A hands-on tutorial on Optimal Transport

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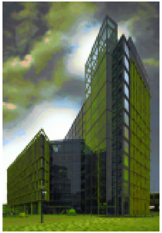


github.com/felipe-tobar/OT-tutorial

Overview

1. **Introduction**
2. **Part I**
   The Optimal Transport Problem
3. **Part II**
   The Wasserstein distance and metric properties
4. **Part III (if time allows)**
   OT for time series: The Wasserstein-Fourier distance

Preliminary remarks

- Based on the Tutorial **Optimal Transport for Signal Processing** given at IEEE MLSP 2024 w/ Laetitia Chapel (IRISA)
- Examples based on **POT: Python Optimal Transport Toolbox** (`pythonot.github.io`)
- Tutorial repository: **`github.com/felipe-tobar/OT-tutorial`**
- To clone the tutorial's `conda` environment, run: (tested on OSX and Linux):

```
conda env create -f environment.yml
```

∞ **thanks to:** Elsa Cazelles (Toulouse), Fernando Fetis (U. Chile), Marco Cuturi (Apple/ENSAE), Rémi Flamary (École Polytechnique)

OT for data analysis in a nutshell

Optimal Transportation theory is a set of tools for computing distances between distributions

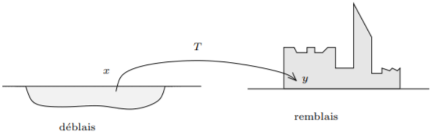
We are interested in OT because

- it gives a geometric-based view of probability distributions
- it enhances the machine learning (generative models), and data analysis (histograms) toolboxes.
- it addresses shortcomings of other divergences
- it is beautiful (but that's subjective)

Figure taken from `https://www.microsoft.com/en-us/research/blog/measuring-dataset-similarity-using-optimal-transport/`.
Credit: David Alvarez-Melis & Nicolo Fusi (Microsoft Research)

Origins of OT: Old and New

Gaspard Monge (1781): How to transport a pile of sand onto a hole in an optimal way?



Leonid Kantorovich (1942): Generalisation of Monge's and dual formulation
Yann Brenier (1987): Connections w/ PDEs, fluid mechanics, probability theory, and more.
A number of Fields Medals (2010+) Villani, Hairer, Figalli
Marco Cuturi (2013): Breakthrough in Machine Learning

Part I
The Optimal Transport Problem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CARMÉNÉRE
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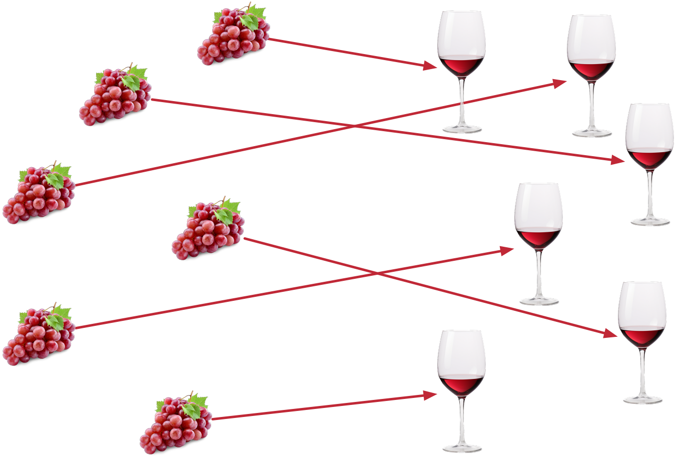
2.3* 1.2 - 90 H

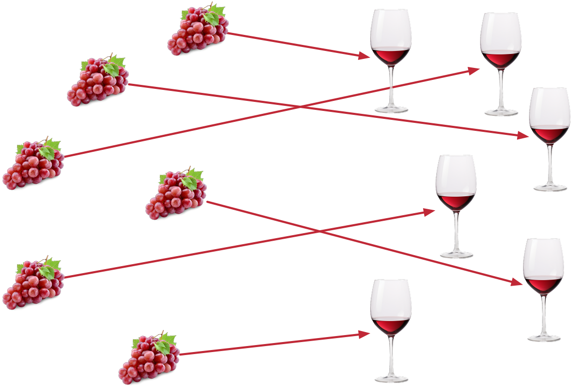
The assignment problem



The assignment problem: encoding the real world

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

(we'll start with a simple case)

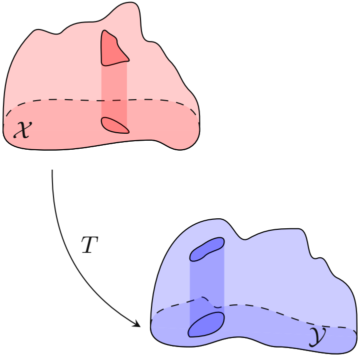


Monge formulation[1]

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

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 $c : (x, y) \in \mathcal{X} \times \mathcal{Y} \mapsto c(x, y) \in \mathbb{R}$.



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 $M_{X,Y} = \{T : \mathcal{X} \to \mathcal{Y},\ s.t.,\ T_{\#\mu} = \nu\}$ is the space of *admissible transport maps.*

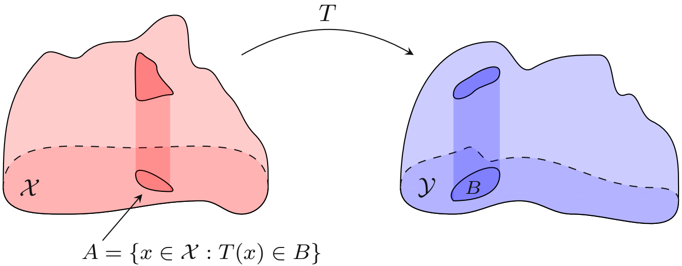
[1] Monge, G. (1781). Mémoire sur la théorie des déblais et des remblais. De l'Imprimerie Royale.

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.

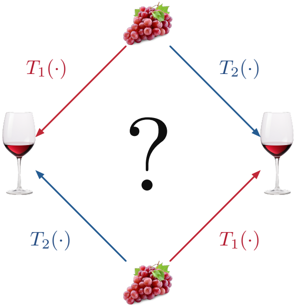


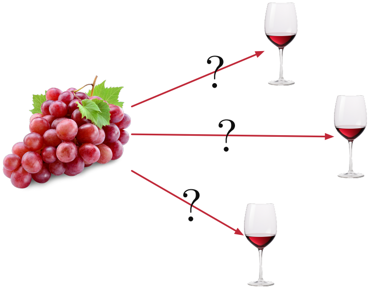
$T\#\mu = \nu$

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

(figure adapted from: Matthew Thorpe, *Introduction to Optimal Transport* 2018)

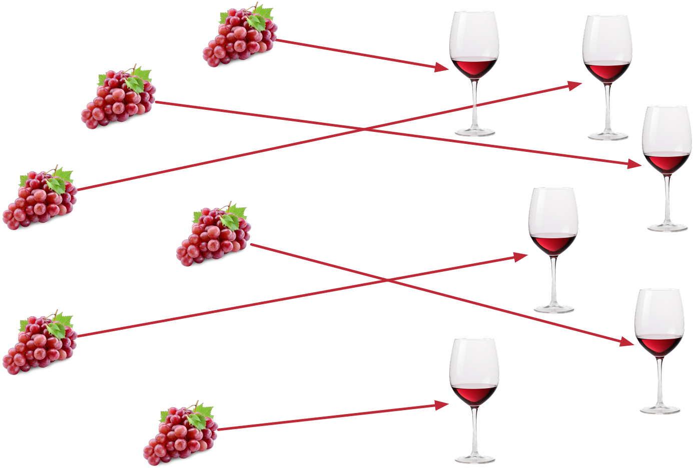
Warning: Neither existence nor uniqueness is guaranteed



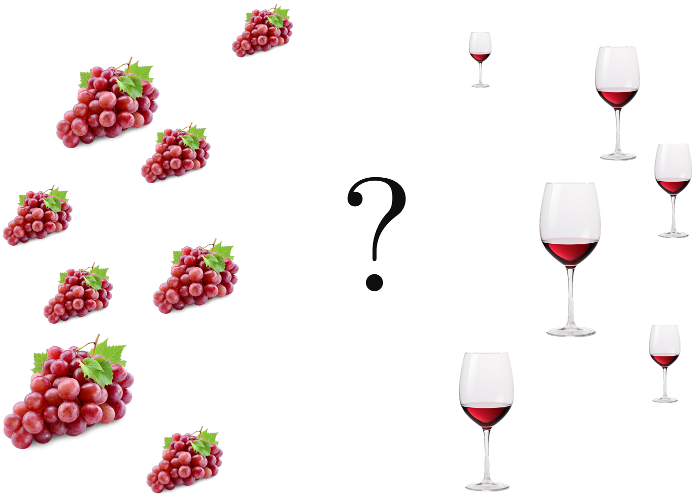


Remark: When both distributions have the same number of same-weight atoms, e.g., pixels or class instances, Monge's formulation can be solved. However, when dealing with different number of *weighted samples*, **Monge's map might be unable to transport the mass.**

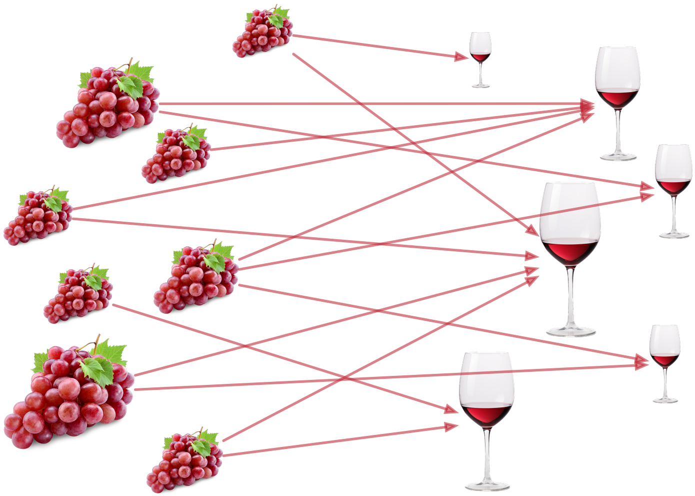
Kantorovich relaxation: mass splitting



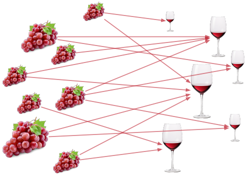
Kantorovich relaxation: mass splitting



Kantorovich relaxation: mass splitting



Kantorovich's *transport plan*

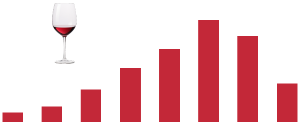


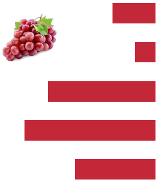
$$\mathrm{OT}\left(\mu,\nu\right)=\inf_{P\in\Pi_{\mu,\nu}}\langle P,C\rangle=\sum_{i,j}^{n,m}C_{ij}P_{ij}$$

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

Transport plan

P





$$\begin{array}{c|cccccccc|} & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\ \hline 1 & ? & ? & ? & ? & ? & ? & ? & ? \\ 2 & ? & ? & ? & ? & ? & ? & ? & ? \\ 3 & ? & ? & ? & ? & ? & ? & ? & ? \\ 4 & ? & ? & ? & ? & ? & ? & ? & ? \\ 5 & ? & ? & ? & ? & ? & ? & ? & ? \\ \hline \end{array}$$

Cost Matrix

C

$$\begin{array}{c|cccccccc|} & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\ \hline 1 & \$ & \$ & \$ & \$ & \$ & \$ & \$ & \$ \\ 2 & \$ & \$ & \$ & \$ & \$ & \$ & \$ & \$ \\ 3 & \$ & \$ & \$ & \$ & \$ & \$ & \$ & \$ \\ 4 & \$ & \$ & \$ & \$ & \$ & \$ & \$ & \$ \\ 5 & \$ & \$ & \$ & \$ & \$ & \$ & \$ & \$ \\ \hline \end{array}$$

Example 0: Compute transport plan (no toolbox)

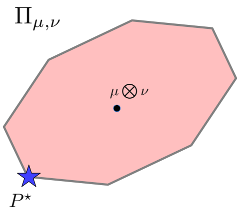
Computing the OT requires solving the linear problem:

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

subject to

$$0 \leq P_{ij} \leq 1, \sum_{i=1}^{m} P_{ij} = \nu_j, \sum_{j=1}^{n} P_{ij} = \mu_i.$$

Feasible set:



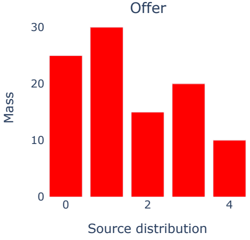
Algorithm:

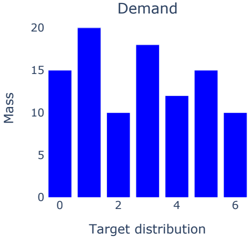
- Input: μ and ν with supports s_μ and s_ν
- Check distributions are valid
- Compute $C = c(s_\mu, s_\nu)$
- Soln: $P^\star = \arg\min \sum_{i,j}^{n,m} C_{ij}P_{ij}$
- Overall cost: $d = \sum_{i,j}^{n,m} C_{ij}P^\star_{ij}$

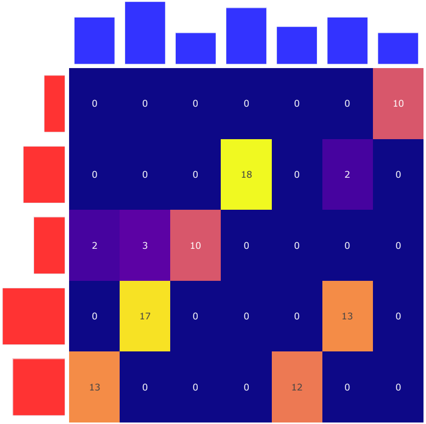
Notebook: Wasserstein_linprog.ipynb

Example 1: Discrete Kantorovich plan

Let consider the following source and target distributions



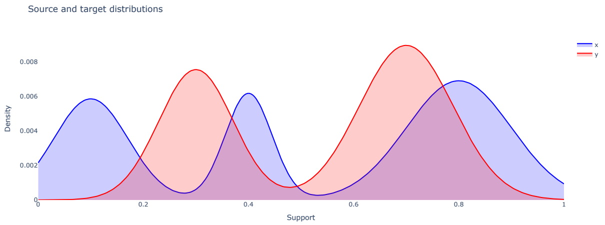


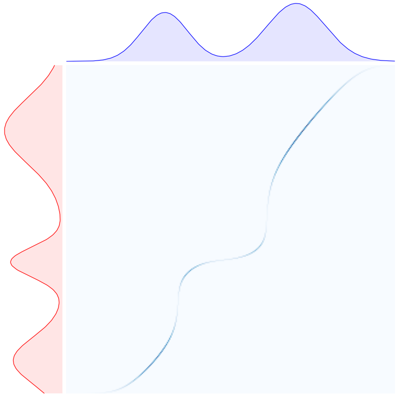


Notebook: kantorovich.ipynb

Example 2: Continuous Kantorovich plan

Let us now consider two distributions over a continuous support



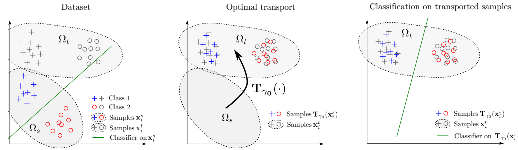


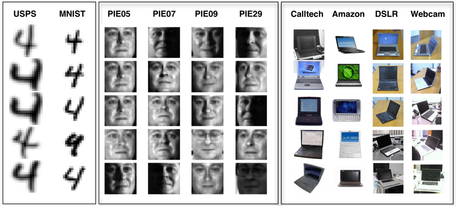
Observe that the plan remained *sparse*, i.e., the mass did not spread much
(bear this in mind, explanation to follow)

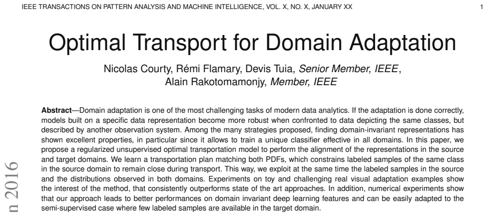
Notebook: kantorovich.ipynb

Motivation: Domain adaptation

Same tasks, different domains







IEEE TRANSACTIONS ON PATTERN ANALYSIS AND MACHINE INTELLIGENCE, VOL. X, NO. X, JANUARY XX 1

Optimal Transport for Domain Adaptation

Nicolas Courty, Rémi Flamary, Devis Tuia, *Senior Member, IEEE*, Alain Rakotomamonjy, *Member, IEEE*

Abstract—Domain adaptation is one of the most challenging tasks of modern data analytics. If the adaptation is done correctly, models built on a specific data representation become more robust when confronted to data depicting the same classes, but described by another observation system. Among the many strategies proposed, finding domain-invariant representations has shown excellent properties, in particular since it allows to train a unique classifier effective in all domains. In this paper, we propose a regularized unsupervised optimal transportation model to perform the alignment of the representations in the source and target domains. We learn a transportation plan matching both PDFs, which constrains labeled samples of the same class in the source domain to remain close during transport. This way, we exploit at the same time the labeled samples in the source and the distributions observed in both domains. Experiments on toy and challenging real visual adaptation examples show the interest of the method, that consistently outperforms state of the art approaches. In addition, numerical experiments show that our approach leads to better performances on domain invariant deep learning features and can be easily adapted to the semi-supervised case where few labeled samples are available in the target domain.

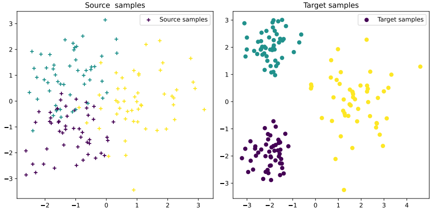
n 2016

Nicolas Courty, Rémi Flamary, Devis Tuia, Alain Rakotomamonjy. Optimal Transport for Domain Adaptation. *IEEE Transactions on Pattern Analysis and Machine Intelligence* 2016, 39 (9), pp.1853- 1865.

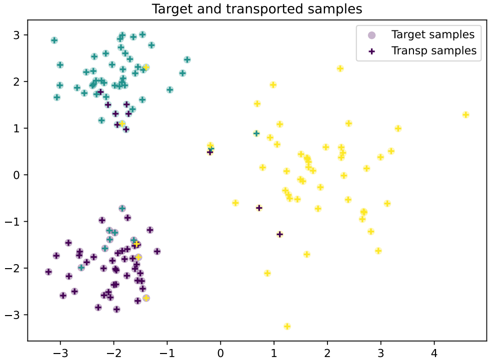
Link: arxiv.org/abs/1507.00504

Example 3: Domain adaptation

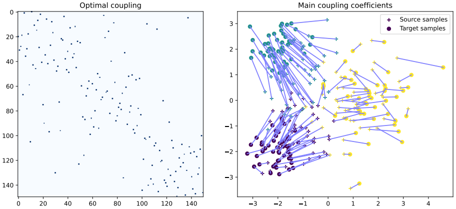
Two datasets: same task



Domain: adapted



Transport



Notebook: Domain_adaptation.ipynb

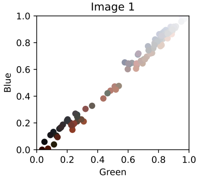
Example 4: Colour transfer

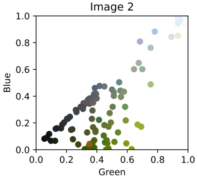
Original images

Image 1

Image 2

Histograms





Notebook: Colour_transfer.ipynb

Ferradans, S., Papadakis, N., Peyre, G., & Aujol, J. F. (2014). Regularized discrete optimal transport. *SIAM Journal on Imaging Sciences*, 7(3), 1853-1882.

Transported images

Image 1

Image 1 (transported)

Image 2

Image 2 (transported)

Remarks

- We've been using the cost $c(x, y) = |x - y|^p, p \geq 1$. In this case, if μ and ν are absolutely continuous wrt the Lebesgue measure, the Kantorovich problem has a unique solution. Furthermore, this solution coincides with that of Monge's problem.
- If $p = 2$, the optimal map is the gradient of a convex function, thus *preserving orientation*
- In some cases, the optimal plan will require to mass splitting (e.g., in the case of atomic measures) and thus Monge's solution may fail to exist.
- From a (Kantorovich) transport plan we can always extract a transport map, e.g., via the barycentric projection

Solving discrete OT

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

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

- Linear problem: it can be rewritten in a vectorial form $\min_{t \geq 0} F(t) = c^T t$
- Linear constraints of the form $\pi \mathbb{1}_m = \mu$ and $\pi^T \mathbb{1}_n = \nu$

$\Longrightarrow$ Linear problem + linear constraints: complexity is $\mathcal{O}(n^3 \log(n))$

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

Regularization of OT

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

Advantages of regularizing the optimisation problem:

- Fast and *smoother* solutions
- Encoding task's prior knowledge
- Better posed problem (convexity, stability).

Regularisation functionals

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

Entropy regularized OT [Cuturi, 2013]

The solution of

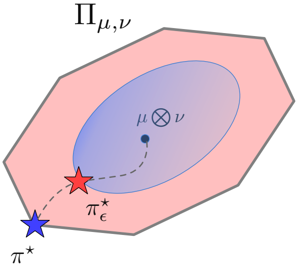
$$\mathrm{OT}(\mu, \nu) = \min_{\pi \in \Pi(a,b)} \langle C, \pi \rangle + \varepsilon \sum_{i,j} \pi_{ij} \log(\pi_{ij})$$

is of the form

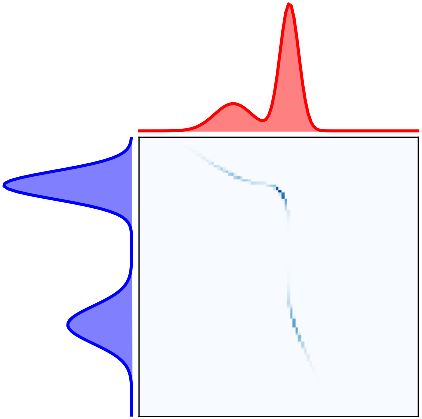
$$\pi^*_\varepsilon = \mathrm{diag}(u) \exp\left(-\frac{C}{\varepsilon}\right) \mathrm{diag}(v)$$

where u and v follow an alternating recursive formula.

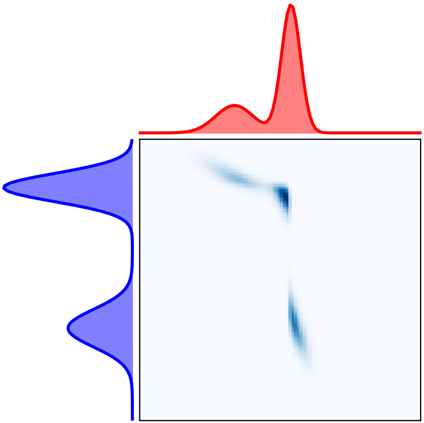
- From Sinkhorn theorem [Sinkhorn, 1964], we know that $\mathrm{diag}(u)$ and $\mathrm{diag}(v)$ exist and are unique.
- Sinkhorn-Knopp algorithm [Knight, 2008] allows to solve it efficiently



Example 5: Sinkhorn regularisation and effect



Transport plan using EMD
Cost: 0.046352152252243212
time: 0.0019245147705078125



Transport plan Sinkhorn
Cost: 0.047175892427394304
time: 0.006723642349243164

Notebook: sinkhorn.ipynb

Part II
The Wasserstein distance and metric properties

OT *lifts* a distance from the measures' support

A family of distances between measures

The **Kantorovich problem**

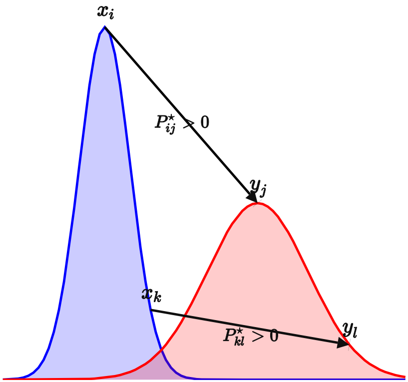
$$P^\star \in \inf_{P\in\Pi_{\mu,\nu}} \langle P, C\rangle = \sum_{i,j}^{n,m} C_{ij}P_{ij}$$

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

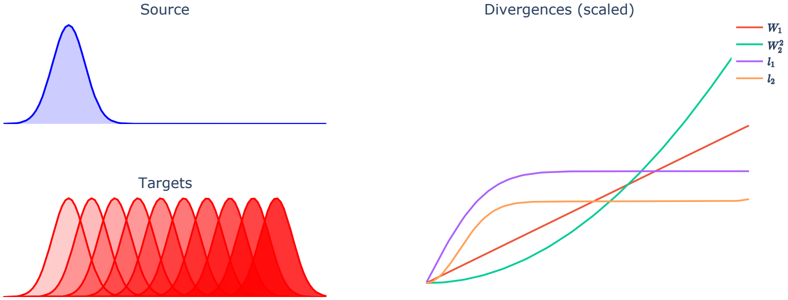
- ✓ **symmetry**
- ✓ **identity of indiscernibles**
- ✓ **triangular inequality**



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 in 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 $\delta_{x_i}, x_i \to x_0$

OT allows for **assessing** convergence and **constructing** convergent sequences

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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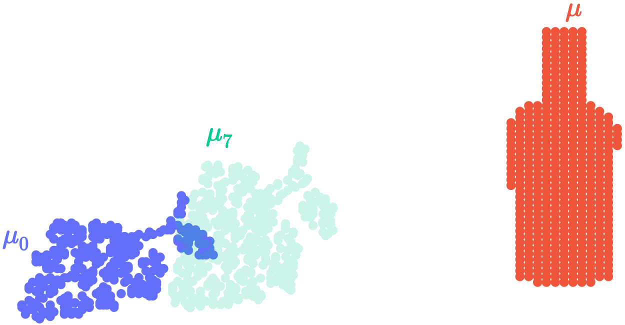

Notebook: Wasserstein Gradient Flows.ipynb

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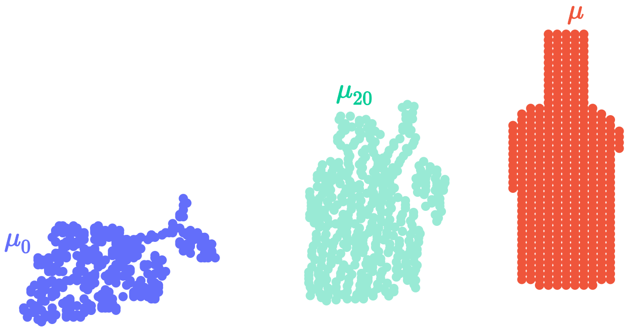

Notebook: Wasserstein Gradient Flows.ipynb

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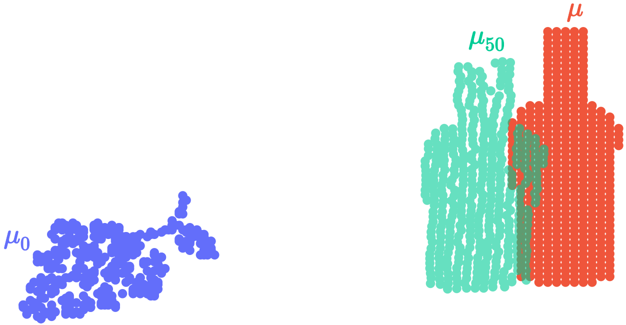


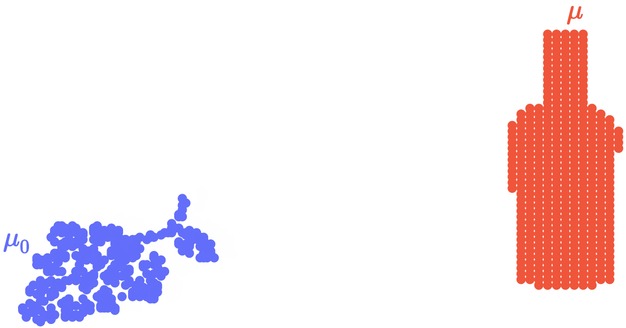
Notebook: Wasserstein Gradient Flows.ipynb

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

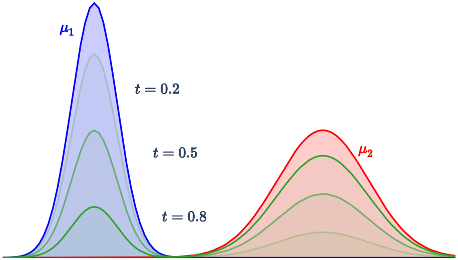
Geodesic paths between distributions

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

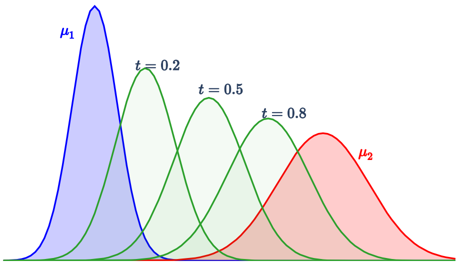
Geodesic properties of the Wasserstein space

$\mathbb{W}_p$ 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 barycentre

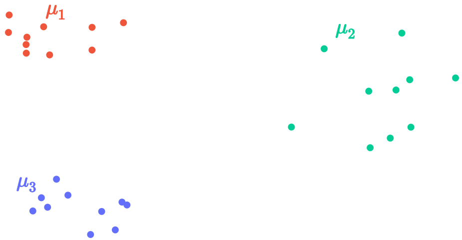
Given a set of distributions μ_s, compute:

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

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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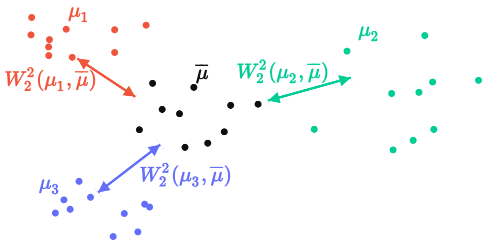


Notebook: Wasserstein barycenter.ipynb

The Wasserstein barycentre

Example on averaging over images

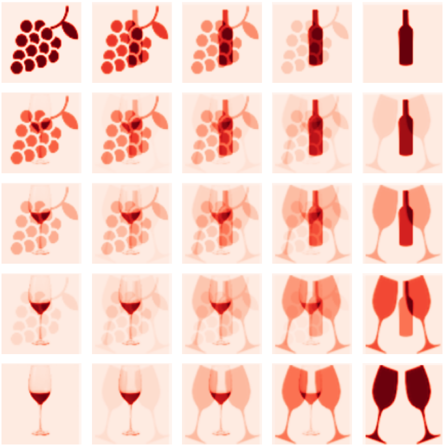


Figure 1: In the **Euclidean** space

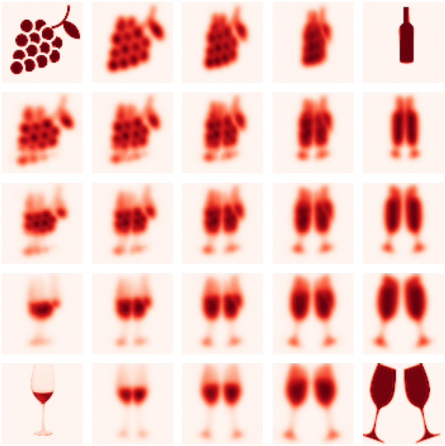


Figure 2: In the **Wasserstein** space

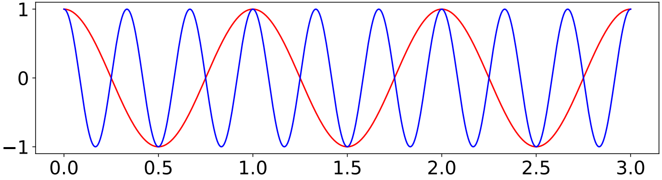
Notebook: Wass bary 4 distribs.ipynb

(if time allows)

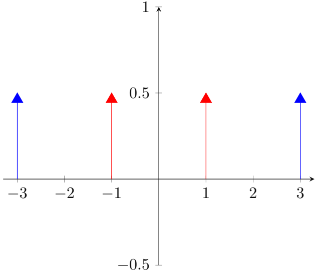
Part III
OT for time series: The Wasserstein-Fourier distance

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:

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

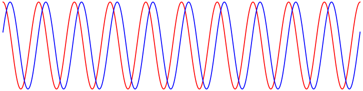
Theorem

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.

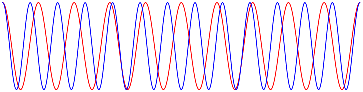
Basics properties of the WF distance

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



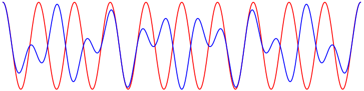
$$\mathrm{WF}\left([x],[y]\right) = 0$$

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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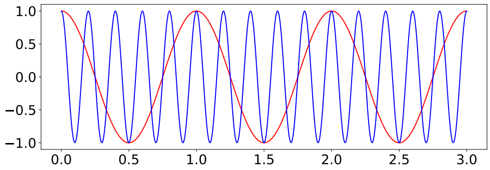

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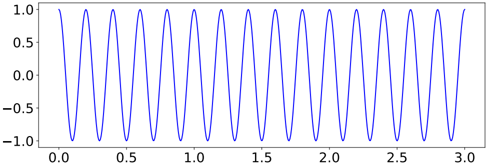
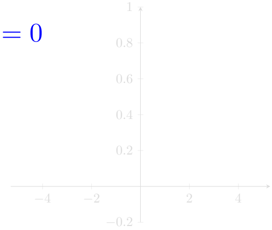


Frequency domain

$\gamma = 0$



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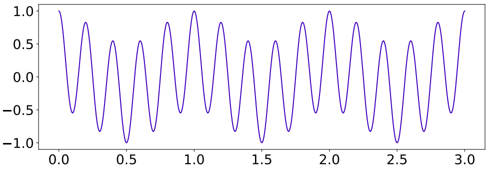
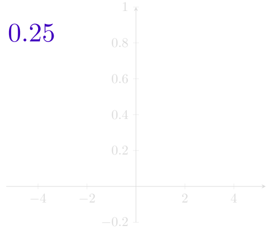


$\gamma = 0.25$

Frequency domain



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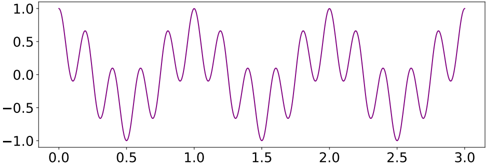
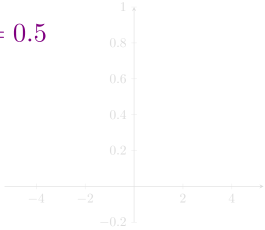


Frequency domain

$\gamma = 0.5$



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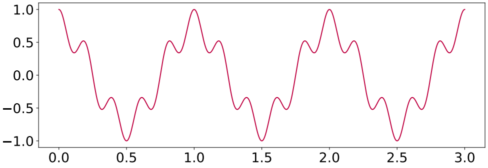
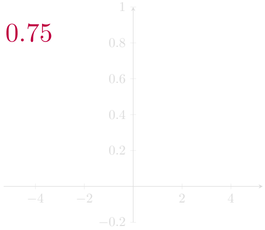


Frequency domain

$\gamma = 0.75$



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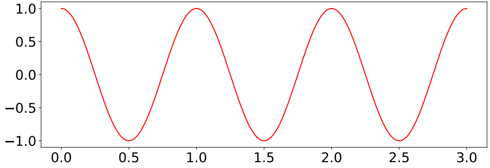
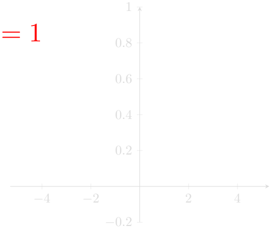


Frequency domain

$\gamma = 1$



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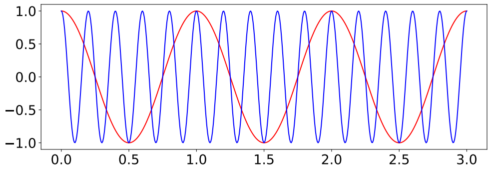
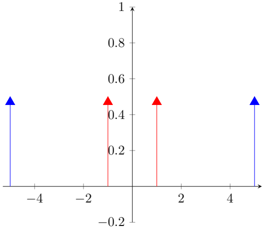


Frequency domain



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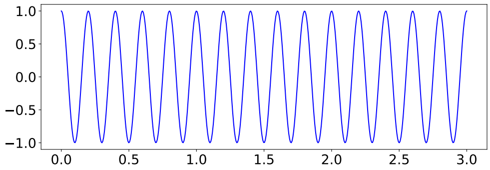

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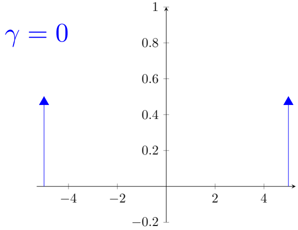

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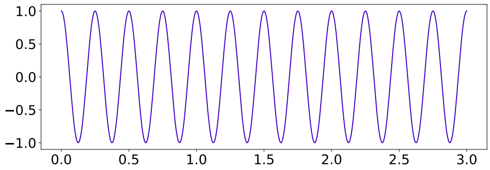
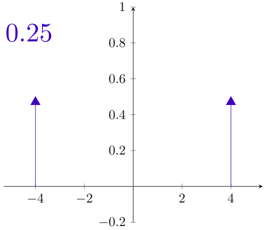


Frequency domain

$\gamma = 0.25$



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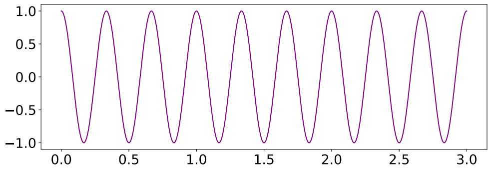

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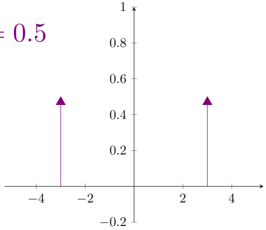

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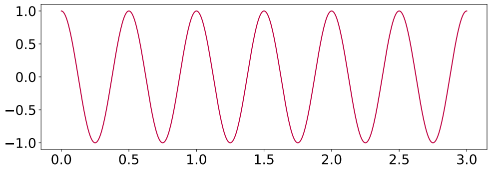
Time domain



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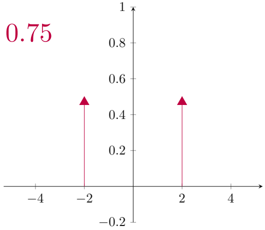

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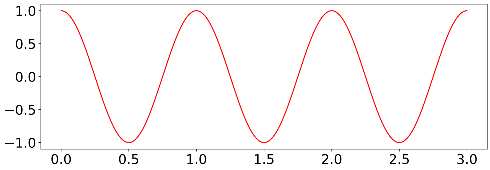
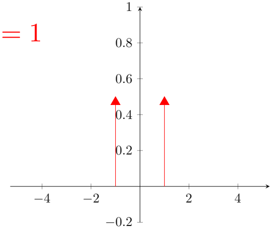
Time domain



Frequency domain

$\gamma = 1$



An interpolation path between two times series

Time domain

Frequency domain

NPSD

x_1, x_2

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.

Inverse Fourier transform

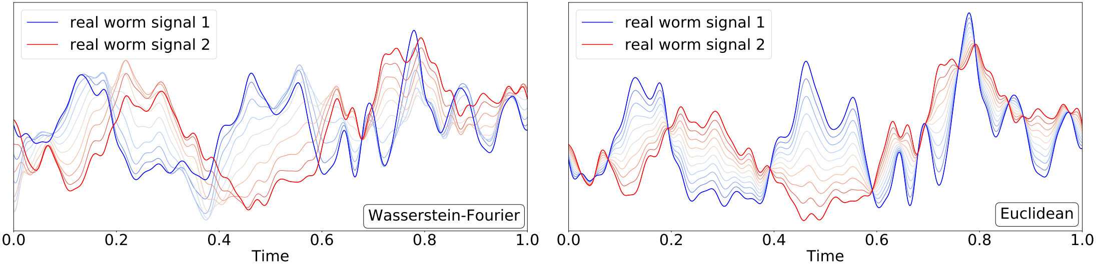
$(x_\gamma)_{\gamma\in[0,1]}$

Interpolant between x_1 and x_2

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

- $p_\gamma(u,v) = (1-\gamma)u + \gamma v$, 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 barycentre** 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

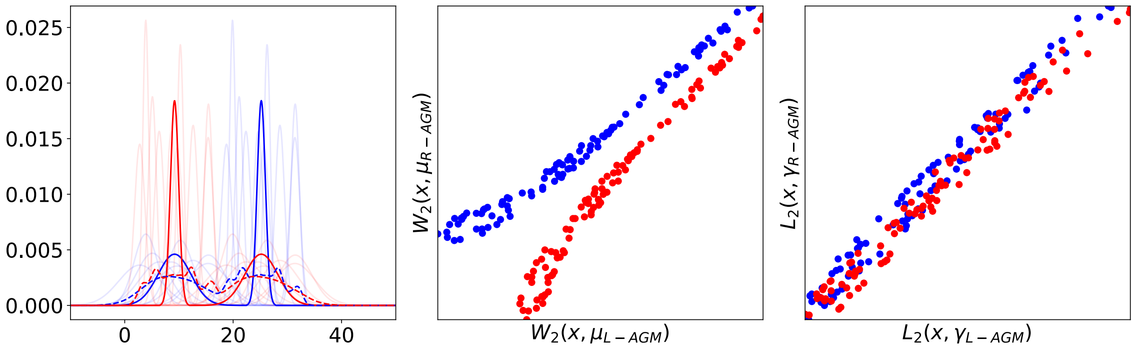


Illustration of the linear separability made possible by the Wasserstein-Fourier distance.

Real-world example: urban audio recordings[2]

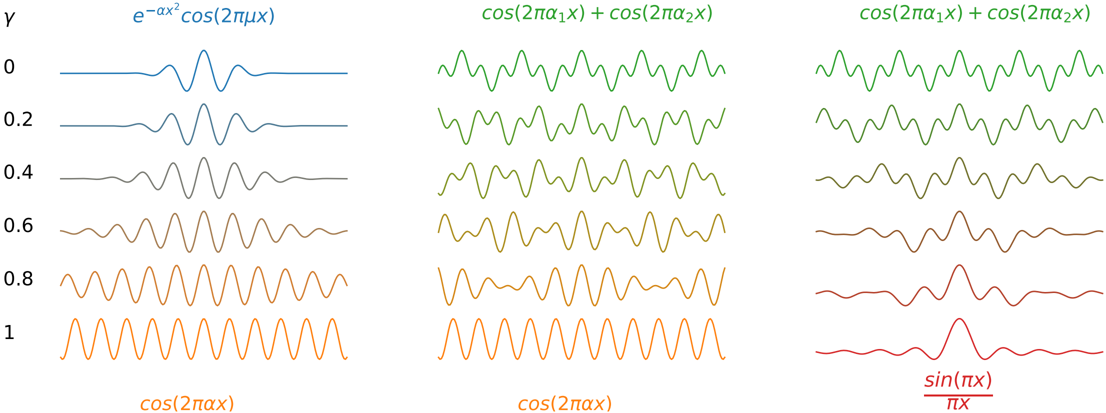
	$\mathcal{L}_{W_2}$	$\mathcal{L}_{\mathbb{L}_2}$	$\mathcal{L}_{KL}$
air conditioner	**0.732** ($\pm$0.072)	0.718 ($\pm$0.047)	0.650 ($\pm$0.090)
car horn	0.588 ($\pm$0.077)	0.743 ($\pm$0.043)	**0.790** ($\pm$0.037)
children playing	**0.751** ($\pm$0.027)	0.685 ($\pm$0.031)	0.736 ($\pm$0.023)
dog bark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

[2] 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

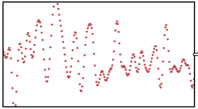
How Gaussian processes are trained

Maximum likelihood: Standard (very expensive) approach.

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

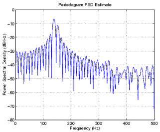
Frequency-based metrics: Compute **Periodogram** and use any density-based metric: KL, Bergamn, Itakura-Saito, and Wasserstein.

Data



Compute

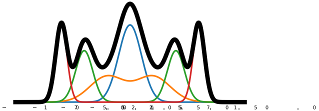
Periodogram:
$\hat{S} = \mathcal{F}\hat{K}$



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 $S = \mathcal{F}\left\{K\right\}$.
- 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

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

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

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

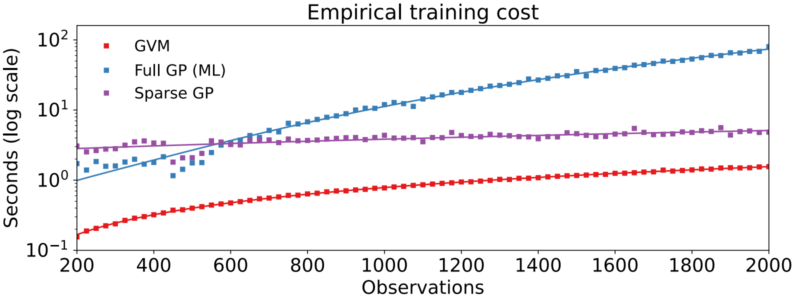
yes it is, provided that:

- **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

- Dual formulation of the Kantorovich problem
- 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 **data analysis**, **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)

A hands-on tutorial on Optimal Transport

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Appendix: what we didn't see

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)

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

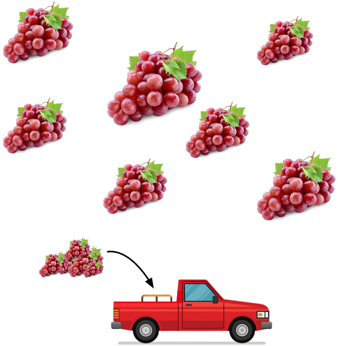
with

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

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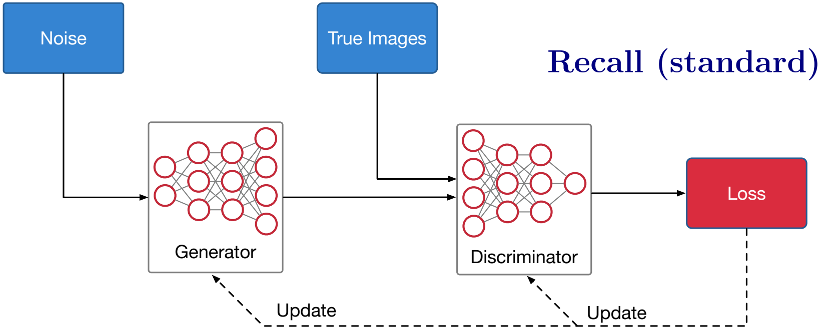
- Negative price are allowed!
- Does the vendor have a competitive offer? Her pricing scheme implies that transferring one kilo of grapes from vineyard x_i to plant y_j costs exactly $\alpha_i + \beta_j$.
- Recall the primal problem: the cost of shipping one unit from x_i to y_j is $C_{i,j}$.
- Feasible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