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

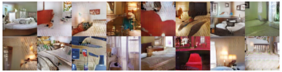
- Examples based on **POT: Python Optimal Transport Toolbox** (`pythonot.github.io`)
- Tutorial repository: `github.com/felipe-tobar/OT-tutorial-MLSP-2024`

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

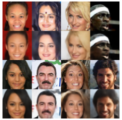
OT as a loss for classification
[Frogner, 2015]

Wasserstein style transfer
[Mroueh, 2020]

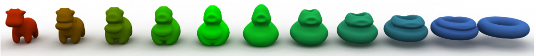


Wasserstein GAN
[Arjovsky 2017]

Wasserstein AE
[Tolstikhin 2018]

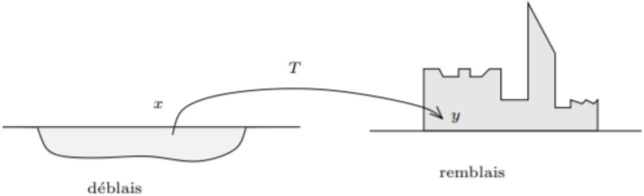


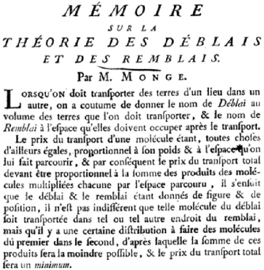
Shape interpolation
[Solomon, 2015]



Origins of OT: Gaspard Monge (1781)

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

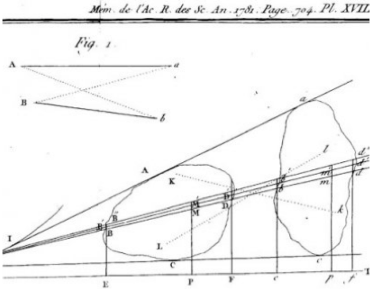




MÉMOIRE
SUR LA
THÉORIE DES DÉBLAIS
ET DES REMBLAIS.
Par M. MONGE.

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.

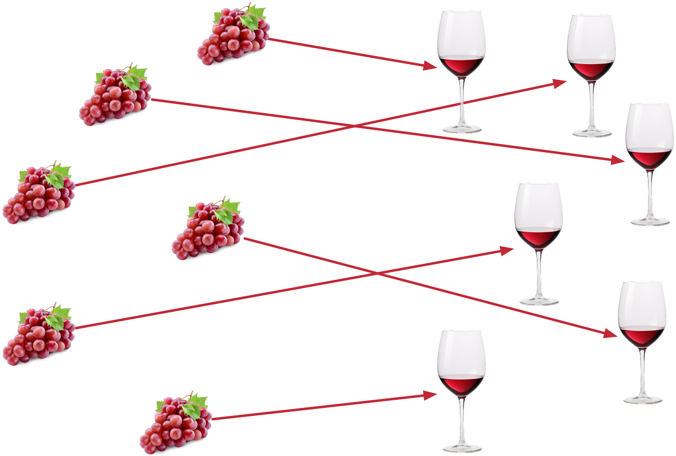
Le prix du tranſport d'une molécule étant, toutes choſes d'ailleurs égales, proportionnel à ſon poids & à l'eſpace qu'on lui fait parcourir, & par conſéquent le prix du tranſport total devant être proportionnel à la ſomme des produits des molécules multipliées chacune par l'eſpace parcouru, il s'enſuit 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

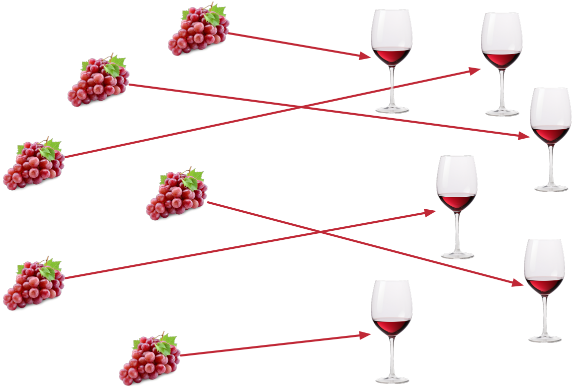

CUARTEL C2
CARMÉNÉRE
2.1 HA - 1994
2.3* 1.2 - 90 H

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

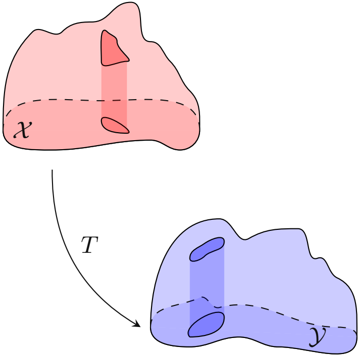


Monge formulation[1]

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

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

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

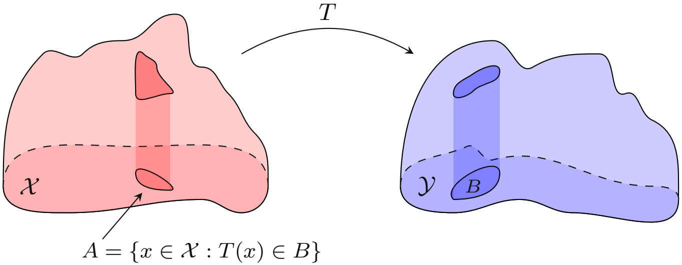
[1] Monge, G. (1781). Mémoire sur la théorie des déblais et des remblais. De l'Imprimerie Royale.

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.



$T\#\mu = \nu$

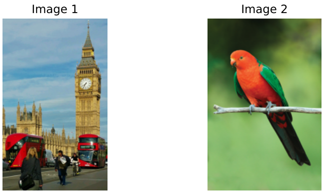
i.e., $\mu(A) = \nu(B)$

Figure adapted from Thorpe's book.[2]

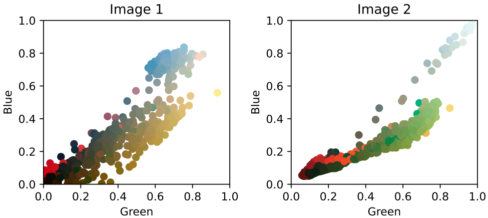
[2]Infinite thanks to Elsa Cazelles (IRIT, CNRS) for kindly sharing these beautiful `tikz` figures.

Example 1: Colour transfer

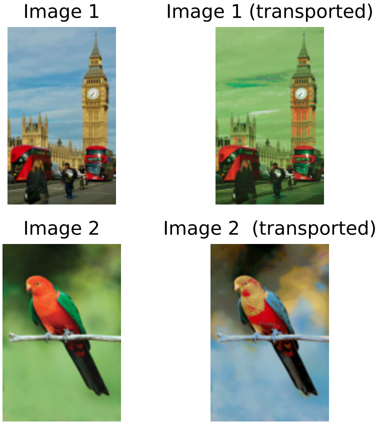
Original images



Histograms



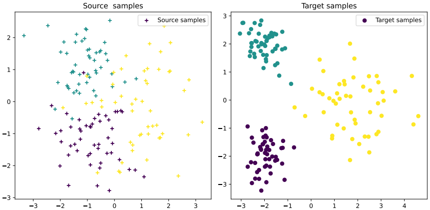
Histograms



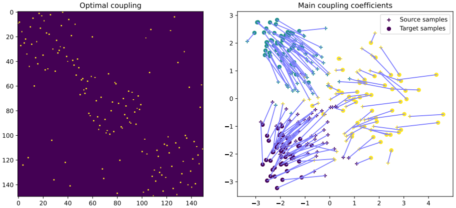
Notebook: Colour_transfer.ipynb

Example 2: Domain adaptation

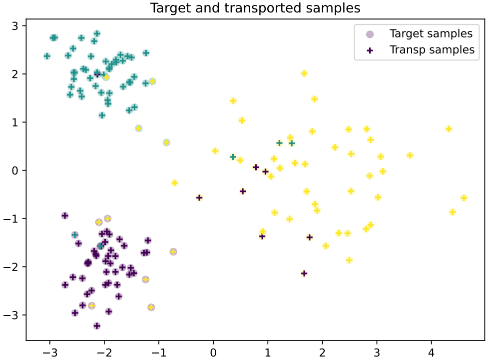
Original images



Histograms

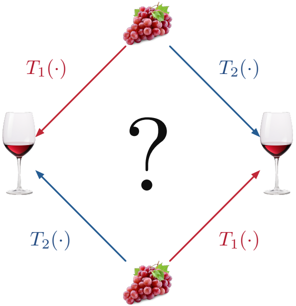


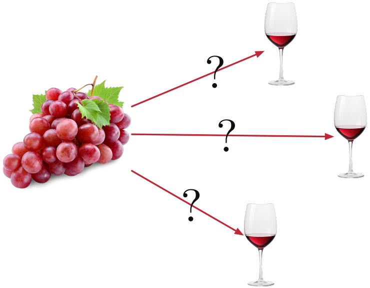
Histograms



Notebook: Domain_adaptation.ipynb

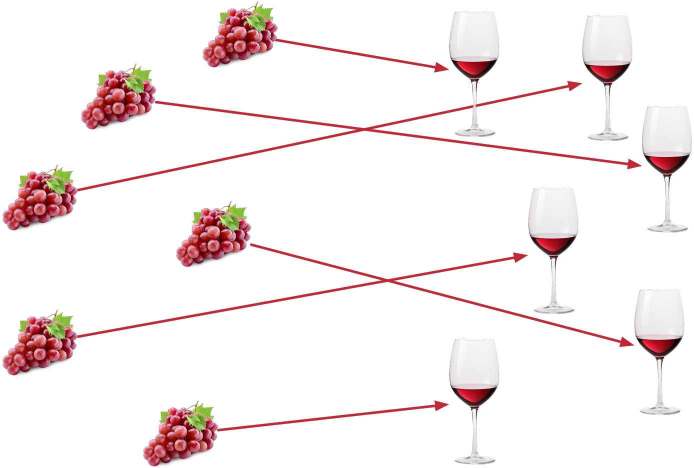
Neither existence nor uniqueness is guaranteed



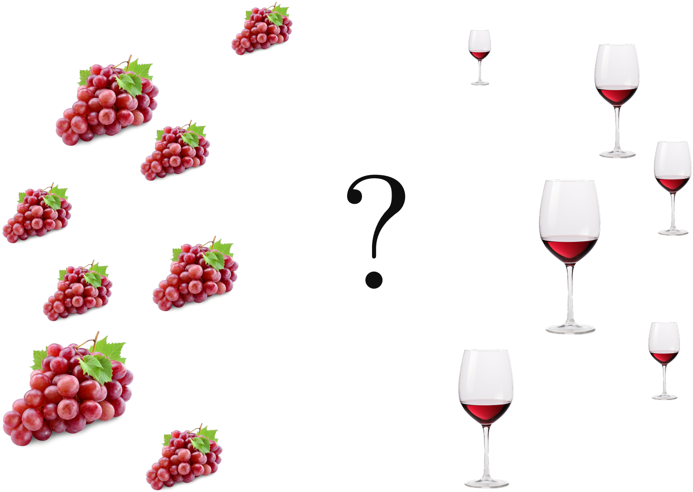


Observation: In the two examples above, each sample *weights the same*, i.e., pixels, class instances. In some cases, we might have *weighted samples*. In such cases, **Monge's map might be unable to transport the mass.**

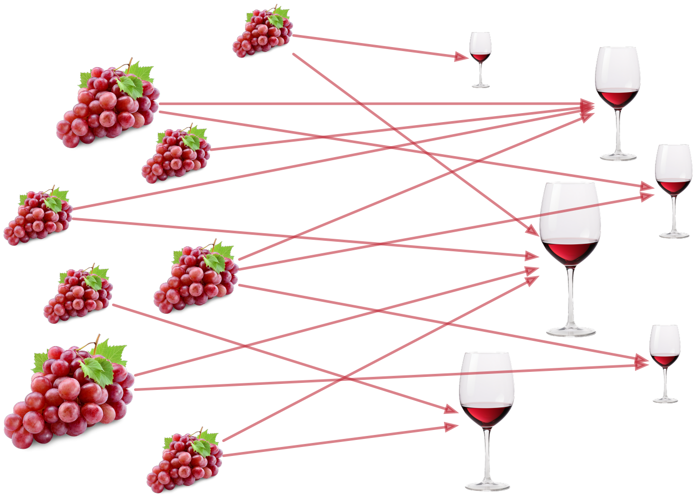
Kantorovich formulation: mass splitting



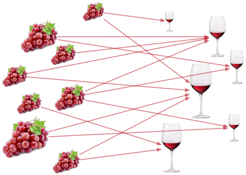
Kantorovich formulation: mass splitting



Kantorovich formulation: mass splitting



Transport *plan*

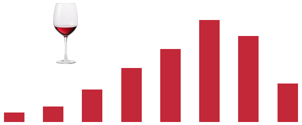


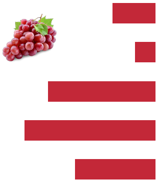
$$\mathrm{OT}(\mu,\nu) = \inf_{P\in\Pi_{\mu,\nu}} \langle P, C\rangle = \sum_{i,j}^{n,m} C_{ij}P_{ij}$$

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





	1	2	3	4	5	6	7	8
1	?	?	?	?	?	?	?	?
2	?	?	?	?	?	?	?	?
3	?	?	?	?	?	?	?	?
4	?	?	?	?	?	?	?	?
5	?	?	?	?	?	?	?	?

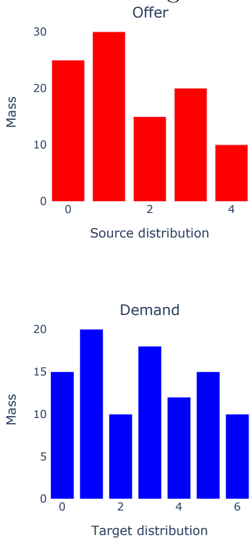
Cost Matrix

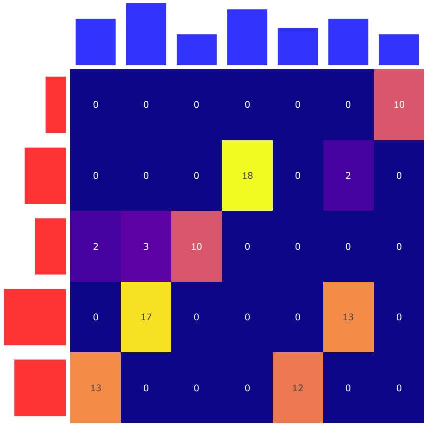
C

	1	2	3	4	5	6	7	8
1	$	$	$	$	$	$	$	$
2	$	$	$	$	$	$	$	$
3	$	$	$	$	$	$	$	$
4	$	$	$	$	$	$	$	$
5	$	$	$	$	$	$	$	$

Example 3: Discrete Kantorovich plan

Let consider the following source and target distributions

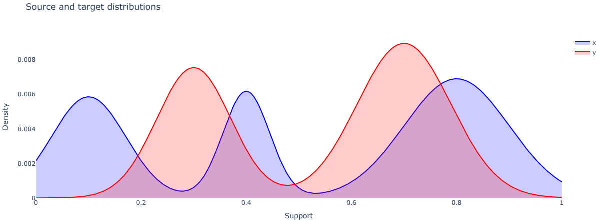


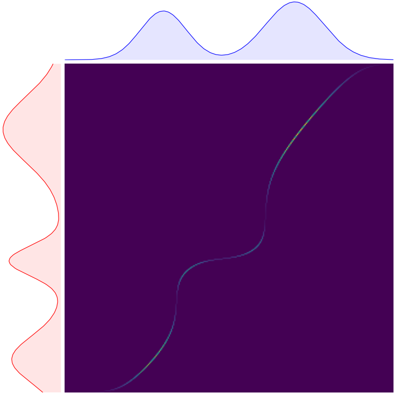


Notebook: kantorovich.ipynb

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

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

- 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)

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

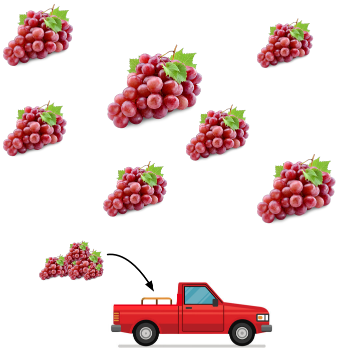
with

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

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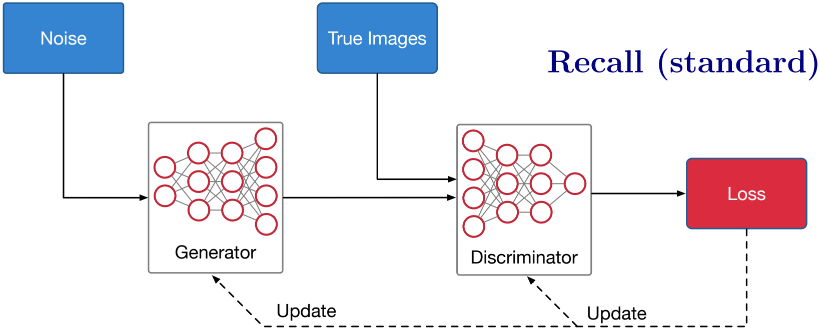
- Negative price are allowed!
- Does the vendor have a competitive offer? Her pricing scheme implies that transferring one kilo of grapes from vineyard x_i to plant y_j costs exactly $\alpha_i + \beta_j$.
- Recall the primal problem: the cost of shipping one unit from x_i to y_j is $C_{i,j}$.
- Feasible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



Recall (standard) 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 $\nu = \sum_{j=1}^{m} \delta_{y_j}$

$$\pi^* \in \underset{\pi \in \Pi(\mu,\nu)}{\arg\min} \; \langle C, \pi \rangle$$

- 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 $\pi \mathbb{1}_m = \mu$ and $\pi^T \mathbb{1}_n = \nu$

$\Longrightarrow$ 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).

Regularization of OT

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Regularization terms :

- Entropic regularization [Cuturi, 2013]
- KL, Itakura Saito, β-divergences, [Papadakis & Papadakis, 2018]

Entropy regularized OT [Cuturi, 2013]

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

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

- From Sinkhorn theorem [Sinkhorn, 1964], we get that $\mathrm{diag}(u)$ and $\mathrm{diag}(v)$ exist and are unique.
- Sinkhorn-Knopp algorithm [Knight, 2008] allows to solve it efficiently

Part II
The Wasserstein distance and metric properties

OT *lifts* a distance from the ground

A family of distances between measures

The **Kantorovich problem**

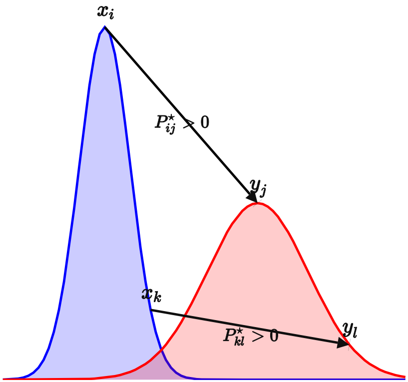
$$P^\star \in \inf_{P\in\Pi_{\mu,\nu}} \langle P, C\rangle = \sum_{i,j}^{n,m} C_{ij}P_{ij}$$

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

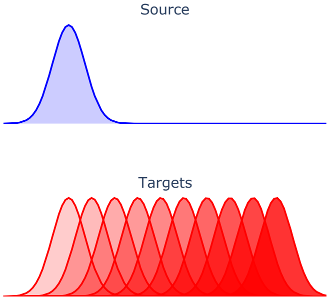
- ✓ **symmetry**
- ✓ **identity of indiscernibles**
- ✓ **triangular inequality**

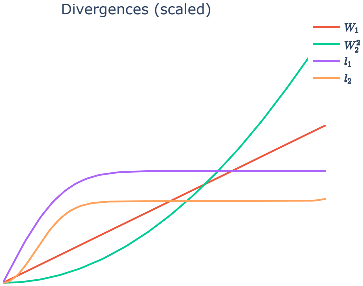


Notebook: Horizontal distance.ipynb

The Wasserstein distance (vs others)

- 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** divergence D.

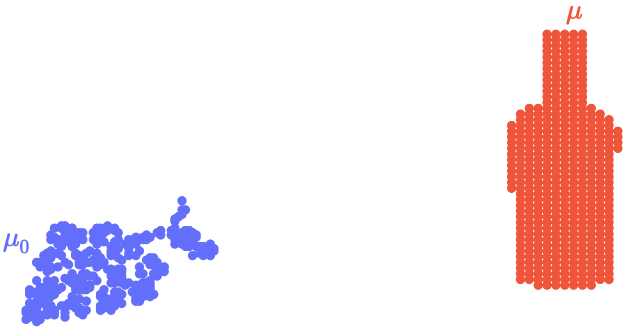
Discussion: Consider δ_{x_0} and $\delta_{x_i}, x_i \to x_0$

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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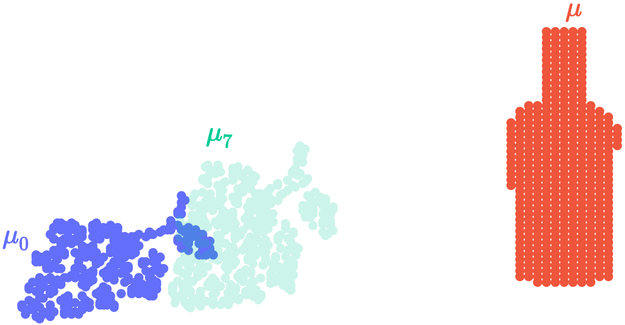

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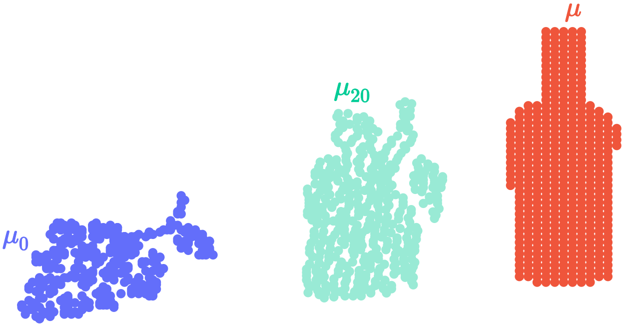

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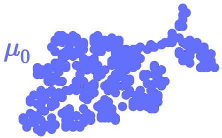

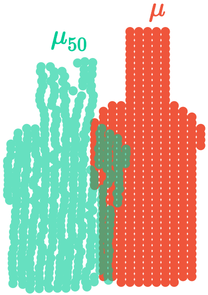

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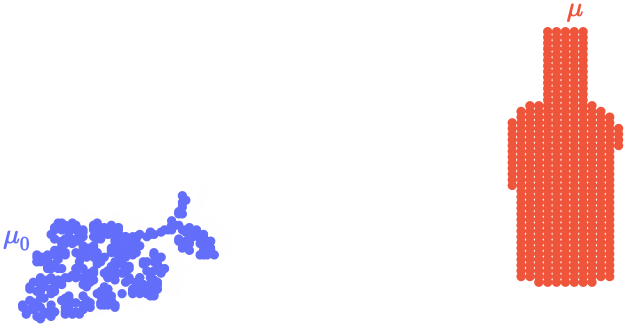


Notebook: Wasserstein Gradient Flows.ipynb

Geodesic paths between distributions

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

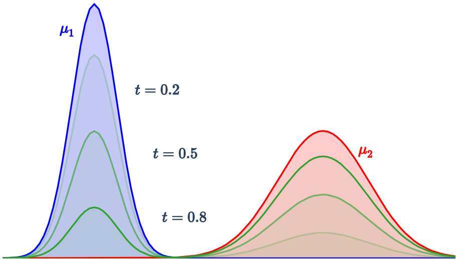
It is a curve that represents the shortest path between two manifolds

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



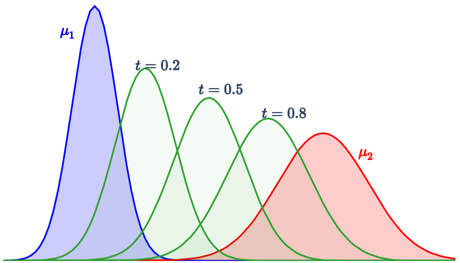
Geodesic properties of the Wasserstein space

$\mathbb{W}_p$ 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

The Wasserstein barycenter

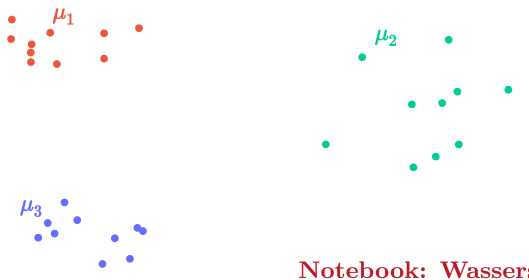
Given a set of distributions μ_s, compute:

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

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.



Notebook: Wasserstein barycenter.ipynb

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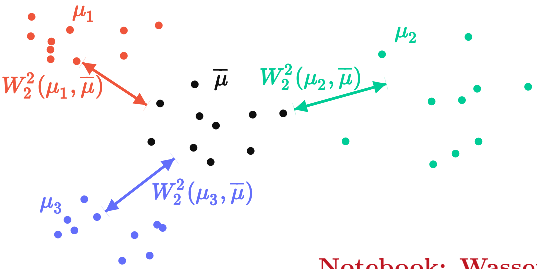


Notebook: Wasserstein barycenter.ipynb

The Wasserstein barycenter

Example on averaging over images

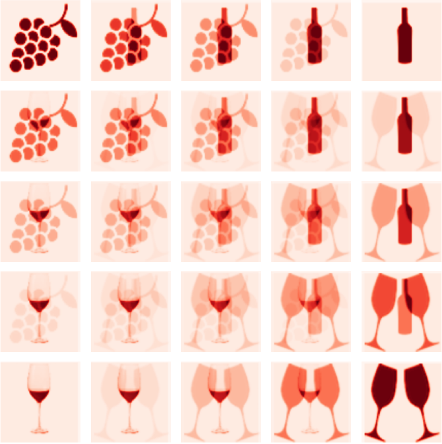


Figure 1: In the **Euclidean** space

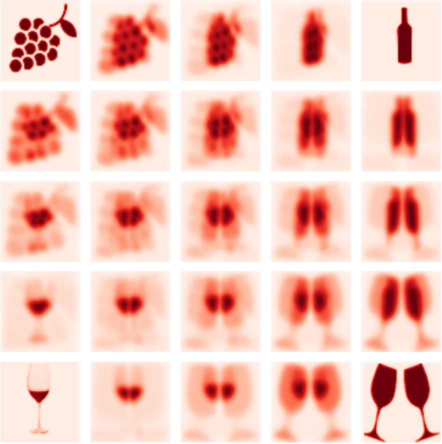


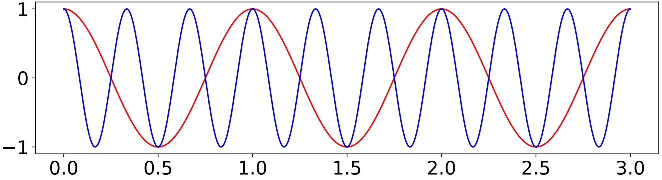
Figure 2: In the **Wasserstein** space

Notebook: Wass bary 4 distribs.ipynb

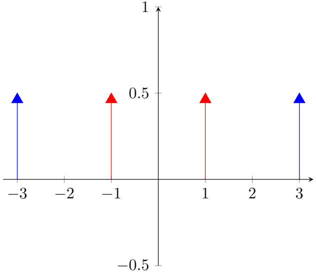
Part III
OT for time series: The Wasserstein-Fourier distance

Applying the Wasserstein distance to time series

Two cosine signals with frequencies 1 and 3.



The associated PSD functions .



$\mathbb{L}_2 = 1/\sqrt{2}$

$W_2 = 2$

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 normalised PSD (NPSD)

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

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

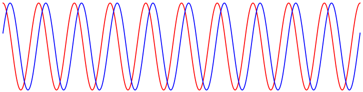
Theorem

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.

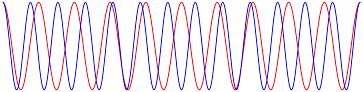
Basics properties of the WF distance

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



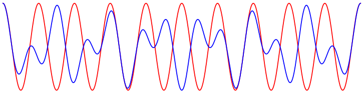
$$\mathrm{WF}\left([x],[y]\right) = 0$$

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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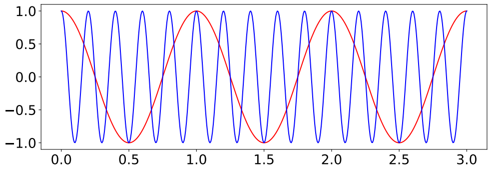

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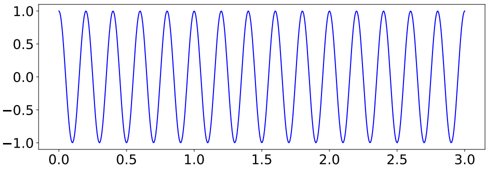
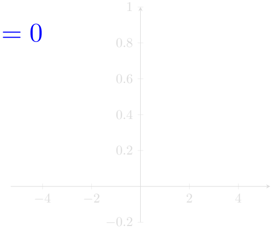


Frequency domain

$\gamma = 0$



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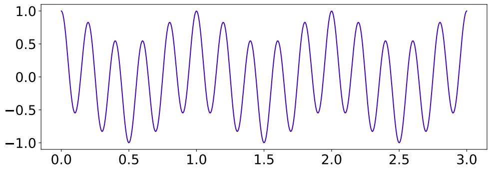
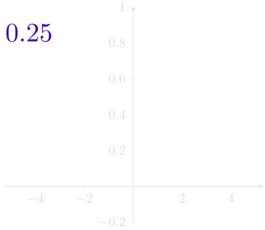


$\gamma = 0.25$

Frequency domain



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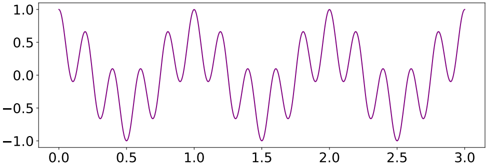
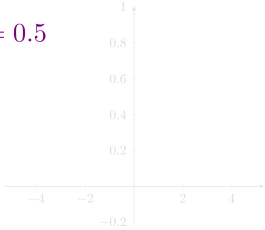


Frequency domain

$\gamma = 0.5$



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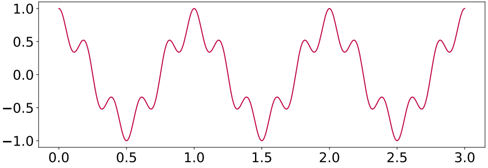
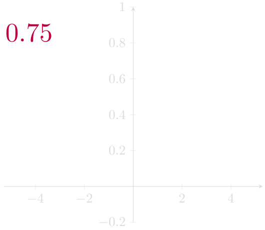


Frequency domain

$\gamma = 0.75$



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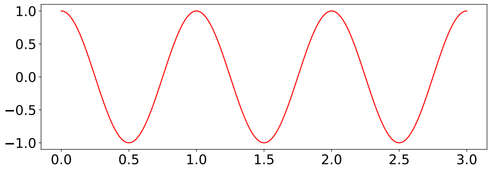
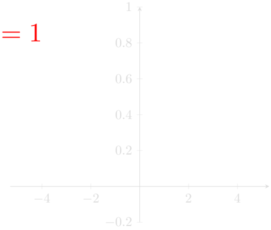


Frequency domain

$\gamma = 1$



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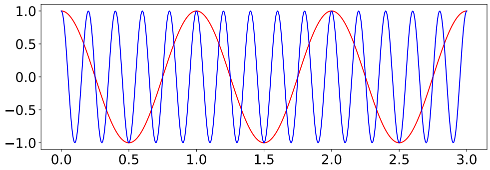

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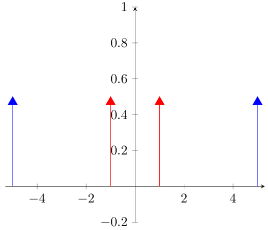

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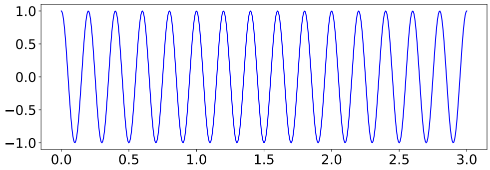
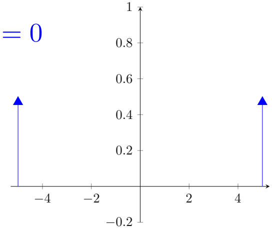


Frequency domain

$\gamma = 0$



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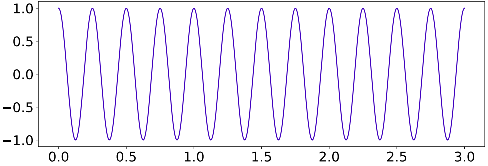
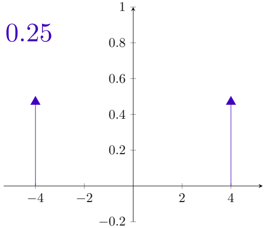


Frequency domain

$\gamma = 0.25$



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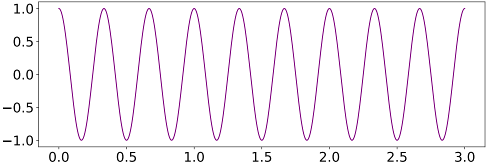

Frequency domain

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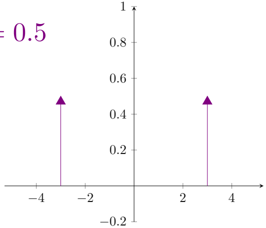

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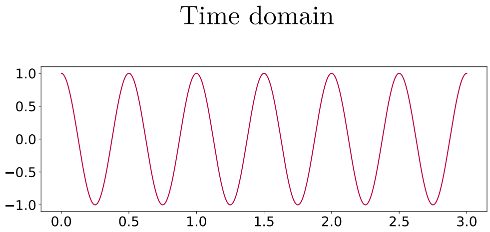

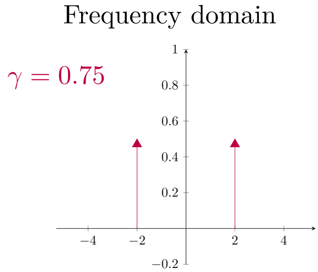

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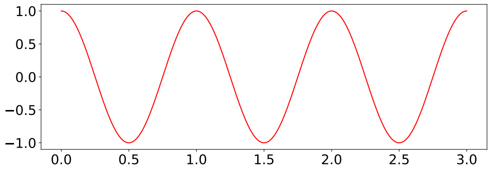
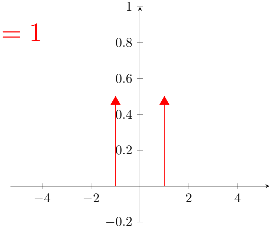


Frequency domain

$\gamma = 1$



An interpolation path between two times series

Time domain

Frequency domain

NPSD

$x_1, x_2 \xrightarrow{\text{NPSD}} s_1, s_2$

McCann's interpolant (or constant-speed geodesic, Ambrosio et. al (2008)) $(g_\gamma)_{\gamma\in[0,1]}$ between s_1 and s_2.

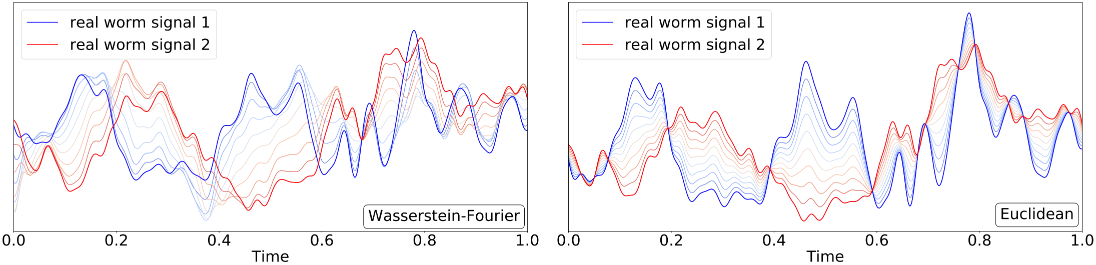
$g_\gamma = p_\gamma \# \pi^*, \gamma \in [0, 1]$

Inverse Fourier transform

$(x_\gamma)_{\gamma\in[0,1]}$
Interpolant between x_1 and x_2

- $p_\gamma(u, v) = (1-\gamma)u + \gamma v$, for $u, v \in \mathbb{R}$
- π^* optimal transport plan between s_1 and s_2
- $\# =$ pushforward operator

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 $(s_i)_{i=1,\ldots,n}$ 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

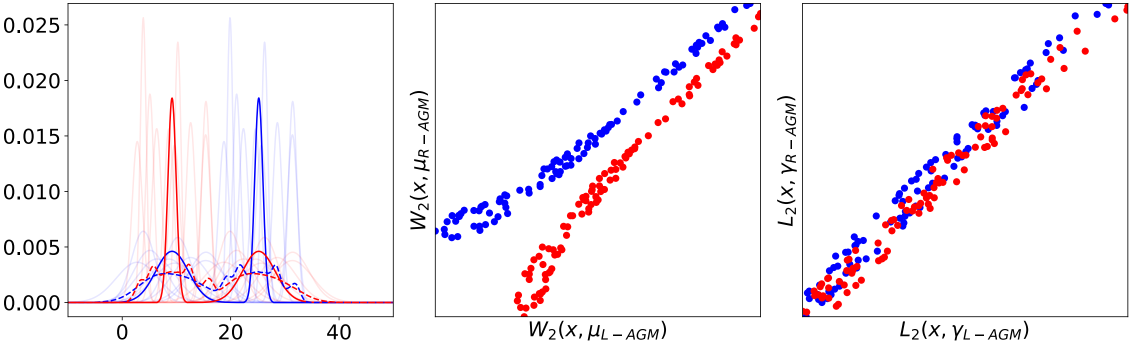


Illustration of the linear separability made possible by the Wasserstein-Fourier distance.

Real-world example: urban audio recordings[3]

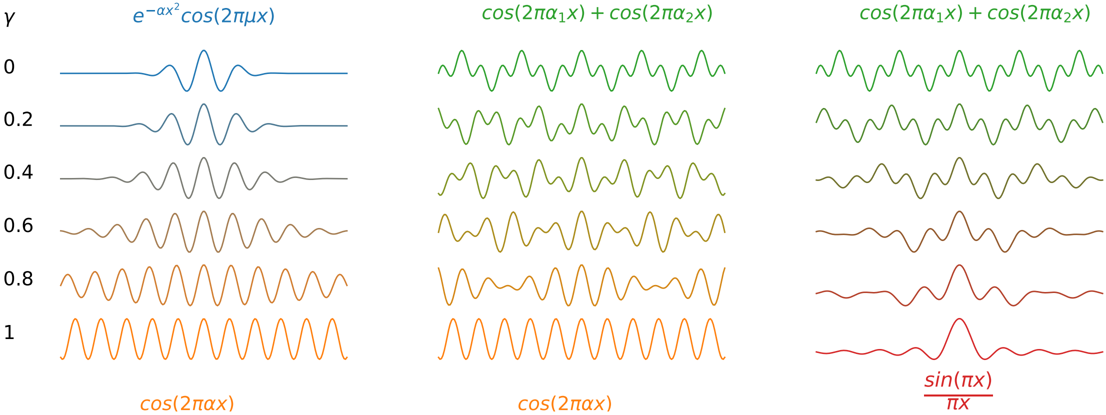
	$\mathcal{L}_{W_2}$	$\mathcal{L}_{\mathbb{L}_2}$	$\mathcal{L}_{KL}$
air conditioner	**0.732** ($\pm$0.072)	0.718 ($\pm$0.047)	0.650 ($\pm$0.090)
car horn	0.588 ($\pm$0.077)	0.743 ($\pm$0.043)	**0.790** ($\pm$0.037)
children playing	**0.751** ($\pm$0.027)	0.685 ($\pm$0.031)	0.736 ($\pm$0.023)
dog bark	**0.743** ($\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.



Spoiler: GPs can be trained in this way at a linear cost

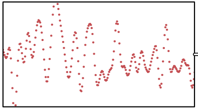
How Gaussian proceeses are trained

Maximum likelihood: Standard (very expensive) approach.

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

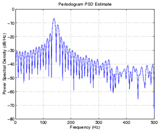
Frequency-based metrics: Compute **Periodogram** and use any density-based metric: KL, Bergamn, Itakura-Saito, and Wasserstein.

Data



Compute

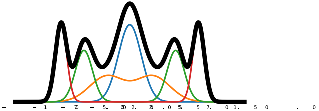
Periodogram:
$\hat{S} = \mathcal{F}\hat{K}$



Minimise

$$\theta^\star = \arg\min D(\hat{S}, S_\theta)$$

Parametric PSD:



$$S(\xi) = \sum_{q=1}^{Q} \sigma_q^2 \frac{1}{\sqrt{2\pi l_q^2}} \exp\left(-\frac{1}{2l_q^2}(\xi \pm \mu_q)^2\right)$$

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 $\mathcal{O}(n)$. I.e., no need of a gradient flow, as solution is exact and closed form.

Theoretical aspects

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

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

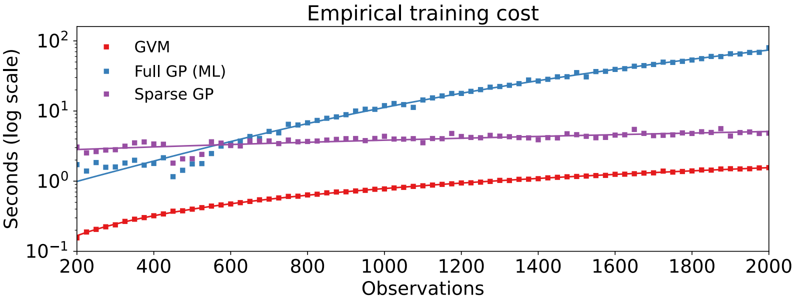
yes it is, provided that:

- **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



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 in the toolkit for many fields spanning **signal processing**, **machine learning**, data science and AI.
- OT defines a meaningful distance between distributions, and gives a procedure for **moving particles to minimise such distance**
- Some open challenges:
  - computational **complexity**
  - **curse of dimensionality:** samples for approximations grow exponentially with the dimension
  - **robustness of the solution** with statistical guarantees (noise? outliers?)
  - OT on **different spaces** than Euclidean ones
  - adding some extra constraints (such as 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

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22 September, 2024