Optimal Transport for Signal Processing

A tutorial at MLSP 2024

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22 September, 2024

github.com/felipe-tobar/OT-tutorial-MLSP-2024

Overview

Speaker's presentation

Felipe Tobar

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Research themes: Gaussian Processes, Optimal Transport, Diffusion Models
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Laetitia Chapel

Full Professor in Computer Science
IRISA Lab, France

Research themes: Optimal Transport, machine learning on structured data
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Forenote on implementation

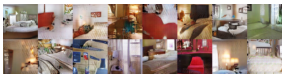
- Examples based on **POT: Python Optimal Transport Toolbox** (`pythonot.github.io`)
- Tutorial repository: **`github.com/felipe-tobar/OT-tutorial-MLSP-2024`**

Why Optimal Transport?

- Need for a **meaningful** measure of distance between probability measures
- Probability distributions are ubiquitous in machine learning and signal processing
- Lots of applications in MLSP

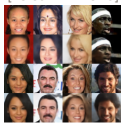
OT as a loss for classification
[Frogner, 2015]

Wasserstein style transfer
[Mroueh, 2020]



Wasserstein GAN
[Arjovsky 2017]

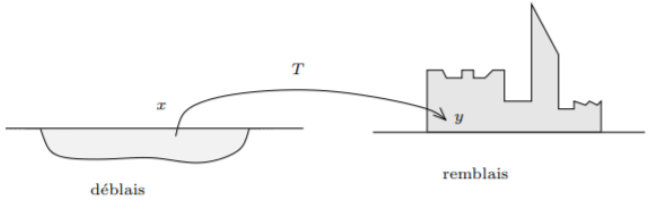
Wasserstein AE
[Tolstikhin 2018]



Shape interpolation
[Solomon, 2015]

Origins of OT: Gaspard Monge (1781)

How to transport a pile of sand onto a hole in an optimal way?

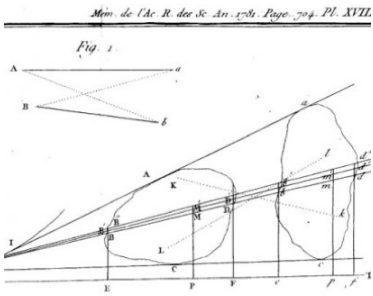


MÉMOIRE
SUR LA
THÉORIE DES DÉBLAIS
ET DES REMBLAIS.

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 *Remblai* à l'eſpace qu'elles doivent occuper après le tranſport.

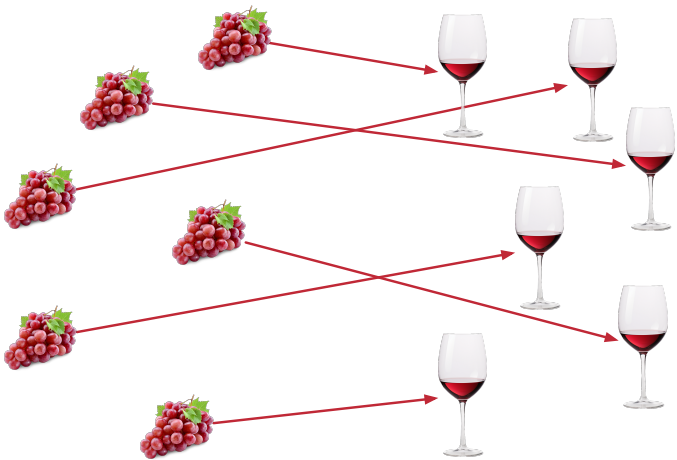
Le prix du tranſport d'une molécule étant, toutes choſes d'ailleurs égales, proportionnel à ſon poids & à l'eſpace qu'on lui fait parcourir, & par conſéquent le prix du tranſport total devant être proportionnel à la ſomme des produits des molécules multipliées chacune par l'eſpace parcouru, il s'enſuit que le déblai & le remblai étant donnés de figure & de poſition, il n'eſt pas indifférent que telle molécule du déblai ſoit tranſportée dans tel ou tel autre endroit du remblai, mais qu'il y a une certaine diſtribution à faire des molécules du premier dans le ſecond, d'après laquelle la ſomme de ces produits ſera la moindre poſſible, & le prix du tranſport total ſera un *minimum*.



Part I: The Optimal Transport Problem

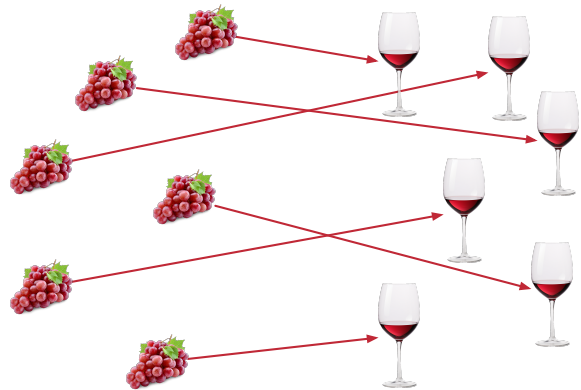

CUARTEL C2
CARMÉNÉRE
2.1 HA - 1994
2.3* 1.2 - 90 H

The assigment problem



The assigment problem: encoding real-world

- Weighted masses
- Different number of sources/targets
- Straight path is not possible
- New source/target becomes available



Monge formulation[1]

Objective: Move a pile of mass from one location to another at a minimum effort

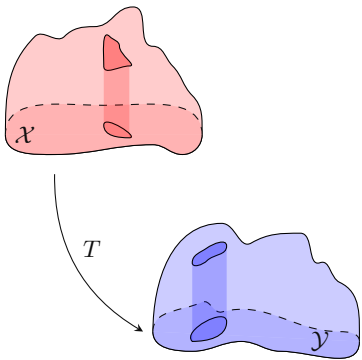
Let us first set up our notation

- **Piles of mass** are probability distributions, μ and ν, corresponding to random variables $X \in \mathcal{X}$ and $Y \in \mathcal{Y}$.
- **Moving procedure** is a function $T : x \in \mathcal{X} \mapsto Y \in \mathcal{Y}$.
- **Moving cost** encoded as $c : (x, y) \in \mathcal{X} \times \mathcal{Y} \mapsto c(x, y) \in \mathbb{R}$.

Solve: Optimise the total transport cost

$$\mathrm{OT}(\mu, \nu) = \min_{T \in M_{X,Y}} \sum_{x \in \mathcal{X}} c(x_i, T(x_i)), \qquad (1)$$

where $M_{X,Y} = \{T : \mathcal{X} \to \mathcal{Y},\ s.t.,\ T_{\#\mu} = \nu\}$.



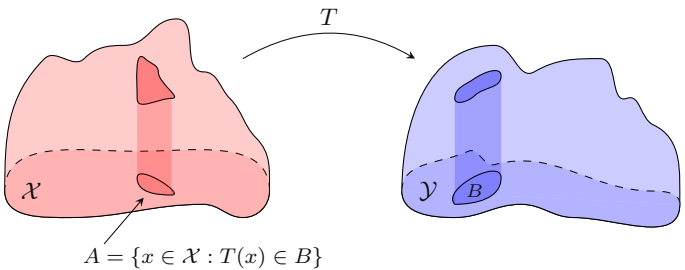
[1] Monge, G. (1781). Mémoire sur la théorie des déblais et des remblais. De l'Imprimerie Royale.

The transport map (aka the *pushforward* operator $T_{\#}$)

T *transports* mass from $\mathcal{X}$ to $\mathcal{Y}$, meaning that for any subset $A \in \mathcal{Y}$, one has

$$\nu(A) = \mu(T^{-1}(A)), \tag{2}$$

where $T^{-1}(A) = \{x \in \mathcal{X}, s.t.\ T(x) \in A\}$ is the preimage of A under T.



$T\#\mu = \nu$

i.e., $\mu(A) = \nu(B)$

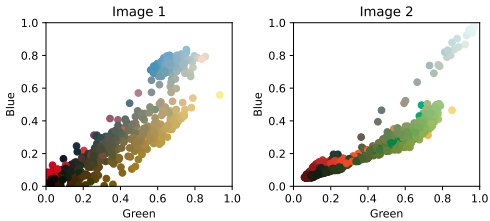
Figure adapted from Thorpe's book.[2]

[2]Infinite thanks to Elsa Cazelles (IRIT, CNRS) for kindly sharing these beautiful `tikz` figures.

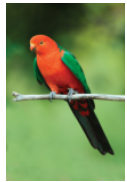
Example 1: Colour transfer

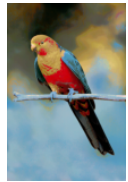
Original images

Histograms



Histograms

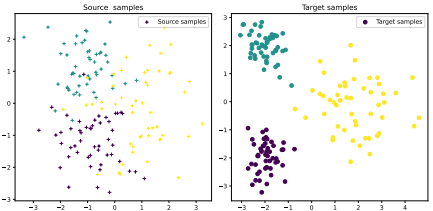




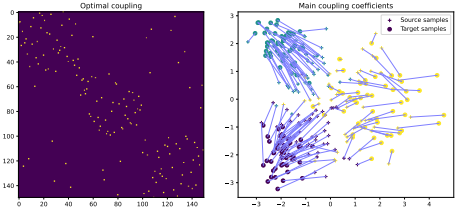
Notebook: Colour_transfer.ipynb

Example 2: Domain adaptation

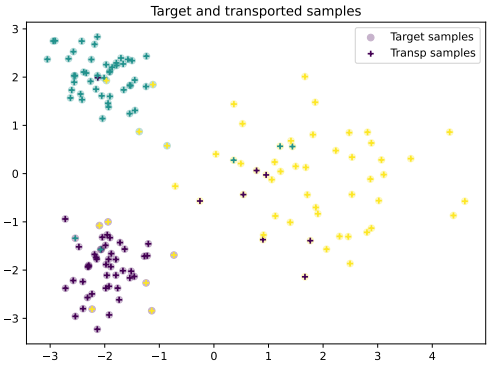
Original images



Histograms

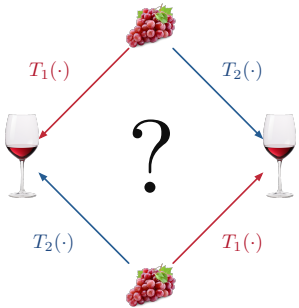


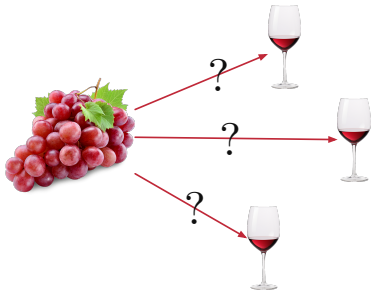
Histograms



Notebook: Domain_adaptation.ipynb

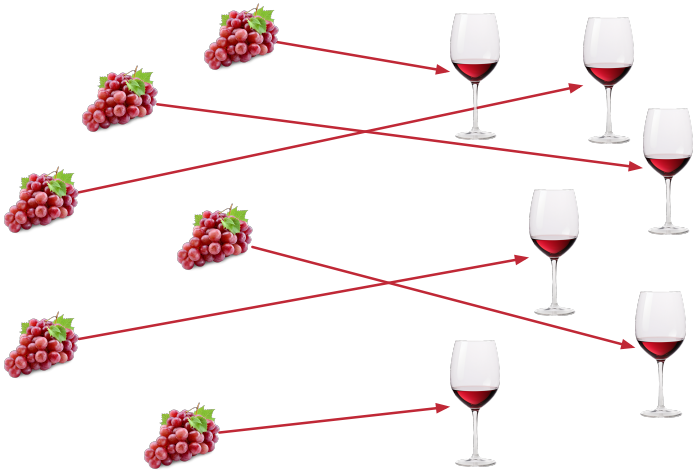
Neither existence nor uniqueness is guaranteed



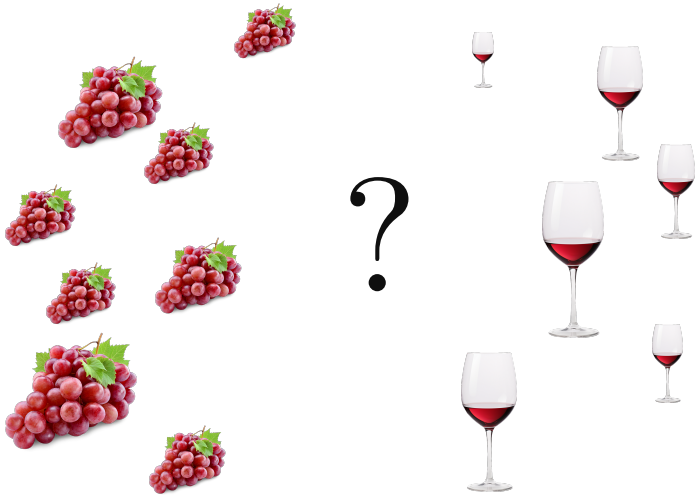


Observation: In the two examples above, each sample *weights the same*, i.e., pixels, class instances. In some cases, we might have *weighted samples*. In such cases, **Monge's map might be unable to transport the mass.**

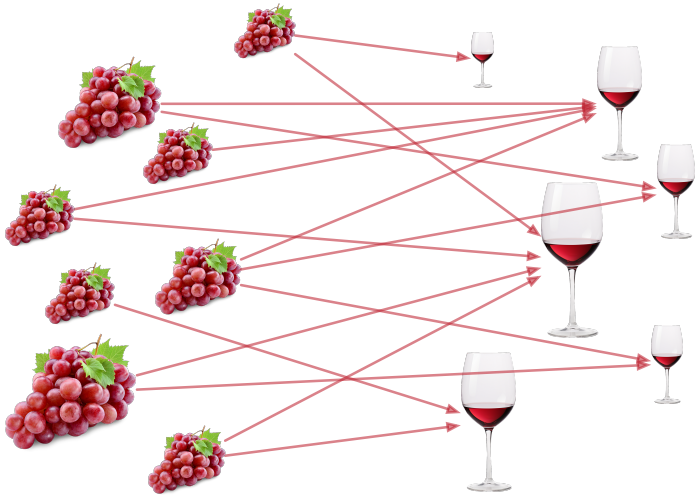
Kantorovich formulation: mass splitting



Kantorovich formulation: mass splitting



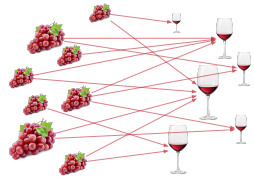
Kantorovich formulation: mass splitting



Transport *plan*

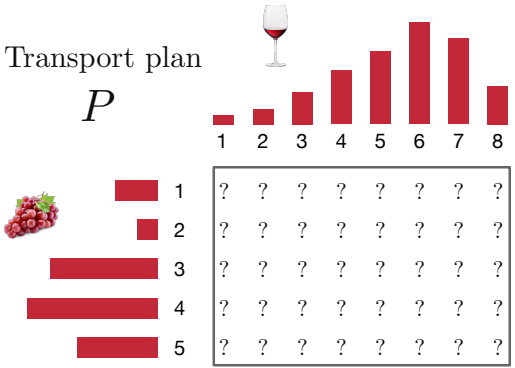
$$\mathrm{OT}(\mu,\nu) = \inf_{P\in\Pi_{\mu,\nu}} \langle P, C\rangle = \sum_{i,j}^{n,m} C_{ij}P_{ij}$$

where $\Pi_{\mu,\nu}\langle P, C\rangle = \{P \in [0,1]^{m\times n} : \sum_{i=1}^{m} P_{ij} = \nu_j, \sum_{j=1}^{n} P_{ij} = \mu_i\}$



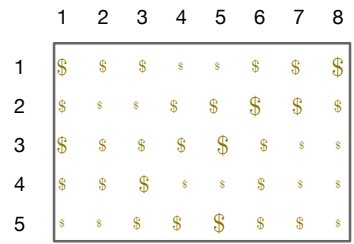
Transport plan

P



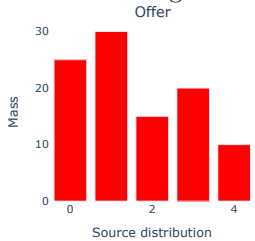
Cost Matrix

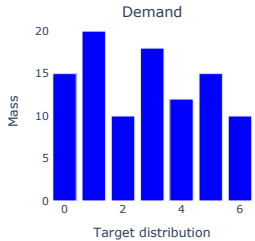
C

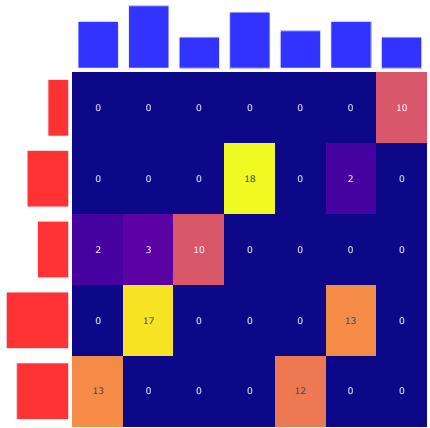


Example 3: Discrete Kantorovich plan

Let consider the following source and target distributions



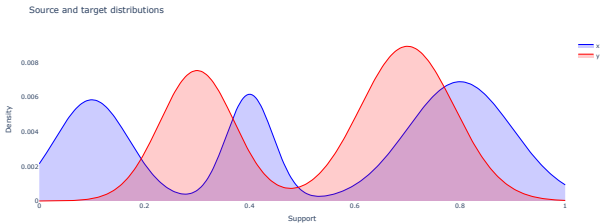


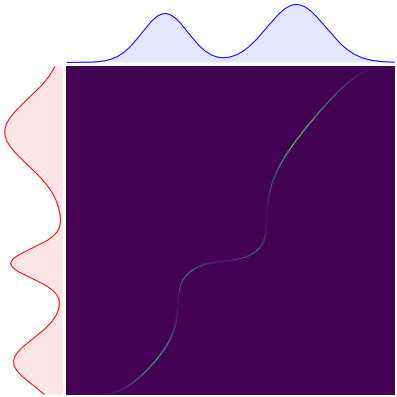


Notebook: kantorovich.ipynb

Example 4: Continuous Kantorovich plan

Let us now consider two distributions over a continuous support





Observe that the plan remained *sparse*, i.e., the mass did not spread much

This motivates the following results

Notebook: kantorovich.ipynb

Observations

- Let us consider a cost $c(x, y) = |x - y|^p, p \geq 1$. Then, if μ and ν are absolutely continuous wrt the Lebesgue measure, the Kantorovich problem as a unique solution. Furthermore, this solution is the same solution of the Monge problem.
- If $p = 2$, the optimal map is the gradient of a convex function
- In some cases the optimal plan will require to split mass (e.g., in the case of atomic measures) and thus Monge's solution may fail to exist.
- Luckily, from a (Kantorovich) transport plan we can always extract a tranport map, e.g., via the barycentric projection

Dual formulation

Recall the primal formulation: $\mathrm{OT}(\mu,\nu) = \inf_{\pi\in\Pi(\mu,\nu)} \iint c(x,y)\mathrm{d}\pi(x,y)$

Dual problem

$$\mathrm{OT}(\mu,\nu) = \sup_{(\phi,\psi)\in\Phi_c} \left(\int_{\mathcal{X}} \phi d\mu + \int_{\mathcal{X}} \psi d\nu \right),$$

where

$$\Phi_c := \{(\phi,\psi) \in L_1(\mu) \times L_1(\nu),\ \text{s.t. } \phi(x) + \psi(y) \leq c(x,y)\}\,.$$

- ϕ and ψ are scalar function also known as **Kantorovich potentials**
- Primal-dual relationship: the support of $\pi \in \Pi^*(\mu,\nu)$ is such that $\phi(x) + \psi(y) = c(x,y)$.

In the discrete setting:

$$\int_{\mathcal{X}} \phi d\left(\sum_{i=1}^n \mu_i \delta_{x_i}\right) + \int_{\mathcal{X}} \psi d\left(\sum_{j=1}^m \nu_j \delta_{y_i}\right) = \sum_{i=1}^n \mu_i \underbrace{\phi(x_i)}_{\alpha_i} + \sum_{j=1}^m \nu_j \underbrace{\psi(y_j)}_{\beta_j}$$

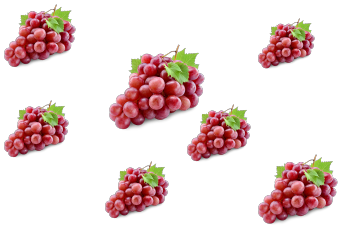
and Φ_c becomes $\{(\alpha,\beta) \in \mathbb{R}^n \times \mathbb{R}^m \text{ s.t. } \alpha_i + \beta_j \leq c(x_i,y_j)\}$

Interpretation of Kantorovich duality (discrete)

$$\mathrm{OT}(\mu,\nu) = \min_{\pi \in \Pi(\mu,\nu)} \langle C, \pi \rangle = \max_{(\alpha,\beta)\in D_c} \langle \alpha, \mu \rangle + \langle \beta, \nu \rangle$$

with

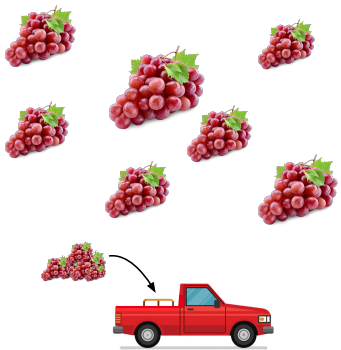
$$D_c := \{(\alpha,\beta) \in \mathbb{R}^n \times \mathbb{R}^m \text{ such that } \forall (i,j) \in \{1,\dots,n\} \times \{1,\dots,m\}, \alpha_i + \beta_j \leq C_{ij}\}$$



Intuition: the shipper's problem

One vendor sets the following:

- α_i = price for **loading** a kilo of grapes at place x_i (no matter which plan it goes)
- β_j = price for **unloading** a kilo of grapes at place y_j (no matter from which vineyard it came from)



Intuition: the shipper's problem

- There are exactly μ_i units at vineyard x_i and ν_j needed at plant y_j; the vendor asks the price **(that she wants to maximize!)**

$$\langle \alpha, \mu \rangle + \langle \beta, \nu \rangle$$

- Negative price are allowed !
- Does the vendor have a competitive offer? Her pricing scheme implies that transferring one kilo of grapes from vineyard x_i to plant y_j costs exactly $\alpha_i + \beta_j$.

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Intuition: the shipper's problem

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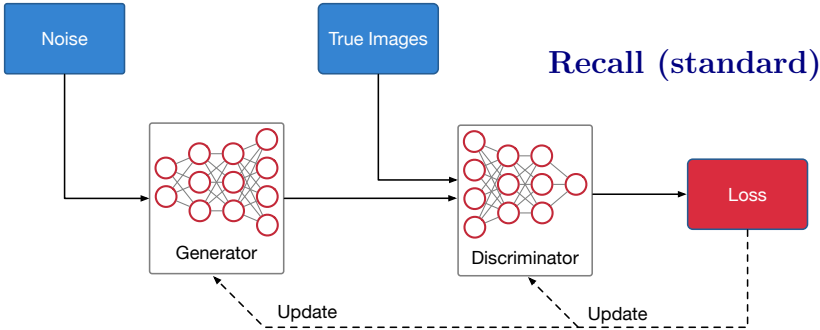
- Negative price are allowed !
- Does the vendor have a competitive offer? Her pricing scheme implies that transferring one kilo of grapes from vineyard x_i to plant y_j costs exactly $\alpha_i + \beta_j$.
- Recall the primal problem: the cost of shipping one unit from x_i to y_j is $C_{i,j}$.
- Feasible deal for the vendor requires that $\alpha_i + \beta_j \leq C_{ij}$.
- The winery checks that the vendor proposition is a better deal by

$$\sum_{i,j} \pi_{ij} C_{ij} \geq \sum_{i,j} \pi_{ij} (\alpha_j + \beta_j) = \left(\sum_i \alpha_i \sum_j \pi_{ij} \right) + \left(\sum_j \beta_j \sum_i \pi_{ij} \right) = \langle \alpha, \mu \rangle + \langle \beta, \nu \rangle$$

.

Critically, when $c(x, y) = |x - y|$, $\alpha = -\beta$, therefore $\mathrm{OT}(\mu, \nu) = \max_\alpha \langle \alpha, \mu \rangle - \langle \alpha, \nu \rangle$

Example 5: Wasserstein GANs



$$\min_G \max_D V(D,G) = \mathbb{E}_{x\sim p_{\text{data}}(x)}[\log D(x)] + \mathbb{E}_{z\sim p_z(z)}[\log(1 - D(G(z))]$$

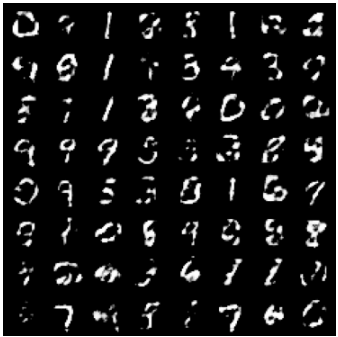
Notice the remarkable similarity between the objectives of the (dual) OT formulation and GANs

Example 5: Wasserstein GANs

GANs vs WGANs: Implementation details

- Discriminator loss no longer a likelihood fn
- Optimised with RMSProp
- Loss for D and G have the same form (Kantorovich potential, $p = 1$)
- Discriminator's inner loop training n_{critic} no longer equal to 1
- Learned parameters are clipped to ensure $||f||_L = 1$

GAN



WGAN

Notebooks: gan.ipynb & wgan.ipynb

Solving discrete OT

Let $\mu = \sum_{i=1}^{n} \delta_{x_i}$ and $\nu = \sum_{j=1}^{m} \delta_{y_j}$

$$\pi^* \in \underset{\pi \in \Pi(a,b)}{\arg\min} \langle C, \pi \rangle$$

Solving discrete OT

Let $\mu = \sum_{i=1}^{n} \delta_{x_i}$ and $\nu = \sum_{j=1}^{m} \delta_{y_j}$

$$\pi^* \in \underset{\pi \in \Pi(a,b)}{\arg\min} \langle C, \pi \rangle$$

- It's a linear problem : it can be rewritten in a vectorial form $\min_{t \geq 0} F(t) = c^T t$
- It has linear constraint $\pi \mathbb{1}_m = a$ and $\pi^T \mathbb{1}_n = b$

$\Longrightarrow$ Linear problem + linear constraints ($(n+m) \times nm$ matrix) : solved in $\mathcal{O}(n^3 \log(n))$ times

Solving discrete OT

Let $\mu = \sum_{i=1}^{n} \delta_{x_i}$ and $\nu = \sum_{j=1}^{m} \delta_{y_j}$

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$\Longrightarrow$ Linear problem + linear constraints ($(n+m) \times nm$ matrix) : solved in $\mathcal{O}(n^3 \log(n))$ times

$\Longrightarrow$ Need for solvers that provide approximate solutions! See [Peyré et Cuturi 2019]

Regularization of OT

$$\pi_\varepsilon = \underset{\pi \in \mathbb{R}_+^{n \times m}}{\arg\min} \ \langle C, \pi \rangle + \varepsilon \ \Omega(\pi)$$

Advantages of regularizing the optimization problem:

- Fast algorithms to solve the OT problem.
- Encode prior knowledge on the data.
- For statistical purposes : smooth the distance estimation
- Better posed problem (convexity, stability).

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Regularization terms :

- Entropic regularization [**?**]
- KL, Itakura Saito, β-divergences, [**?**]

Entropy regularized OT [?]

Adding regularization to the original problem turns the dual computation to an **unconstrained problem** !

$$\mathrm{OT}(\mu,\nu) = \min_{\pi\in\Pi(a,b)} \langle C,\pi\rangle + \varepsilon \sum_{i,j} \pi_{ij}\log(\pi_{ij})$$

The Lagrangian of the optimization problem is

$$\mathcal{L}(\pi,\alpha,\beta) = \sum_{ij} \pi_{ij}C_{ij} + \varepsilon\pi_{ij}(\log(\pi_{ij})-1) + \alpha^T(a-\pi\mathbb{1}_m) + \beta^T(b-\pi^T\mathbb{1}_n)$$

Then, by 1st order condition, we get

$$C_{ij} + \varepsilon\log(\pi_{ij}) + \alpha_i + \beta_j = 0$$

leading to

$$\mathrm{OT}(\mu,\nu) = \max_{\alpha,\beta}\ \alpha^T a + \beta^T b - \frac{1}{\varepsilon}\exp\left(\frac{\alpha}{\varepsilon}\right)^T \mathbf{K}\exp\left(\frac{\beta}{\varepsilon}\right)$$

with $\mathbf{K} = \exp\left(-\frac{C}{\varepsilon}\right)$.

Entropy regularized OT [?]

The solution of

$$\mathrm{OT}(\mu,\nu) = \min_{\pi\in\Pi(a,b)} \langle C,\pi\rangle + \varepsilon \sum_{i,j} \pi_{ij}\log(\pi_{ij})$$

is of the form

$$\pi^*_\varepsilon = \mathrm{diag}(u)\exp\left(-\frac{C}{\varepsilon}\right)\mathrm{diag}(v)$$

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$$\pi^*_\varepsilon = \mathrm{diag}(u) \exp\left(-\frac{C}{\varepsilon}\right) \mathrm{diag}(v)$$

- From Sinkhorn theorem [**?**], we get that $\mathrm{diag}(u)$ and $\mathrm{diag}(v)$ exist and are unique.
- Sinkhorn-Knopp algorithm [**?**] allows to solve it efficiently

Part II: The Wasserstein distance

Motivation

OT defines a family of distances between measures

The **Kantorovitch problem**

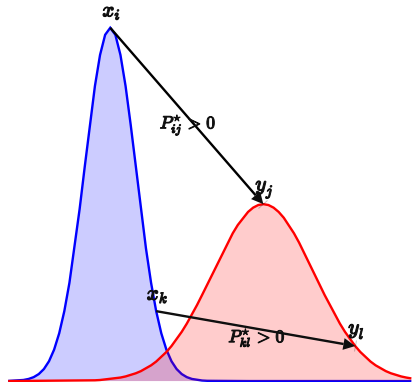
$$P^\star \in \inf_{P \in \Pi_{\mu,\nu}} \langle P, C \rangle = \sum_{i,j}^{n,m} C_{ij} P_{ij}$$

allows defining the **Wasserstein distance** of order p

$$W_p^p(\mu, \nu) = \langle P^\star, C \rangle$$

where the moving cost $c(x, y) = d(x, y)^p = \|x - y\|^p$.
It is often depicted as an "horizontal" distance

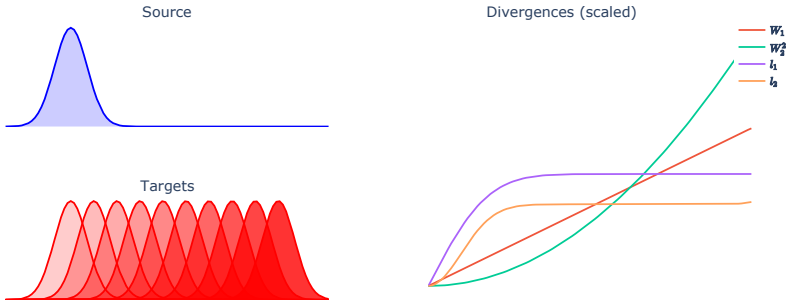
- ✓ **symmetry**
- ✓ **identity of indiscernibles**
- ✓ **triangular inequality**



Notebook: Horizontal distance.ipynb

The Wasserstein distance

- Does not need overlapping support (as KL)
- Determines the *degree of dissimilarity* between distributions



Notebook: Wasserstein_distance.ipynb

On the suitability of W_p for learning

- Thus far we have referred to *spaces of probability functions*, but we are interested in applying W_p on spaces of **generative models**.
- Learning is such a space requires, more than a distance, a notion of **convergence**
- Consider μ_{data} to be the true data distribution. We want to find a model $(P_\theta)_{\theta \in \Theta}$ such that $P_\theta \to \mu_{\text{data}}$, or equivalently, $D(\mu_{\text{data}}, P_\theta) \to 0$ — for a **reasonable** distance D.

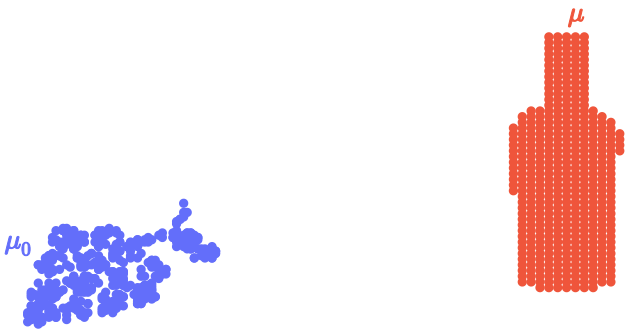
Discussion: Consider δ_{x_0} and $\delta_{x_i}, x_i \to x_0$

Example 6: Gradient flows on Wasserstein space

Wasserstein space $\mathbb{W}_p$: space endowed with the distance W_p

- In the space $\mathbb{W}_p(\mathbb{R}^d)$, we have $W_p(\mu_n, \mu) \to 0$ iff $\mu_n \to \mu$ (weak topology)

Consider the loss $W_2^2(\mu_t, \mu)$. The figure below shows how a distribution μ_0 evolves under de application of gradient flow of this loss.



Notebook: Wasserstein Gradient Flows.ipynb

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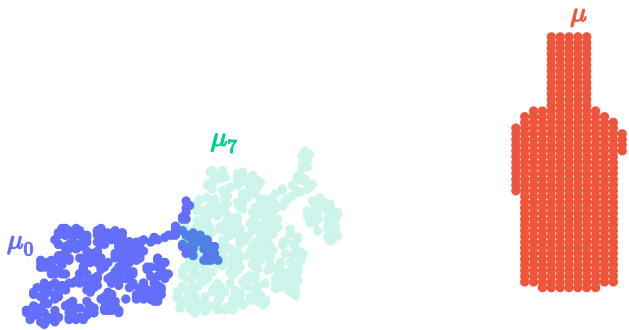

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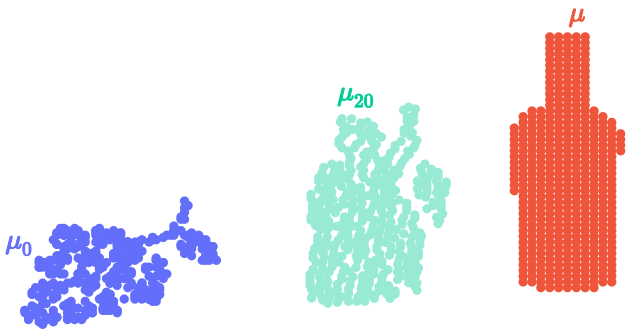

Notebook: Wasserstein Gradient Flows.ipynb

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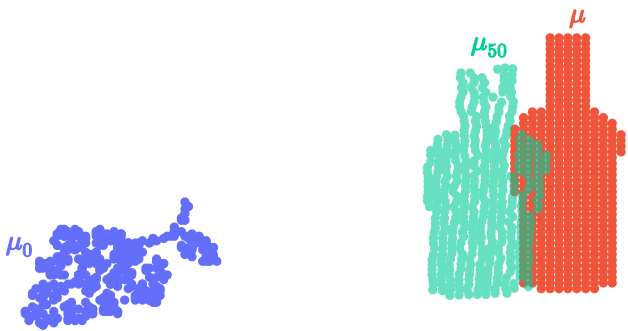

Notebook: Wasserstein Gradient Flows.ipynb

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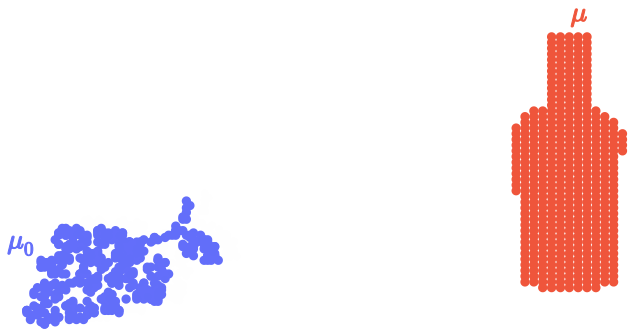


Notebook: Wasserstein Gradient Flows.ipynb

Geodesic paths between distributions

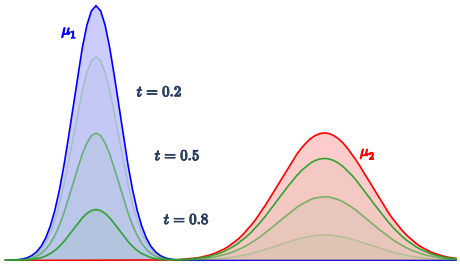
A geodesic generalizes the concept of a straight line between two points

It is a curve that represents the shortest path between two manifolds

Euclidean space with a l_2 distance is a **geodesic space**

$$\forall t \in [0,1], \quad \mu^{1\to 2}(t) = t\mu_2 + (1-t)\mu_1$$

Allows "vertical" interpolation between the distributions



Notebook: Wasserstein Geodesics.ipynb

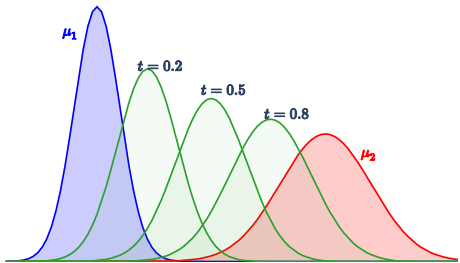
Geodesic properties of the Wasserstein space

$\mathbb{W}_p$ is a **geodesic space**

- Given a Monge map T between μ_1 and μ_2 such that $T_{\#}\mu_1 = \mu_2$, a geodesic curve $\mu^{1\to 2}$ is

$$\forall t \in [0,1], \quad \mu^{1\to 2}(t) = (tT + (1-t)\mathrm{Id})_{\#}\mu_1$$

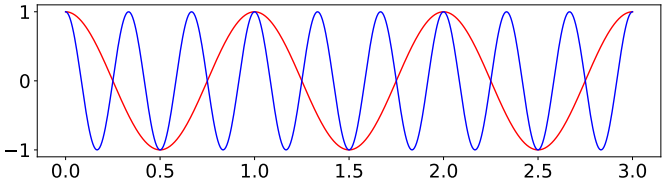
- It represents the shortest path (on the Wasserstein space $\mathbb{W}_p$) between μ_1 and μ_2
- Allows "horizontal" interpolation between the distributions



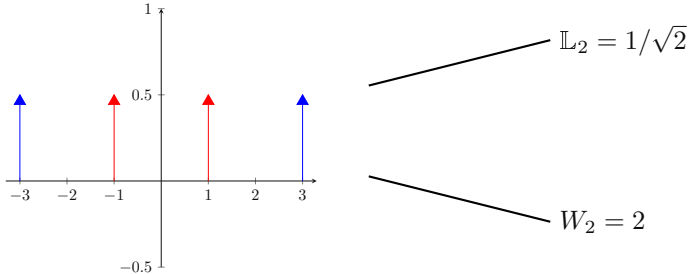
Notebook: Wasserstein Geodesics.ipynb

Motivation: Applying the Wasserstein distance to time series

Two cosine signals with frequencies 1 and 3.



The associated PSD functions .



Definition: The Wasserstein-Fourier distance

Definition

For two signals x and y belonging to two different classes of time series, we denote by

- $[x]$ and $[y]$ their respective class
- s_x and s_y their respective NPSD

We define the proposed *Wasserstein-Fourier* (WF) distance:

$$\mathrm{WF}\left([x],[y]\right) = W_2(s_x, s_y).$$

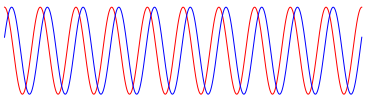
Theorem

WF is a distance over the space of equivalence classes of time series sharing the same NPSD.

E. Cazelles, A. Robert & **F. Tobar**, The Wasserstein-Fourier Distance for Stationary Time Series. *IEEE Trans. on Signal Processing* 2021

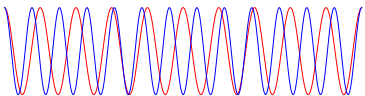
Basics properties of the WF distance

Time shifting : $x(t) = y(t - t_0)$.



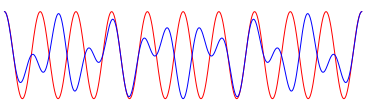
$$\mathrm{WF}\left([x],[y]\right) = 0$$

Time scaling : $x(t) = y(at), a > 0$.



$$\mathrm{WF}\left([x],[y]\right) = |a-1|(\left\langle |Y|^2 \right\rangle_{s_y})^{\frac{1}{2}}$$

Frequency shifting : $x(t) = e^{2i\pi\xi_0 t}y(t)$.



$$\mathrm{WF}\left([x],[y]\right) = |\xi_0|$$

How to interpolate two time series?

The usual $\mathbb{L}_2$ path: a superposition of two signals

$$x_\gamma(t) = \gamma x_1(t) + (1-\gamma)x_2(t), \quad \gamma \in [0,1],$$

Example: For EEG, the $\mathbb{L}_2$ average of multiple responses to a common stimulus would probably convey little information about the true average response and it is likely to quickly vanish due to the random phases.

Toy example: The WF path i.e. Wasserstein interpolation in the frequency domain

Frequency domain

Time domain

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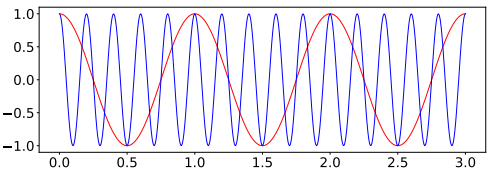

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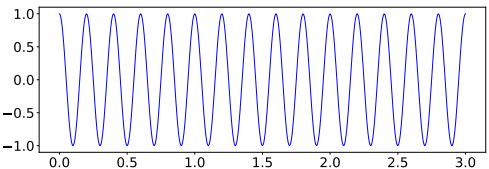

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$\gamma = 0$

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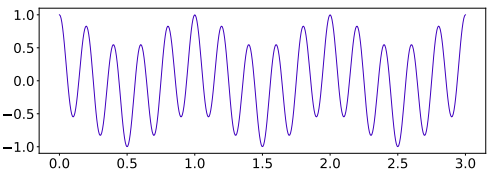

Frequency domain

$\gamma = 0.25$

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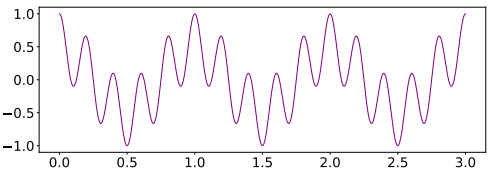
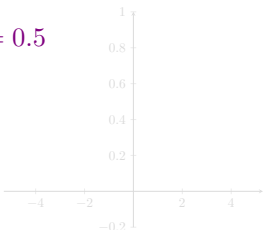


Frequency domain

$\gamma = 0.5$



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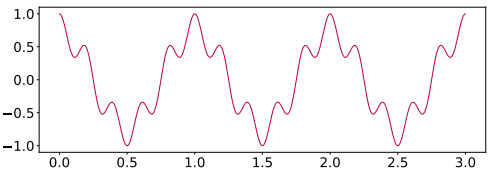

Frequency domain

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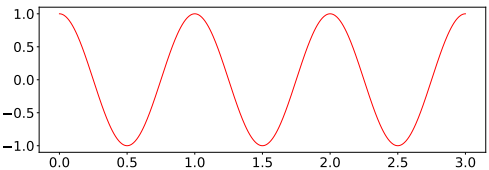
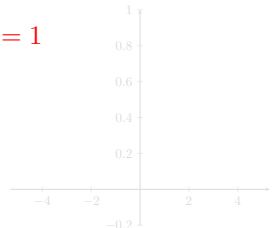


Frequency domain

$\gamma = 1$



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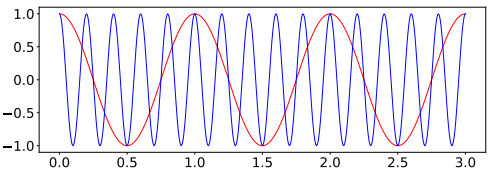

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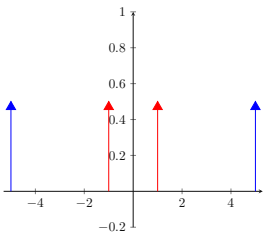

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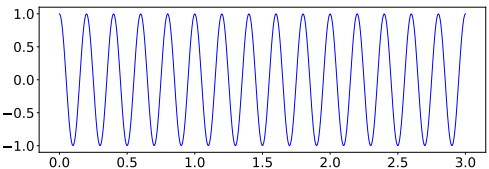
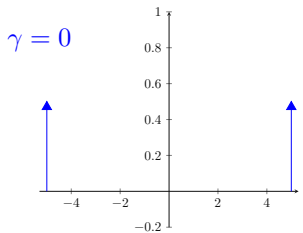


Frequency domain



How to interpolate two time series?

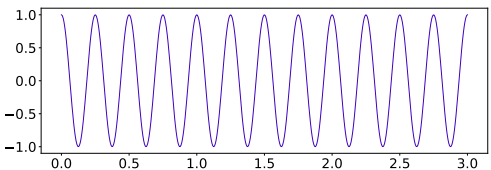
The usual $\mathbb{L}_2$ path: a superposition of two signals

$$x_\gamma(t) = \gamma x_1(t) + (1-\gamma)x_2(t), \quad \gamma \in [0,1],$$

Example: For EEG, the $\mathbb{L}_2$ average of multiple responses to a common stimulus would probably convey little information about the true average response and it is likely to quickly vanish due to the random phases.

Toy example: **The WF path i.e. Wasserstein interpolation in the frequency domain**

Time domain



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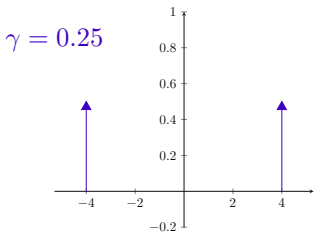

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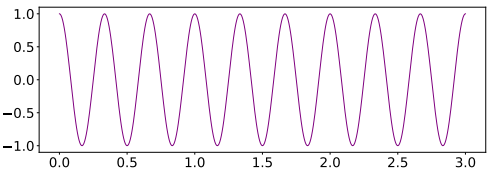

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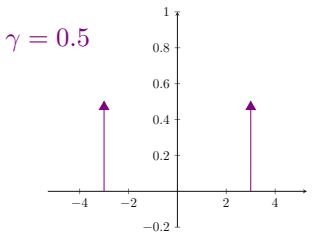

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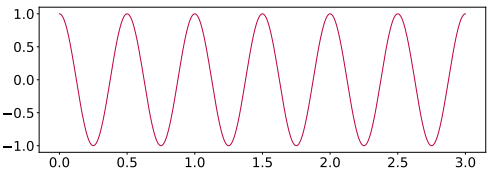

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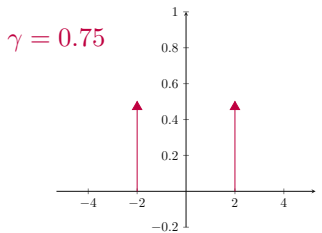

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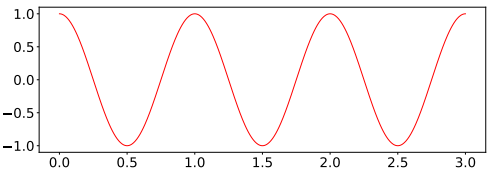

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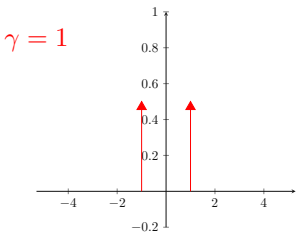
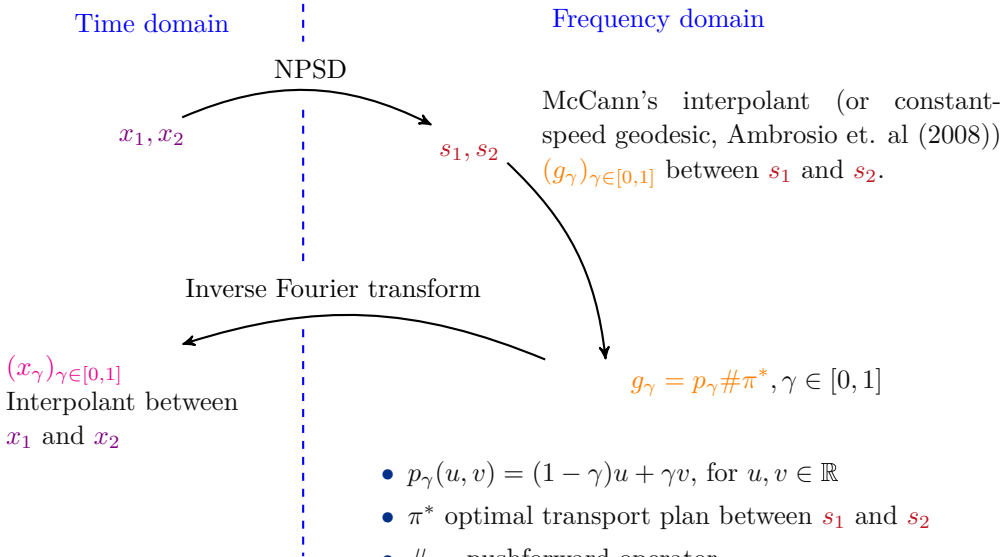
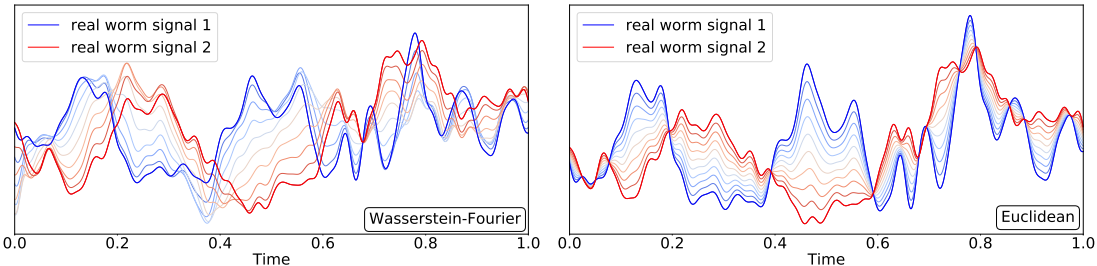


An interpolation path between two times series



Example: interpolation for the *C. Elegans* database



10-step interpolation $(x_\gamma)_{\gamma\in[0,1]}$ between two signals from the *C. elegans* database using the proposed WF distance (top) and the Euclidean distance (bottom): the true signals are shown in solid blue and red, while the interpolations are colour-coded with respect to γ.

Logistic regression of time series

For two classes C_0 and C_1, one defines a binary classification of a sample s as

$$p(C_0|s) = \frac{1}{1 + e^{-\alpha+\beta d(s,\bar{s_0})+\gamma d(s,\bar{s_1})}},$$

where d is a divergence $(\mathbb{L}_2, KL, W_2)$ and $\bar{s_i}$ sums up the information of class C_i.

- $\mathbb{L}_2$ and KL cases:

$$\bar{s} \in \arg\min_s \frac{1}{n}\sum_{i=1}^{n} \|s_i - s\|^2 = \frac{1}{n}\sum_{i=1}^{n} s_i.$$

- W_2 case: a **Wasserstein barycenter** of a family $(s_i)_{i=1,\dots,n}$ of distributions is given by

$$\bar{s} \in \arg\min_s \frac{1}{n}\sum_{i=1}^{n} W_2^2(s_i, s).$$

Logistic regression of time series

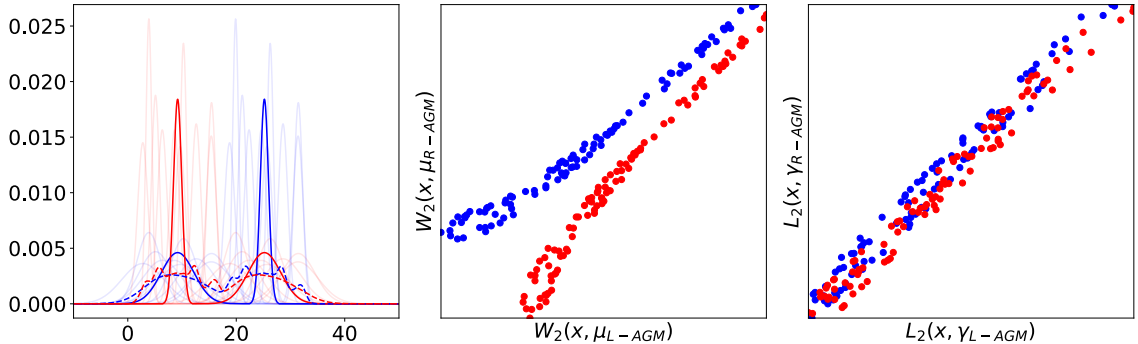


Illustration of the linear separability made possible by the Wasserstein-Fourier distance.

Real-world example: urban audio recordings[3]

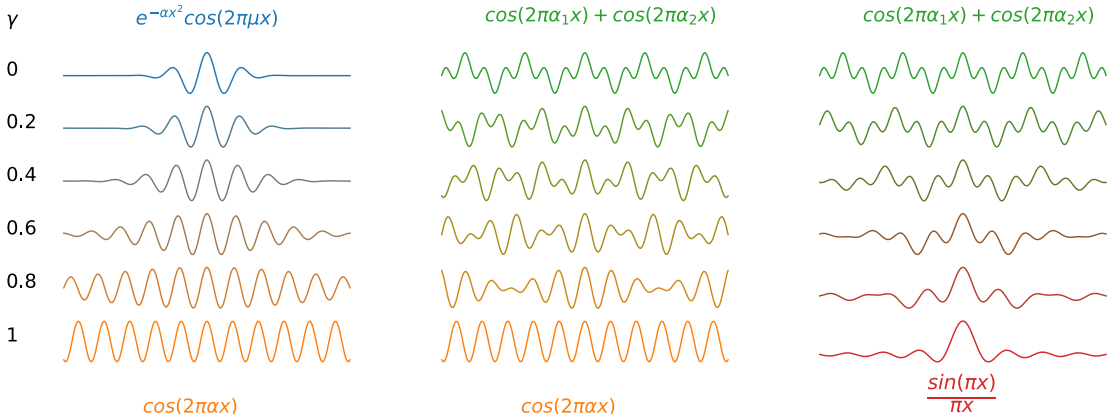
	$\mathcal{L}_{W_2}$	$\mathcal{L}_{\mathbb{L}_2}$	$\mathcal{L}_{KL}$
air conditioner	**0.732** ($\pm$0.072)	0.718 ($\pm$0.047)	0.650 ($\pm$0.090)
car horn	0.588 ($\pm$0.077)	0.743 ($\pm$0.043)	**0.790** ($\pm$0.037)
children playing	**0.751** ($\pm$0.027)	0.685 ($\pm$0.031)	0.736 ($\pm$0.023)
dog bark	**0.743** ($\pm$0.040)	0.720 ($\pm$0.033)	0.728 ($\pm$0.040)
drilling	**0.827** ($\pm$0.027)	0.826 ($\pm$0.026)	0.817 ($\pm$0.026)
engine idling	0.767 ($\pm$0.041)	0.733 ($\pm$0.051)	**0.791** ($\pm$0.042)
jackhammer	0.645 ($\pm$0.087)	0.585 ($\pm$0.095)	**0.669** ($\pm$0.059)
siren	0.803 ($\pm$0.062)	0.878 ($\pm$0.034)	**0.897** ($\pm$0.034)
street music	0.792 ($\pm$0.030)	0.782 ($\pm$0.025)	**0.812** ($\pm$0.029)

Table 1: Classification results for the class *gun shot* against the 9 remaining classes.

[3] Urbansound8k dataset

Geodesic path for Gaussian processes

Gaussian process $\leftrightarrow$ Kernel $\leftrightarrow$ PSD.



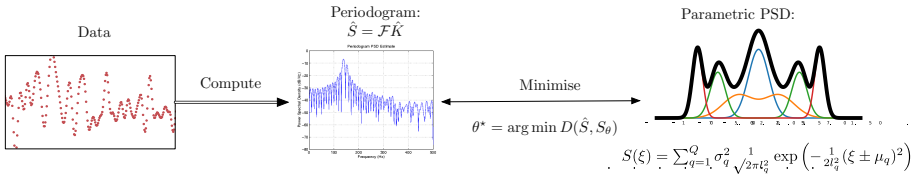
Our conjecture: We can train GPs in this way

Preliminary results: For some PSD families, the cost is convex

How Gaussian proceeses are trained

Covariance-based metrics: Compute sample covariance and apply, e.g., L_p distances.

Frequency-based metrics: Compute **Periodogram** and use any density-based metric: KL, Bergamn, Itakura-Saito, and Wasserstein.



An interesting case

Let us consider:

- Metric: The *Wasserstein* distance applied to the PSD, i.e., W_2 on $S = \mathcal{F}\{K\}$.
- A Location-scatter family of PSD: $\left\{ S_{\mu,\sigma}(\xi) = \frac{1}{\sigma} S_{0,1}\left(\frac{\xi-\mu}{\sigma}\right), \mu \in \mathbb{R}, \sigma \in \mathbb{R}_+ \right\}$

Theorem

For a location-scale family with prototype $S_{0,1}$, the minimiser of $W_2(S, S_{\mu,\sigma})$ is unique, given by

$$\mu^* = \int_0^1 Q(p)dp \qquad \textit{and} \qquad \sigma^* = \frac{1}{\int_0^1 Q_{0,1}^2(p)dp} \int_0^1 Q(p)Q_{0,1}(p)dp \tag{3}$$

where Q is the quantile function of S. The PSD S does not need to be location-scale.

Corollary: Training a GP with the Wasserstein distance has a cost $\mathcal{O}(n)$

Theoretical aspects

Does it converge? I.e., is it true that

$$\theta_n^\star = \arg\min D(\hat{S}_n, S_\theta) \xrightarrow[n\to\infty]{a.s.} \theta^\star = \arg\min D(S, S_\theta) \tag{4}$$

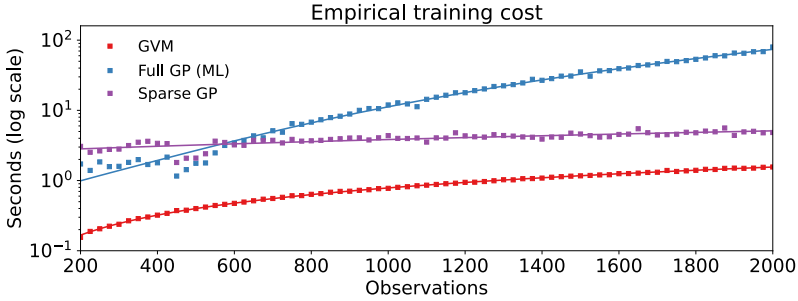
yes it is, provided that:

- **Metric.** D is either the Wasserstein-p or the L_p distances with $p \in \{1, 2\}$
- **Estimator of PSD.** $D(\hat{S}_n, S) \xrightarrow[n\to\infty]{a.s.} 0$
- **Identifiability.** $\theta_n \xrightarrow[n\to\infty]{} \theta \iff D(S_{\theta_n}, S_\theta) \to 0$;
- **Compactness.** the parameter space Θ is compact.

** This applies to temporal (covariance) distances too

OT-powered GP training: Linear complexity

- Computation time vs number of observations
- Exact case (W_2 distance and location-scale family)
- **Unevenly-sampled** observations from an single component SM kernel ($\mu = 0.05, \sigma = 0.01$) in the range $[0, 1000]$
- Compared against: ML estimate starting from the OT value (full GP, 100 iterations), and sparse GP using 200 pseudo inputs



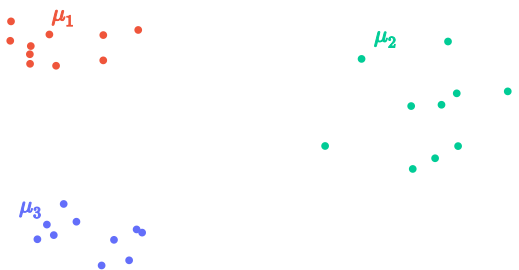
The Wasserstein barycenter

Given a set of distributions μ_s, compute:

$$\overline{\mu} = \arg\min_{\mu} \sum_{i=1}^{s} \lambda_i W_p^p(\mu, \mu_i)$$

where $\lambda_i > 0$ and $\sum_{i=1}^{s} \lambda_i = 1$.

Generalizes the interpolation between more than 2 measures.
For discrete measures $\mu = \sum_{i=1}^{n} a_i \delta_{x_i}$ $\Rightarrow$ we can fix the weights a_i and/or the support x_i.



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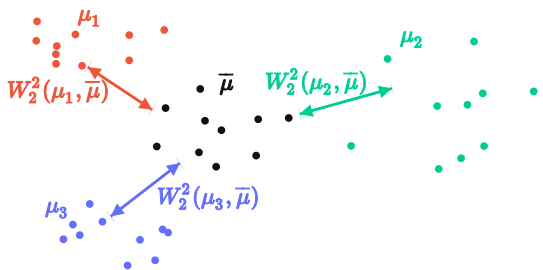

The Wasserstein barycenter

Example on averaging over images

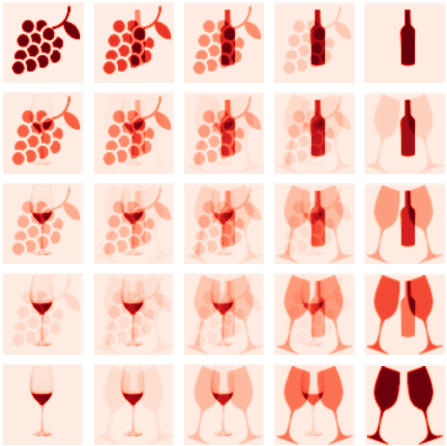

Figure 1: In the **Euclidean** space

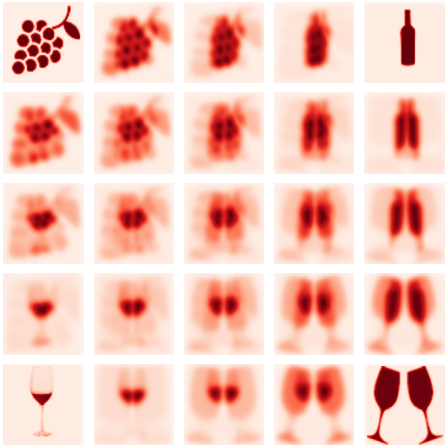

Figure 2: In the **Wasserstein** space

Notebook: Wass bary 4 distribs.ipynb

What we did not see

- Computational OT
- Multimarginal OT
- Unbalanced OT
- Partial OT
- Weak OT
- Particular cases with closed form

Conclusions & the future

- OT is now on the toolkit for many fields such as signal processing, machine learning etc.
- Defines a meaningful distances between distribution, with the extra information on how the particles should be moved
- Some open challenges: computational complexity, curse of dimensionality (number of samples to approximate the solutions depends is exponential with the dimension), robustify the solution with statistical guarantees (noise? outliers?), OT on different spaces than Euclidean ones, adding some extra constraints (like a temporal consistency)

Huge thanks to:

This tutorial handn't been possible without the infinite generosity and kindness of the following colleagues. Thank you for the discussion and the shared resources!

- Elsa Cazelles (IRIT)
- Fernando Fêtis (UChile)
- Joaquín Fontbona (UChile)
- Marco Cuturi (ENSAE/Apple)
- Rémi Flamary (École Polytechnique)

Optimal Transport for Signal Processing

A tutorial at MLSP 2024

Felipe Tobar[1] Laetitia Chapel[2]

[1]Initiative for Data & Artificial Intelligence, Universidad de Chile

[2]IRISA, Obelix team, Institut Agro Rennes-Angers

22 September, 2024