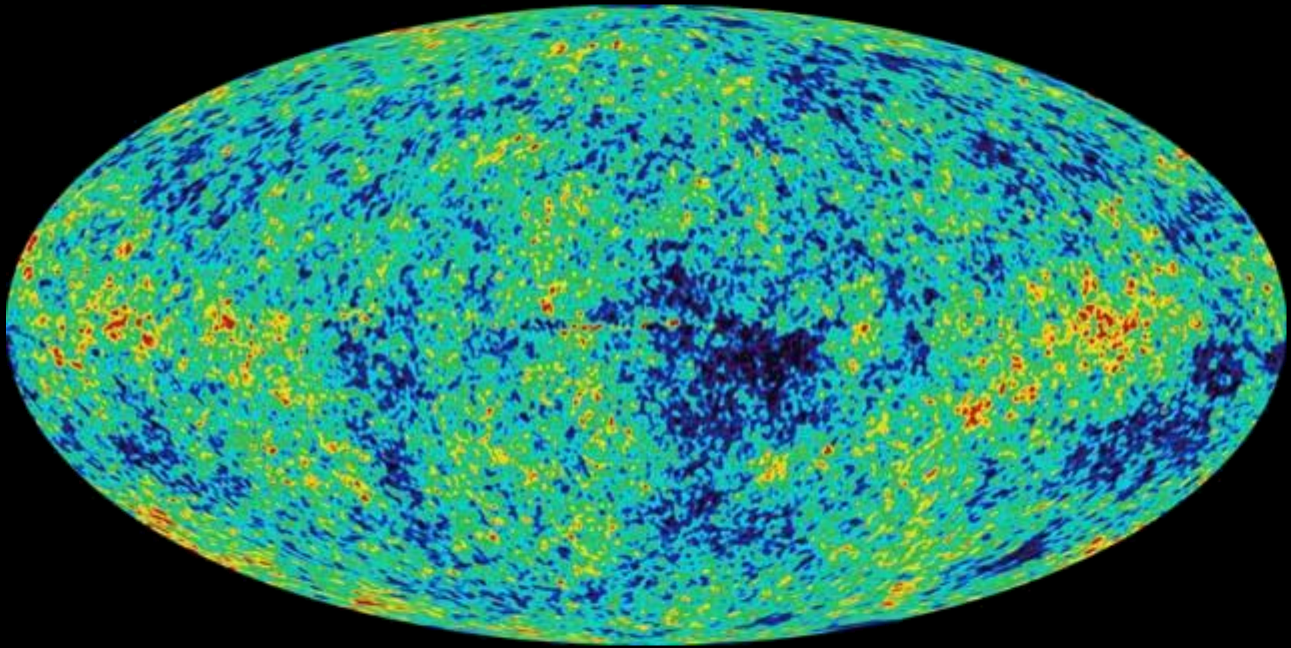
Cosmic Microware Background:
“Fossil light” emitted 380 000 Y after BigBang
and measured now

“Time-warped” map of the universe

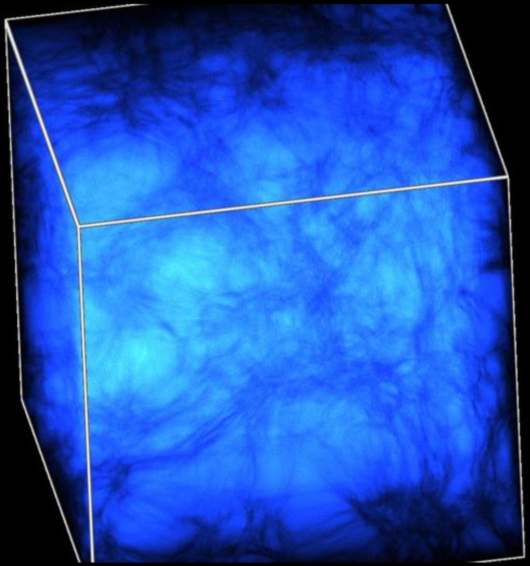


Coop. with MOKAPLAN & Institut d’Astrophysique de Paris & Observatoire de Paris

Early Universe Reconstruction



"Time-warped" map of the universe



Cosmic Microware Background:
"Fossil light" emitted 380 000 Y after BigBang
and measured now

Do they match ?

Coop. with MOKAPLAN & Institut d'Astrophysique de Paris & Observatoire de Paris

Conclusions
Open Questions
References
Online resources

Conclusions – Open questions

* **Connections with physics, Legendre transform and <u>entropy</u> ?**
[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

Topics on Optimal Transportation, 2003
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

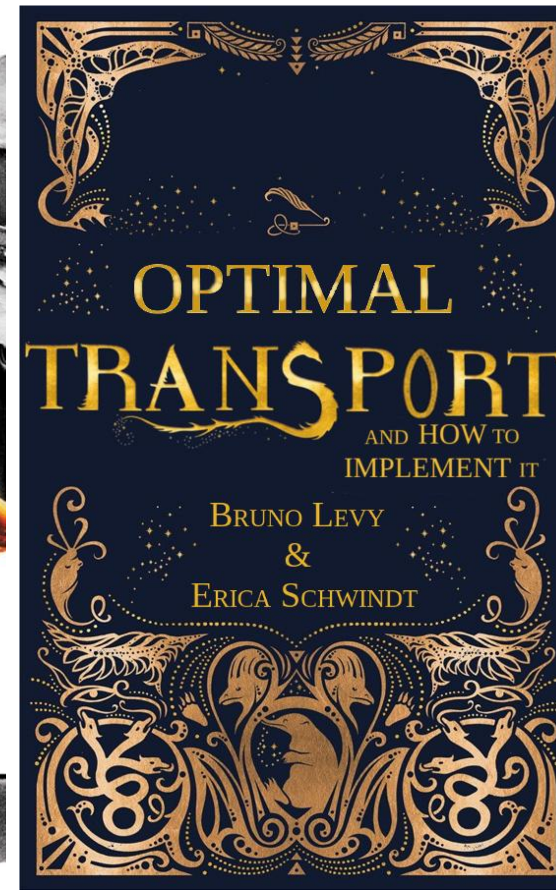
Gabriel Peyré, Marco Cuturi, Computational Optimal Transport, 2018

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.



Bonus Slides

The Isoperimetric Inequality

The isoperimetric inequality

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

The isoperimetric inequality

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

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

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

The isoperimetric inequality

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Consider a compact set Ω such that Vol(Ω) = Vol(B_2^3)
and f = the indicatrix function of Ω

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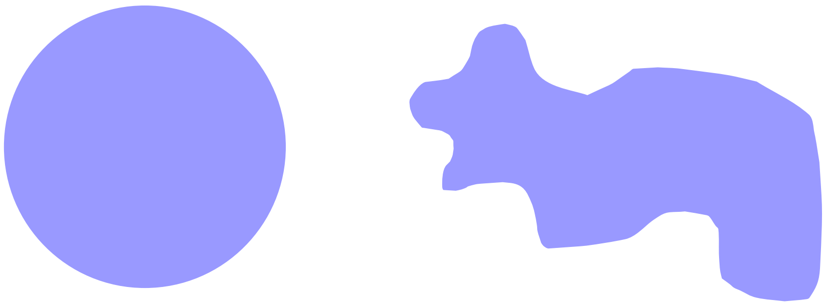

The isoperimetric inequality

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Consider a compact set Ω such that $Vol(\Omega) = Vol(B_2^3)$
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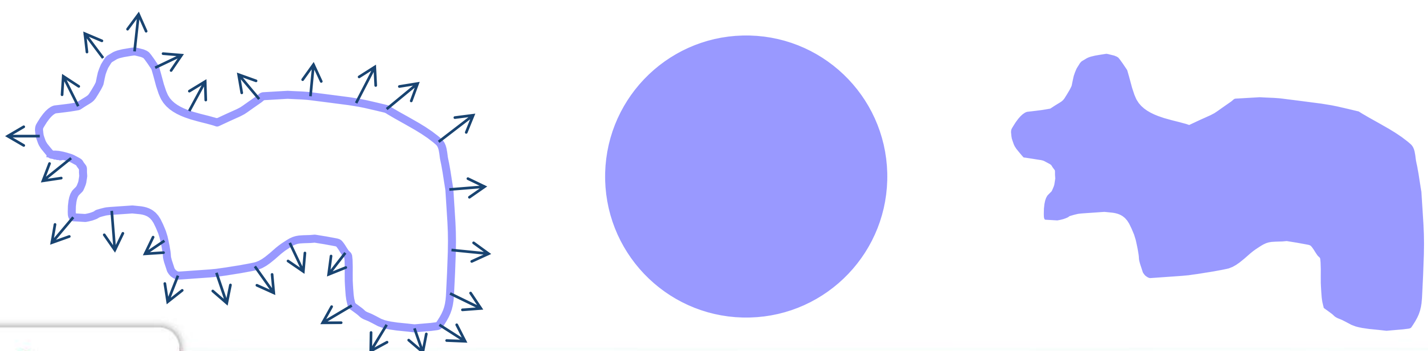
$$\int |\text{ grad } f\,| \;\geq n \; Vol(B_2^n)^{1/n} \left(\int f^{\,n/(n-1)}\right)^{(n-1)/n}$$

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



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

$$\mathrm{Vol}(\partial\Omega) \;\geq\; 4\,\pi \;=\; \mathrm{Vol}(\partial B_2^3)$$

The isoperimetric inequality

L_1 Sobolev inegality: a proof with OT [Gromov]

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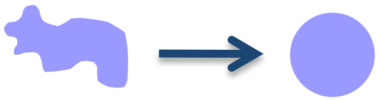
There exists an optimal transport $T = \mathrm{grad}\overline{\Psi}$ between $f^{\,n/(n-1)}(x)dx$ and $\mathbf{1}B_2^n/\mathrm{Vol}(B_2^n)dx$



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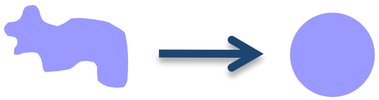

Monge-Ampère equation: $\mathrm{Vol}(B_2^n)\, f^{n/(n-1)}(x) = \det \mathrm{Hess}\, \overline{\Psi}$

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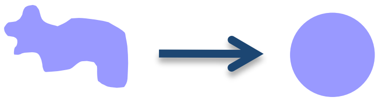

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Arithmetico-geometric ineq: $\det(H)^{1/n} \leq \mathrm{trace}(H)/n$ if H positive

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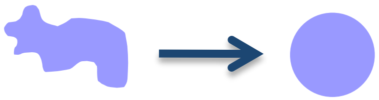

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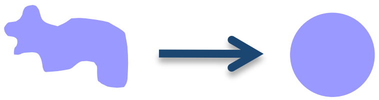

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$\det(\mathrm{Hess}\, \overline{\Psi})^{1/n} \leq \mathrm{trace}(\mathrm{Hess}\, \overline{\Psi})/n$

$\det(\mathrm{Hess}\, \overline{\Psi})^{1/n} \leq \Delta \overline{\Psi} / n$

The isoperimetric inequality

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$$\mathrm{Vol}(B_2^n) = \mathrm{Vol}(B_2^n) \int f^{\,n/(n-1)} = \int f\ \ \mathrm{Vol}(B_2^n)\, f^{\,1/(n-1)}$$

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$\det(\mathrm{Hess} \, \overline{\Psi})^{1/n} \leq (\Delta \, \overline{\Psi})/n$

$$\mathrm{Vol}(B_2^n) = \mathrm{Vol}(B_2^n) \int f^{\, n/(n-1)} = \int f \; \mathrm{Vol}(B_2^n) \, f^{\, 1/(n-1)} \leq 1/n \int f \, \Delta \, \overline{\Psi}$$

$$\int f \, \Delta \, \overline{\Psi} = - \int \operatorname{grad} f \, . \, \operatorname{grad} \overline{\Psi}$$

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

Inria

Bonus Slides

Plotting the potential & optics

Plotting the potential, “optics”

The [AHA] paper summary:

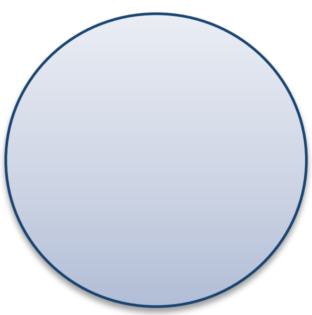
- The optimal weights minimize a convex function
- The gradient and Hessian of this convex function is easy to compute

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

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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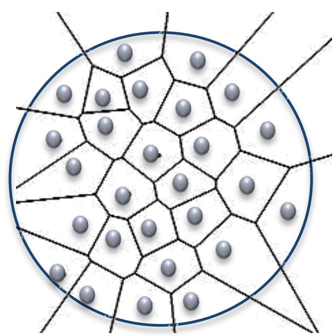

ν

Plotting the potential, “optics”

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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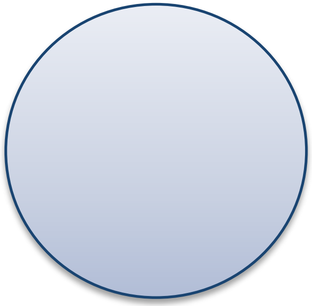

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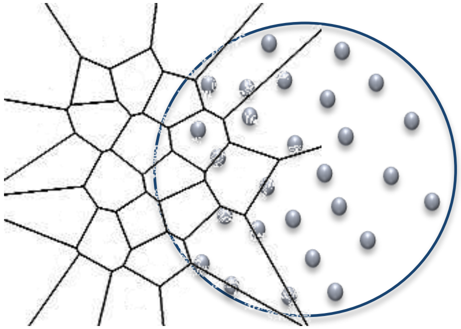

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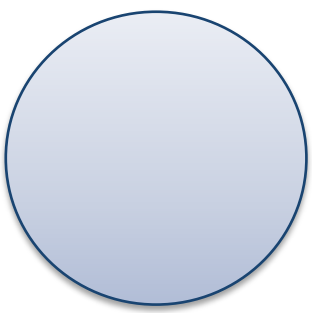

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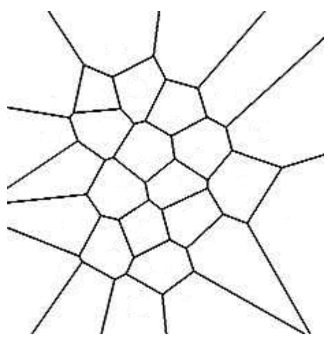

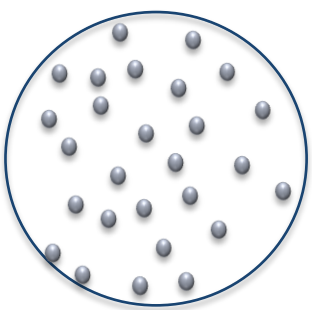

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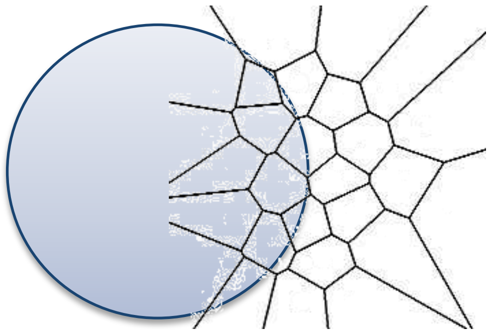

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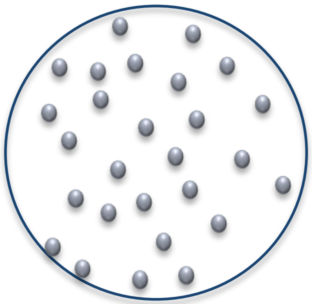

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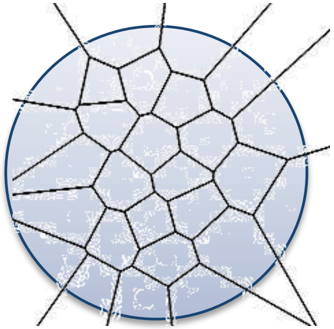

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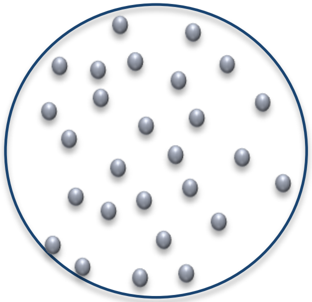

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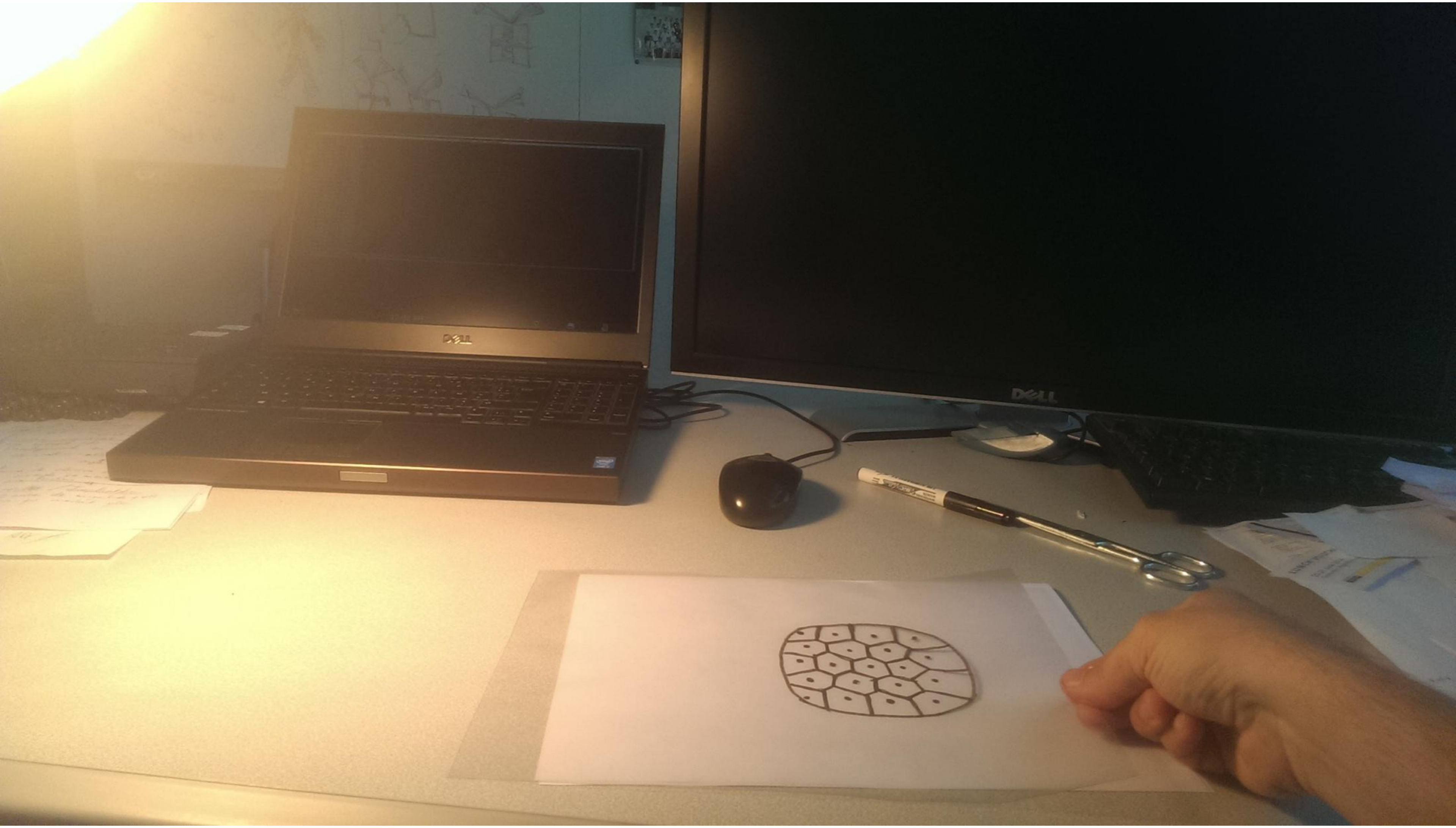

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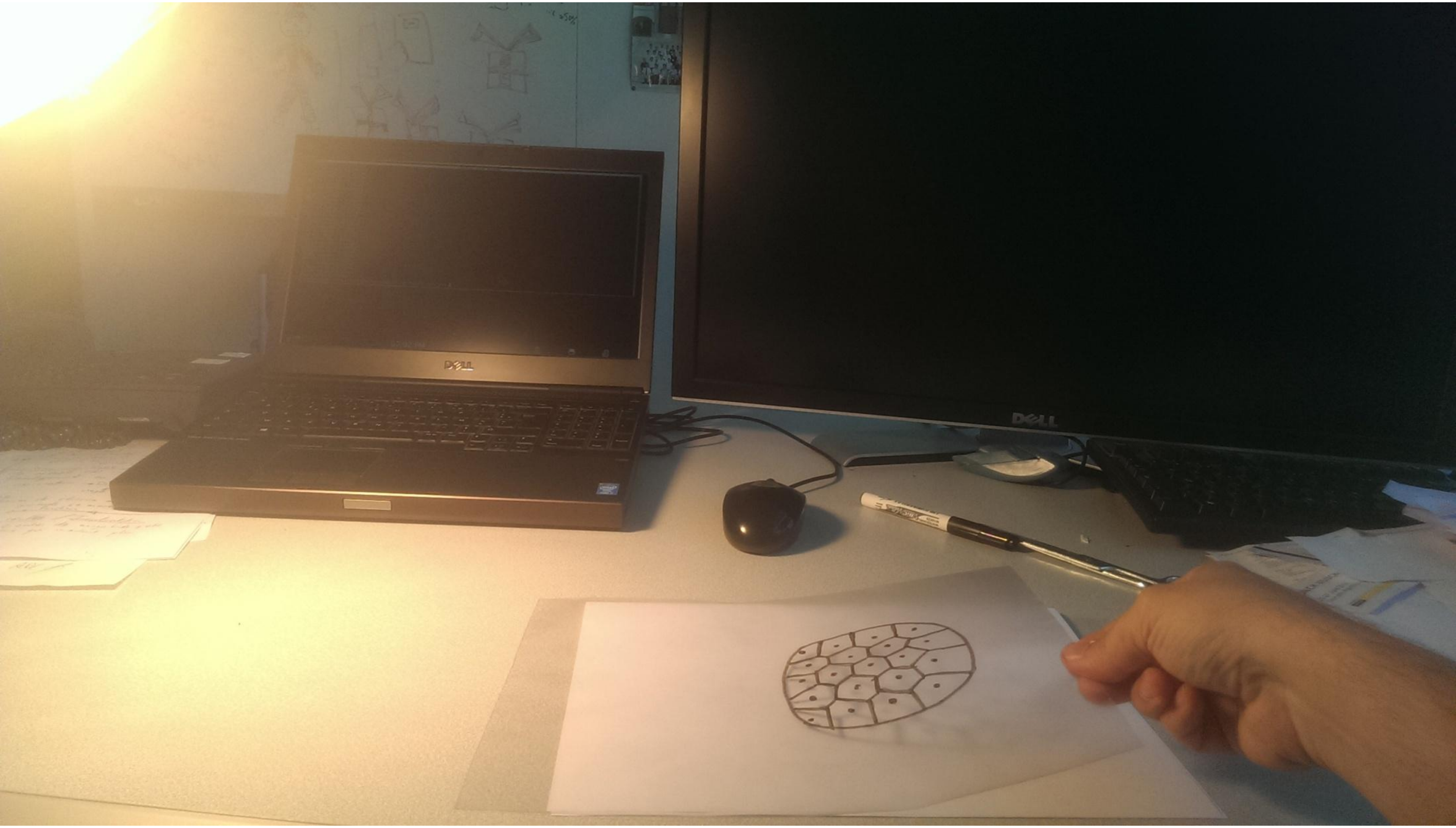

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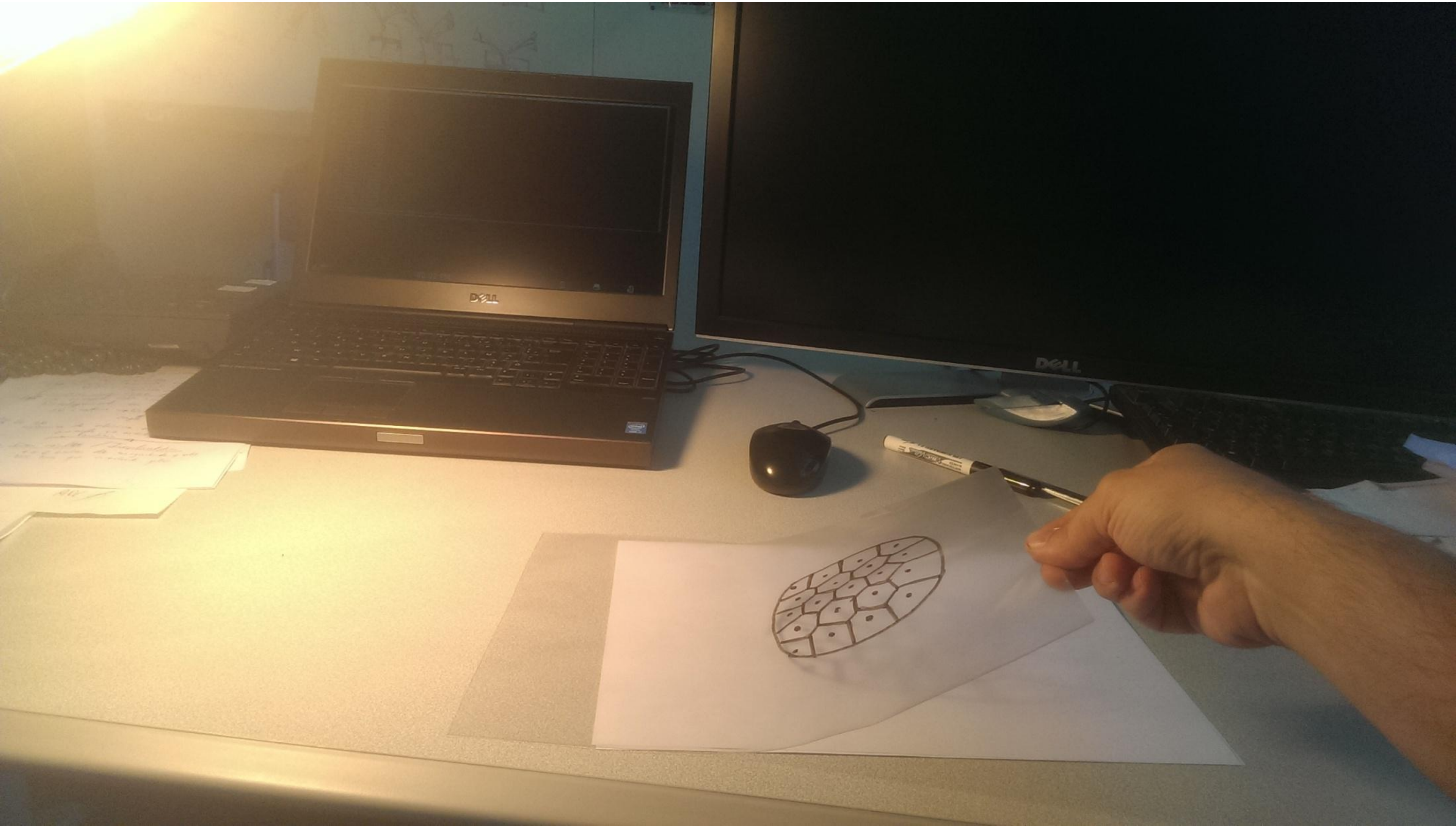

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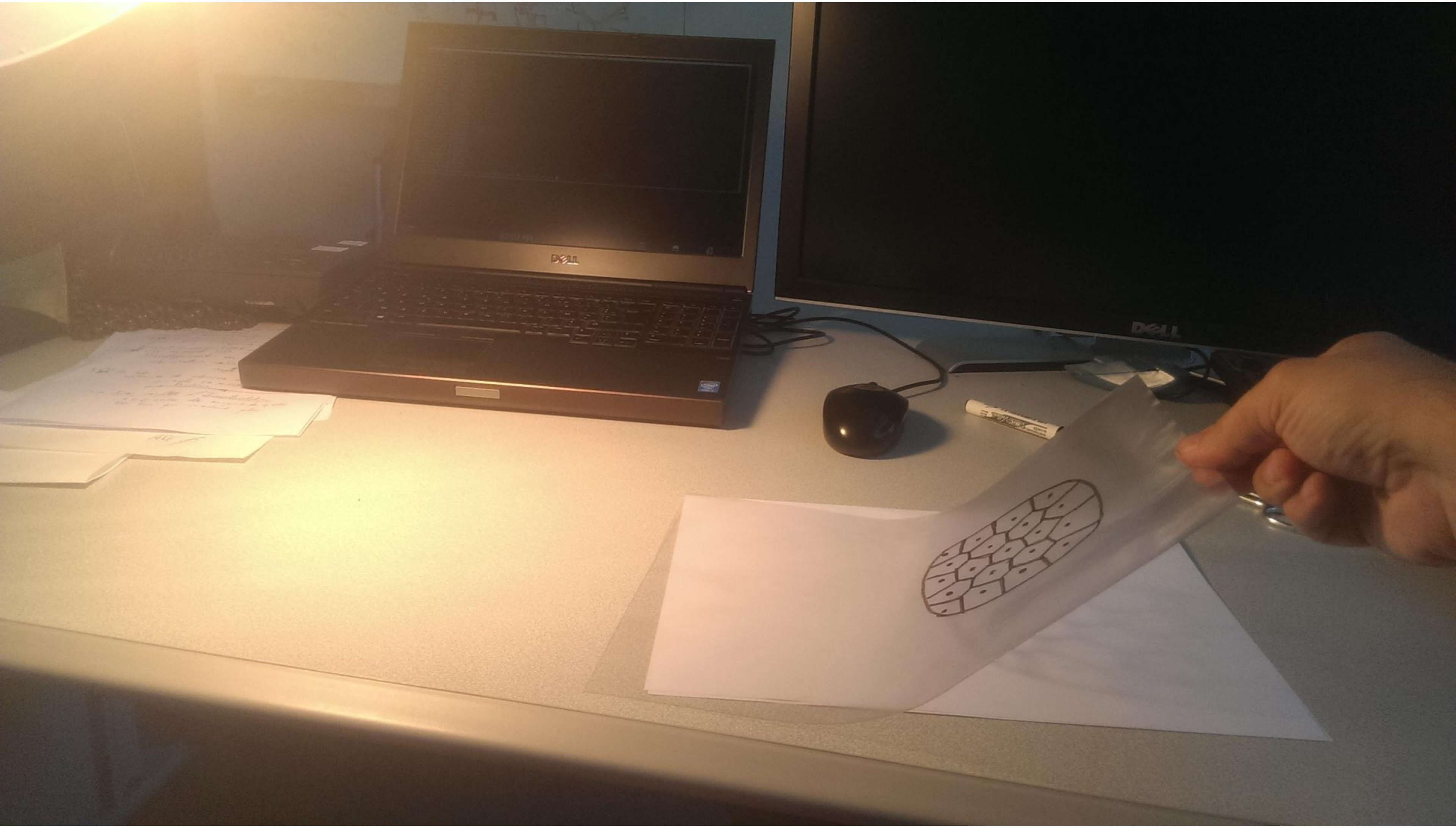

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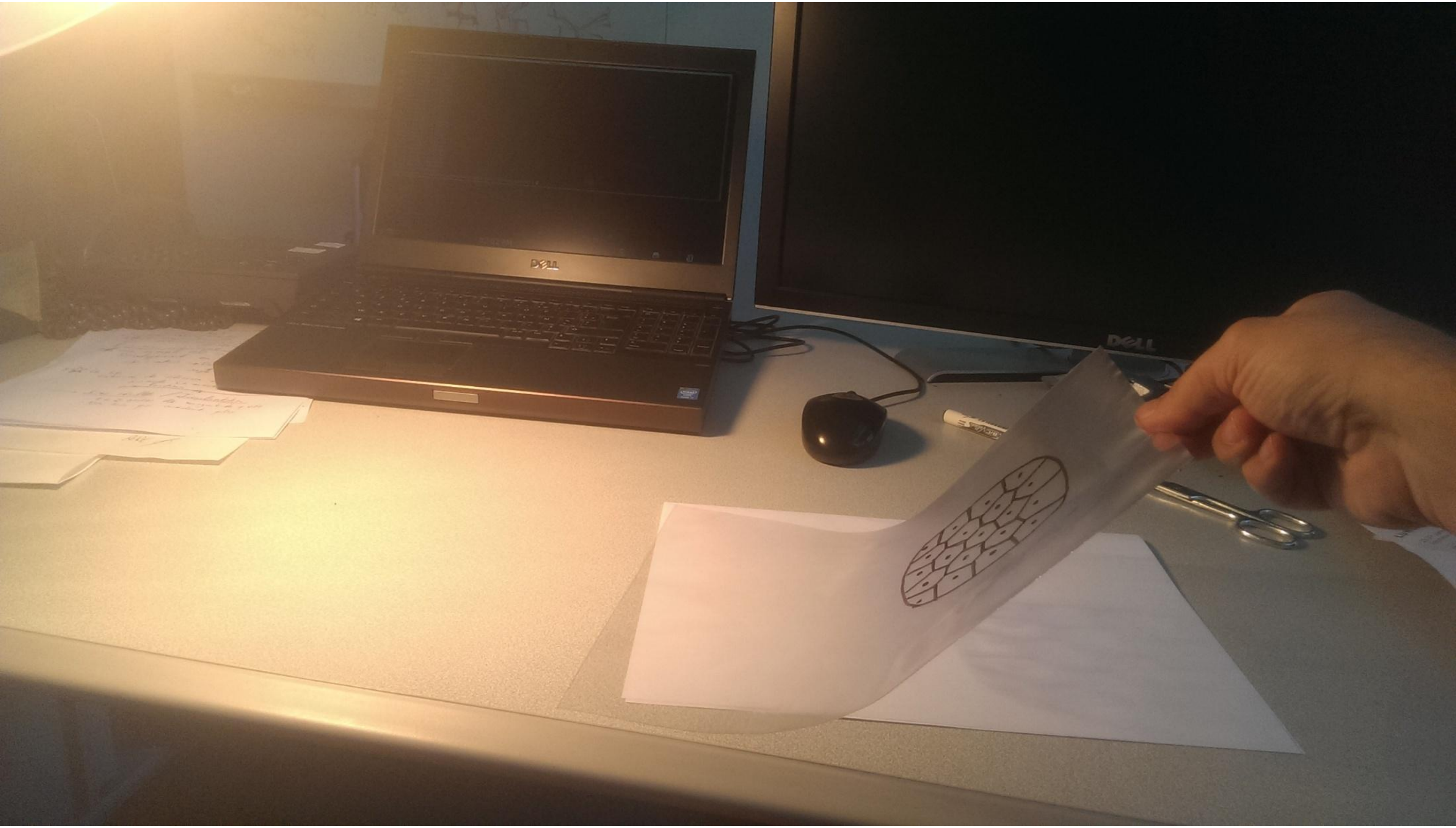

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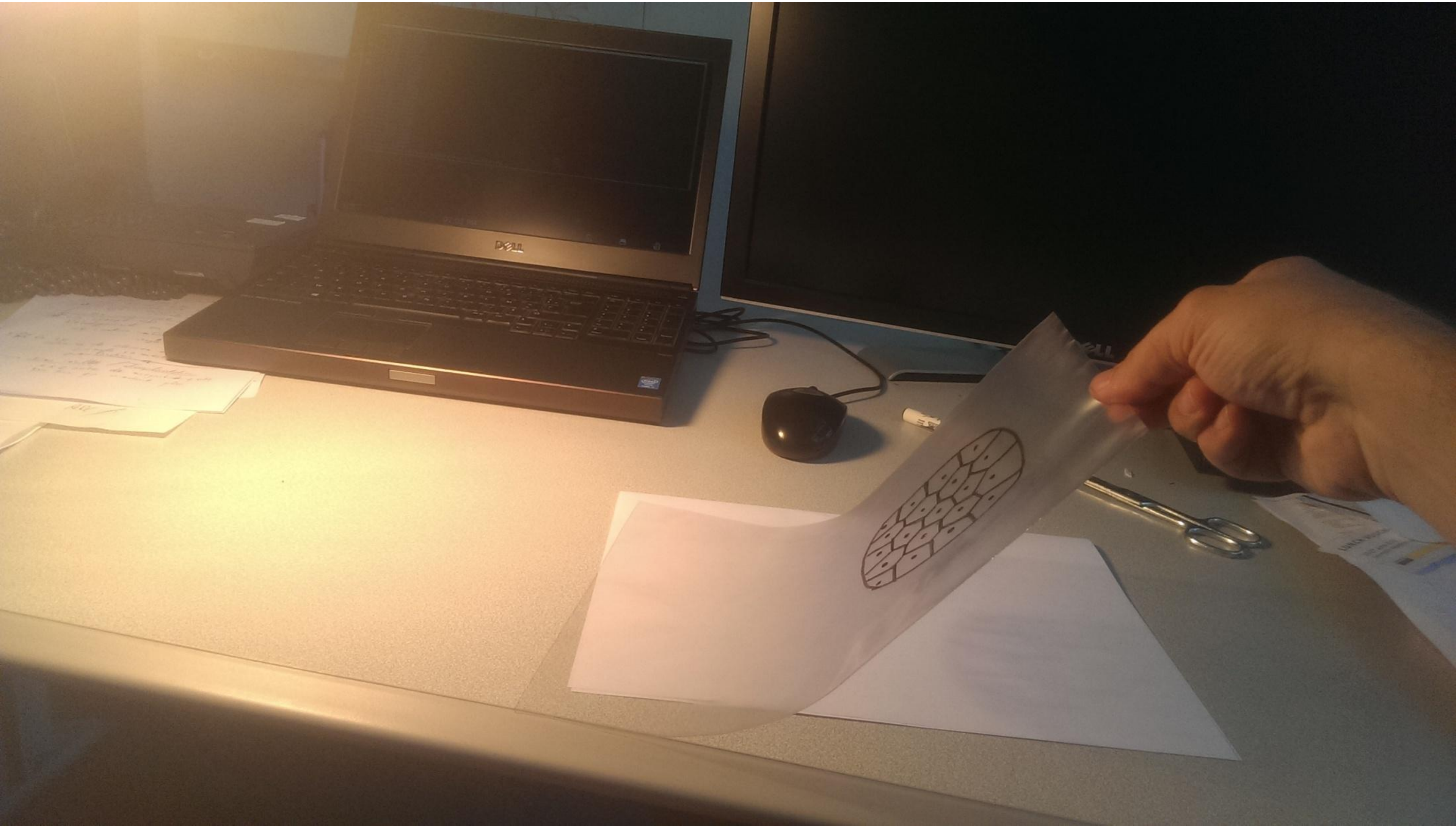

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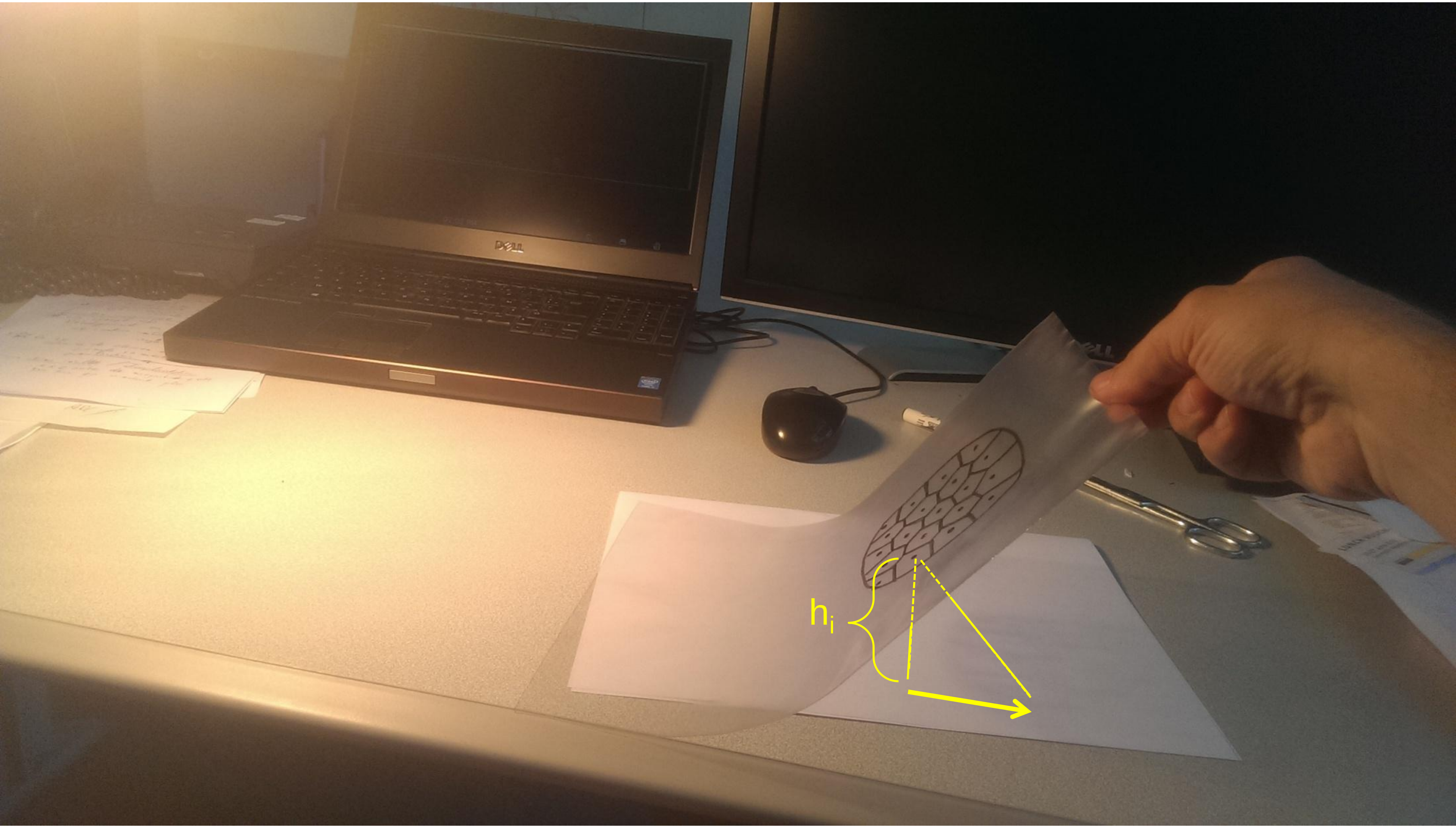

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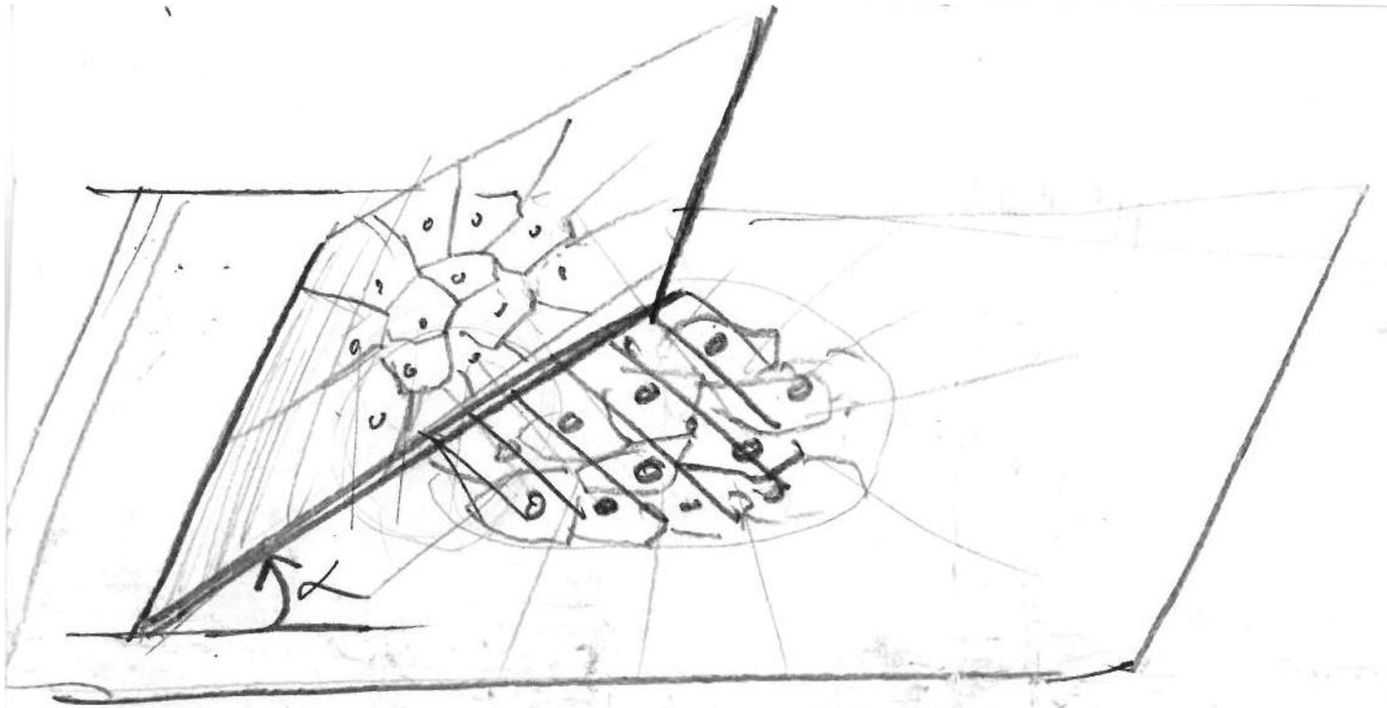
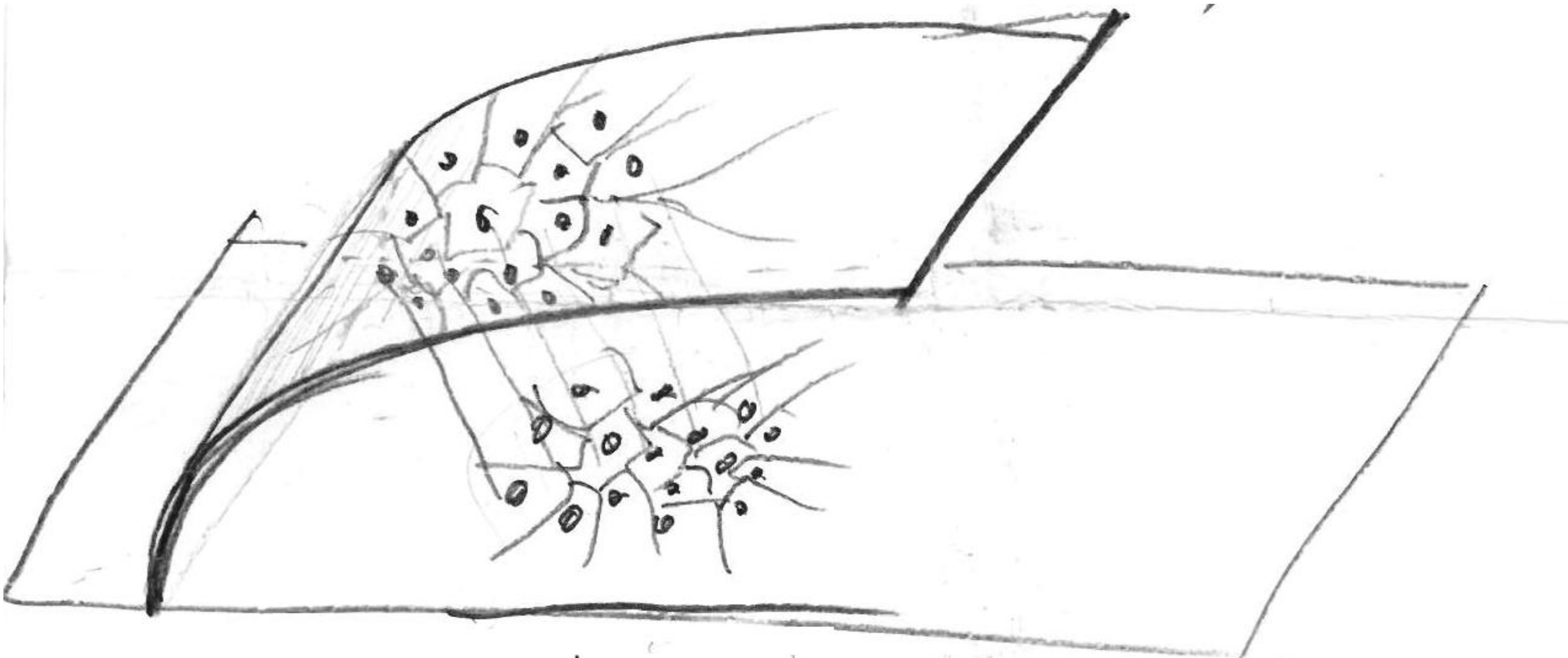


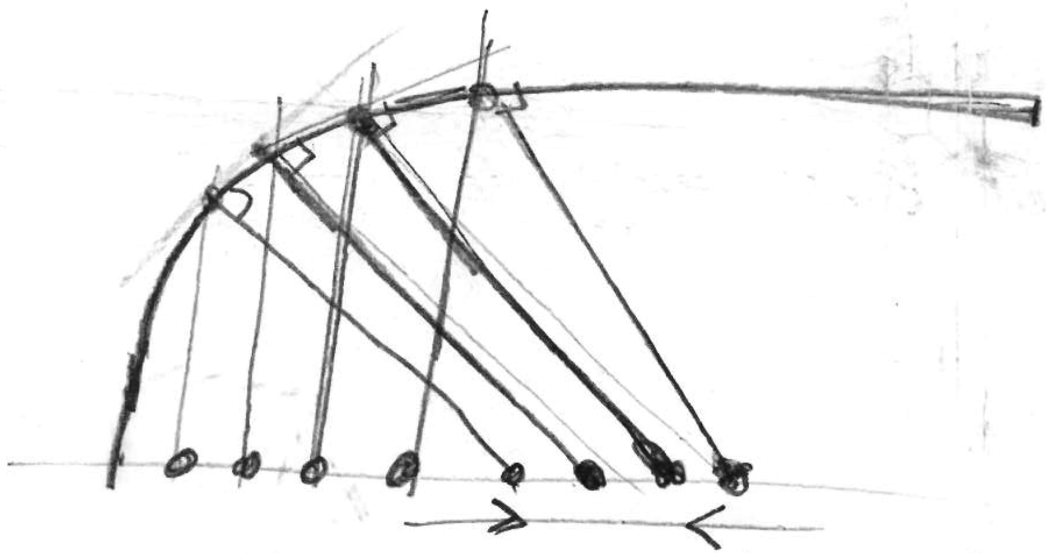
Translating a Voronoi diagram.
1st Try: linear lifting
(FAIL: scales by 1/cos(α))

Plotting the potential, “optics”



2nd Try : Curved lifting

Plotting the potential, “optics”



“converging beams” can compensate the $1/\cos(\alpha)$ expansion by “re-concentrating” the points

Plotting the potential, “optics”

2

$$d^2(p_i,q)\,\Big|^{+h_i^2}_{-w_i} < d^2(p_j,q)\,{}^{+h_i^2}_{-w_j} \quad \forall j$$

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

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

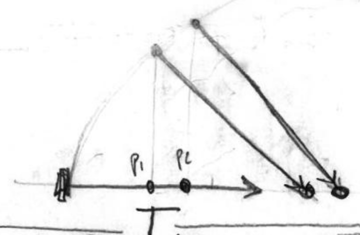
$$d^2(p_i,q) + 2T\cdot(p_i - q) + T^2 < d^2(p_j,q) + 2T\,(p_j - q) + T^2 \quad \forall j$$

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

$$h_i^2 \,\big|\, w_i = -2T\cdot p_i + cte$$

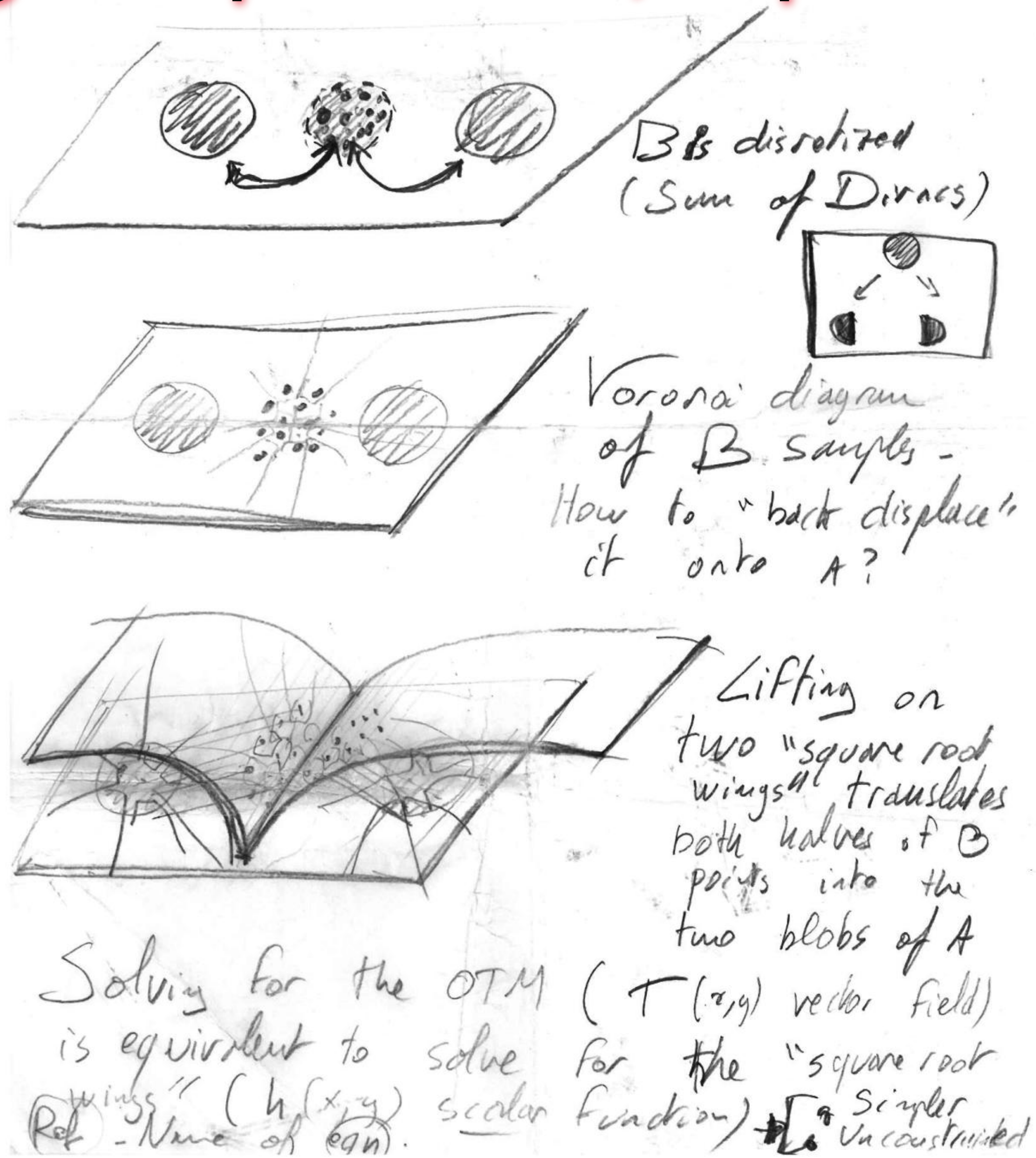
$$h_i^2 = (2T\cdot p_i + Cte)$$

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



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

Plotting the potential, “optics”



Plotting the potential, “optics”

Numerical Experiment: *A disk becomes two disks*

End Of Line.