Optimal Transport Meets Privacy: Gaussian-Smoothed Divergences for Private Distribution Learning and Domain Adaptation

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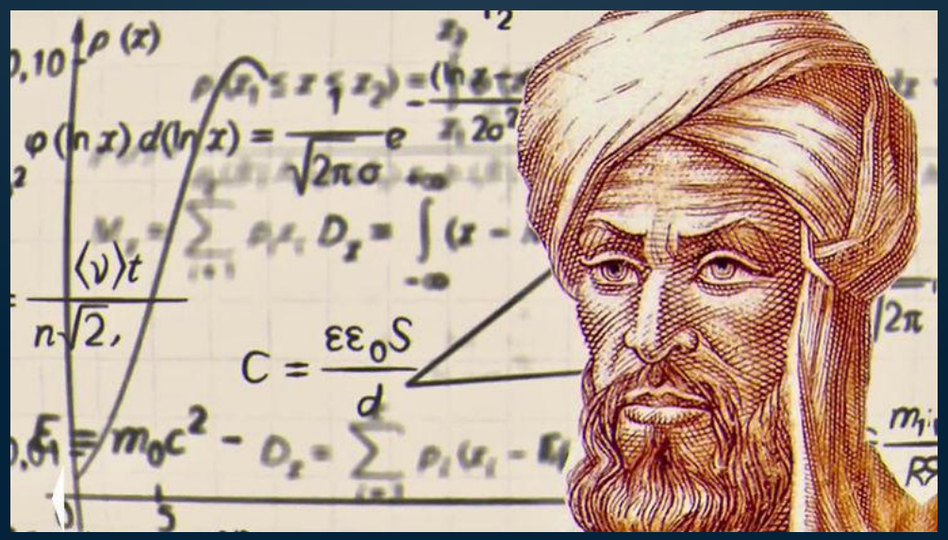
Applied Mathematics Webinar

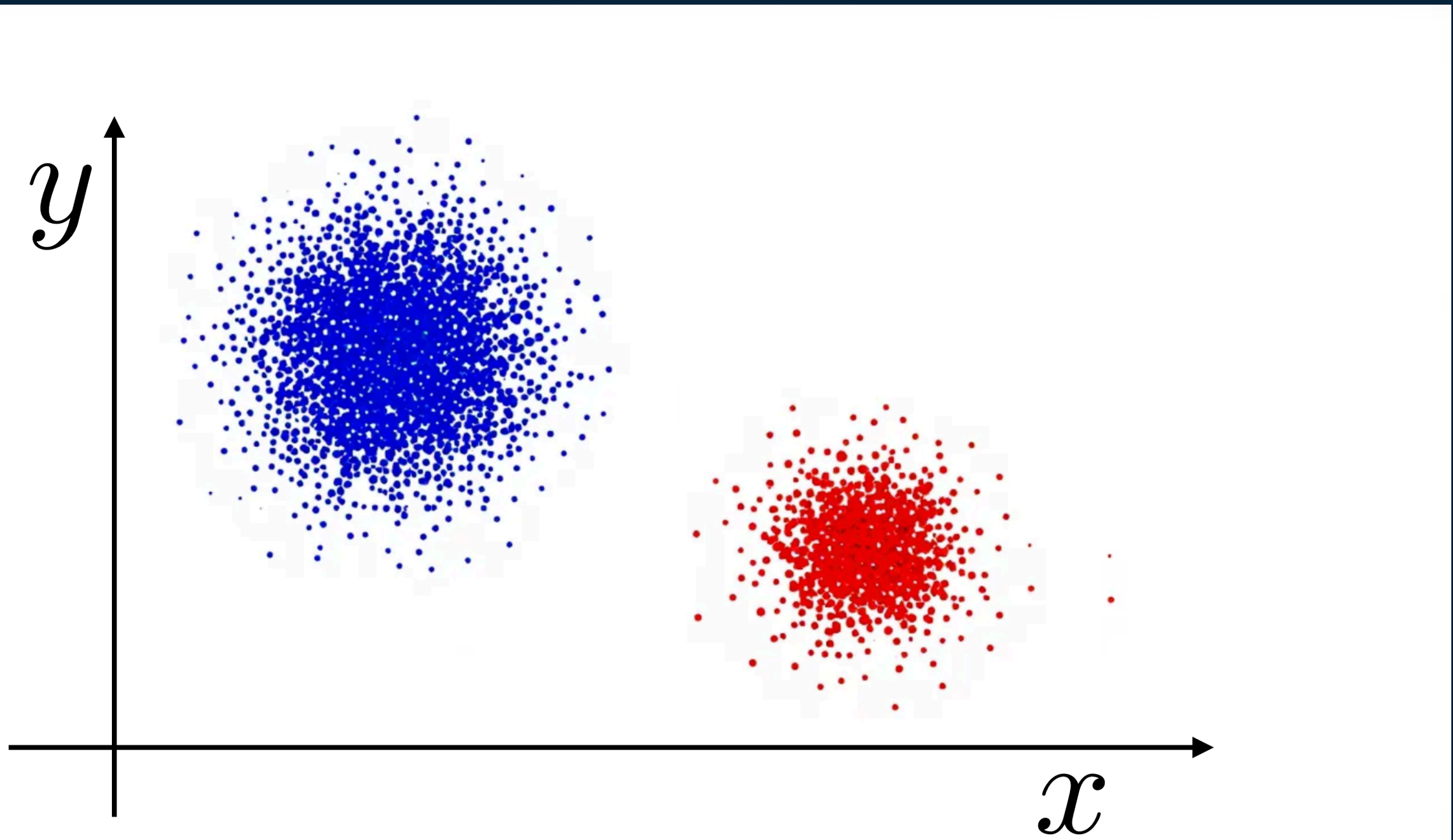


May 12, 2026

I. Motivations

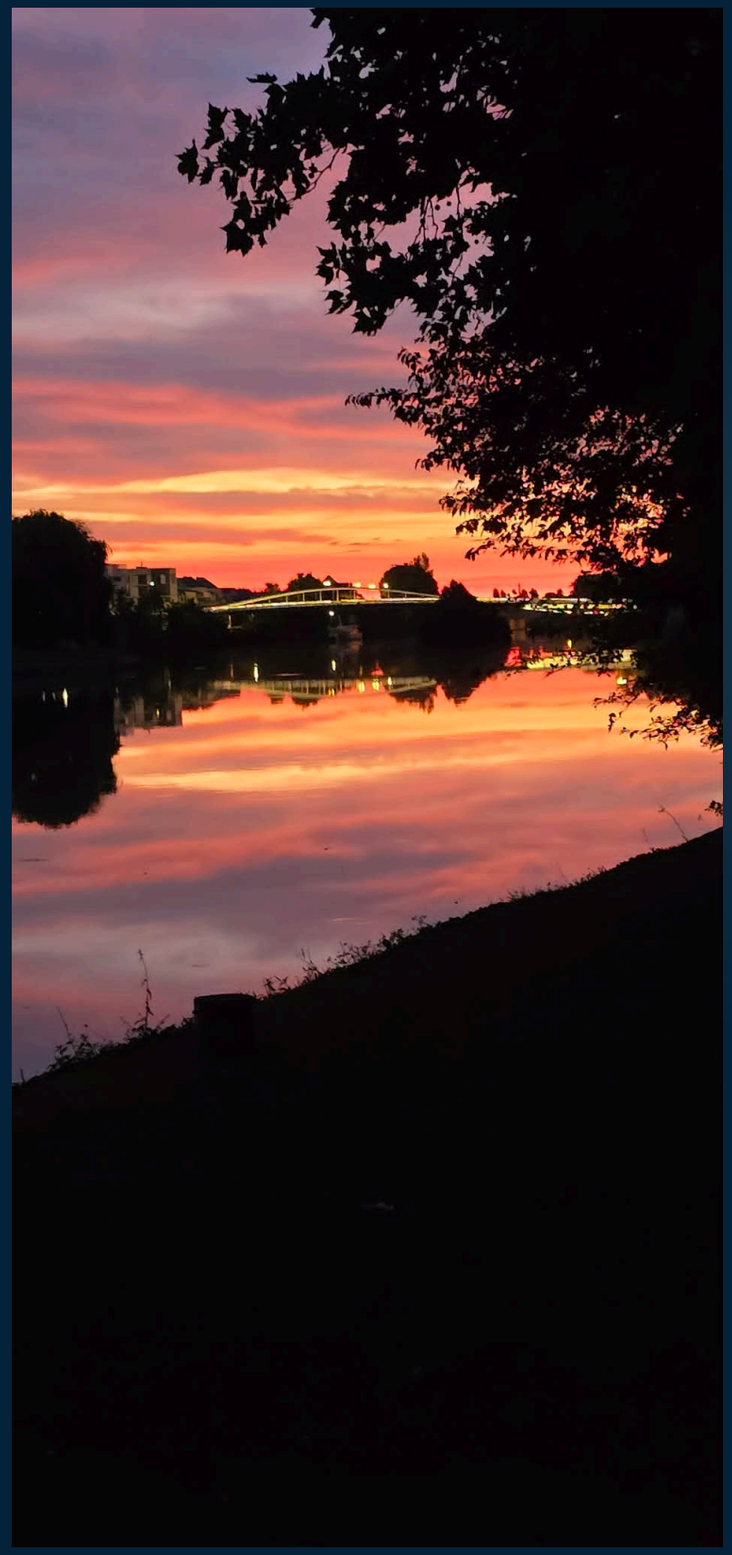
… in Cloud of points

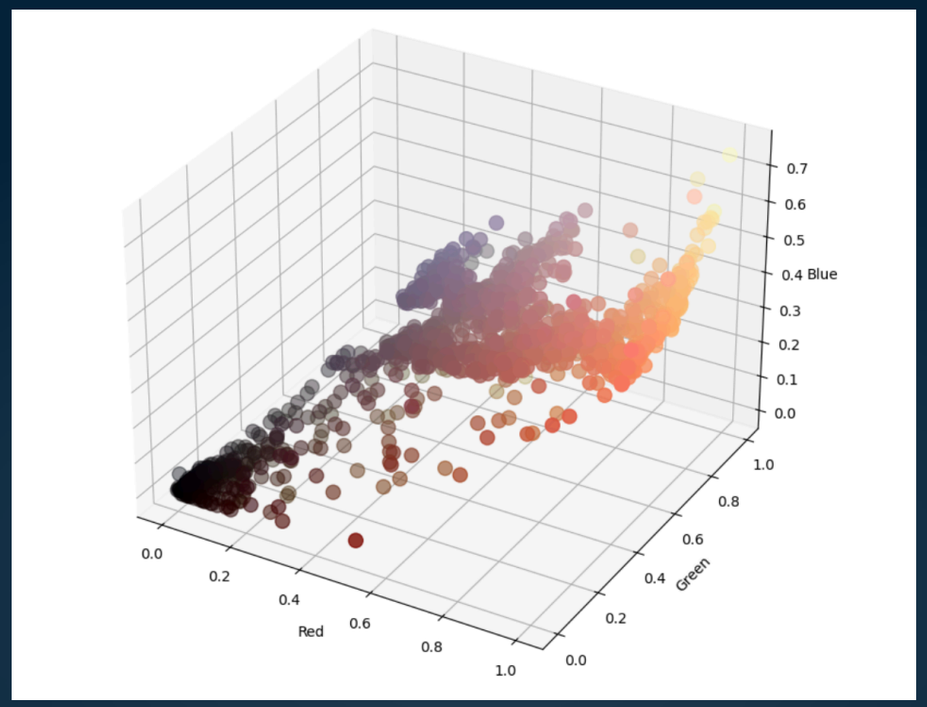
- How to compare two sets of clouds points?

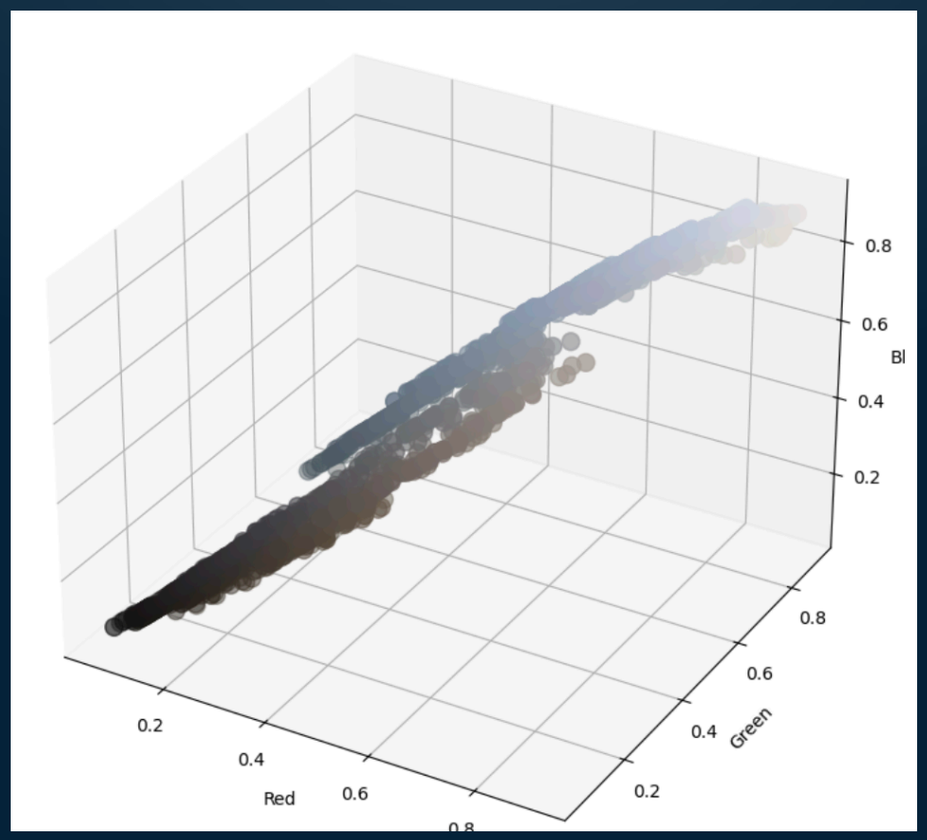


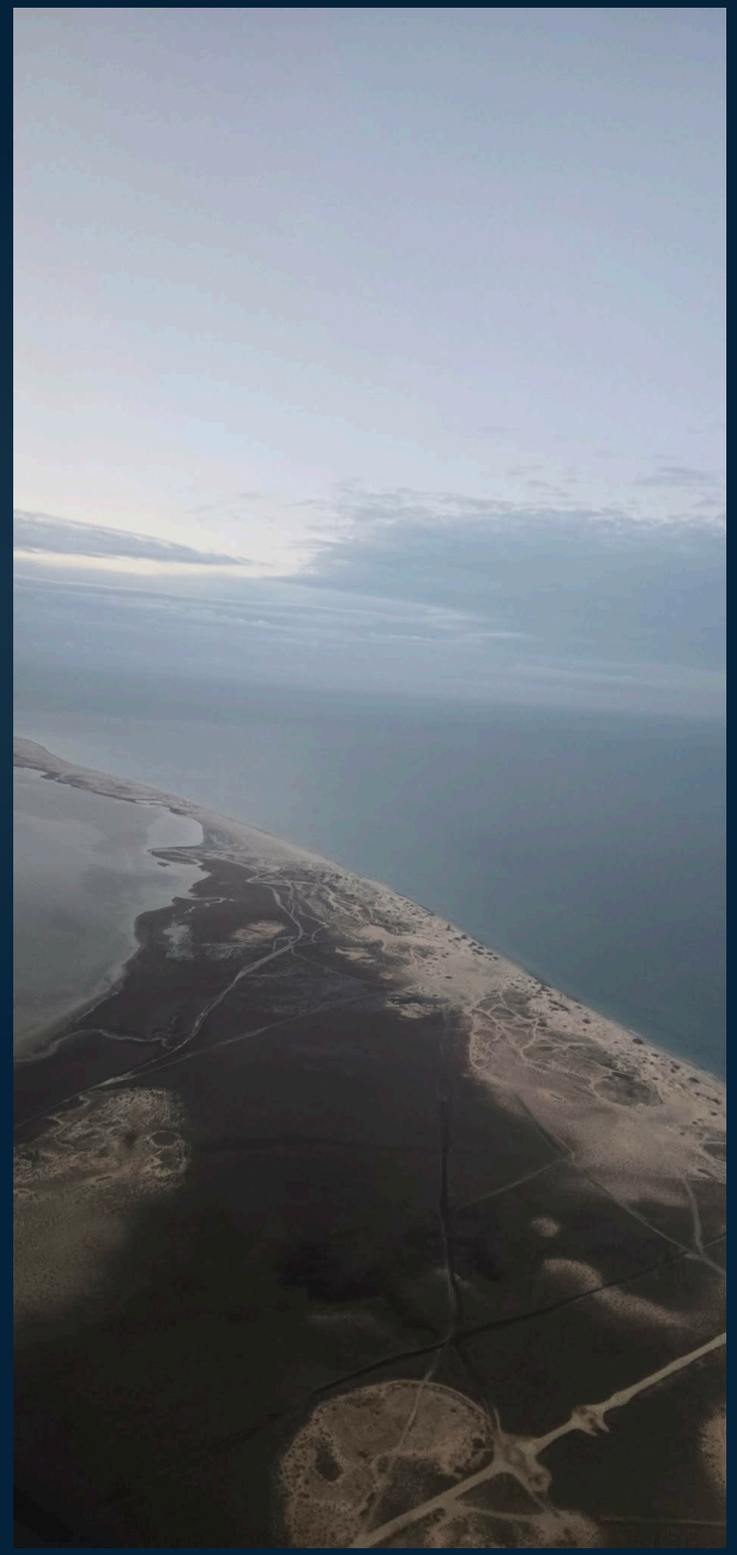
… in Image Processing

- How to measure the similarity between two images?



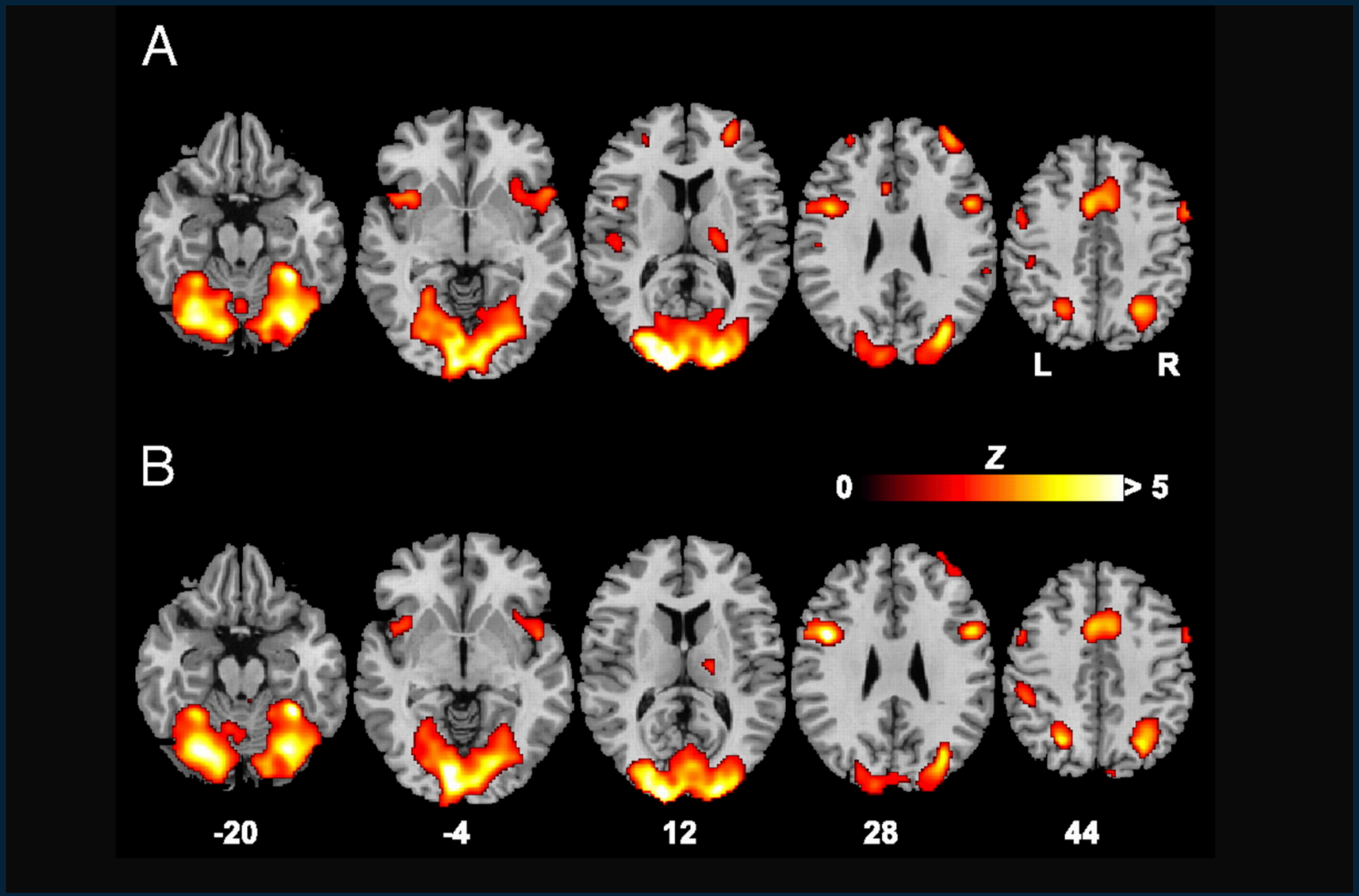






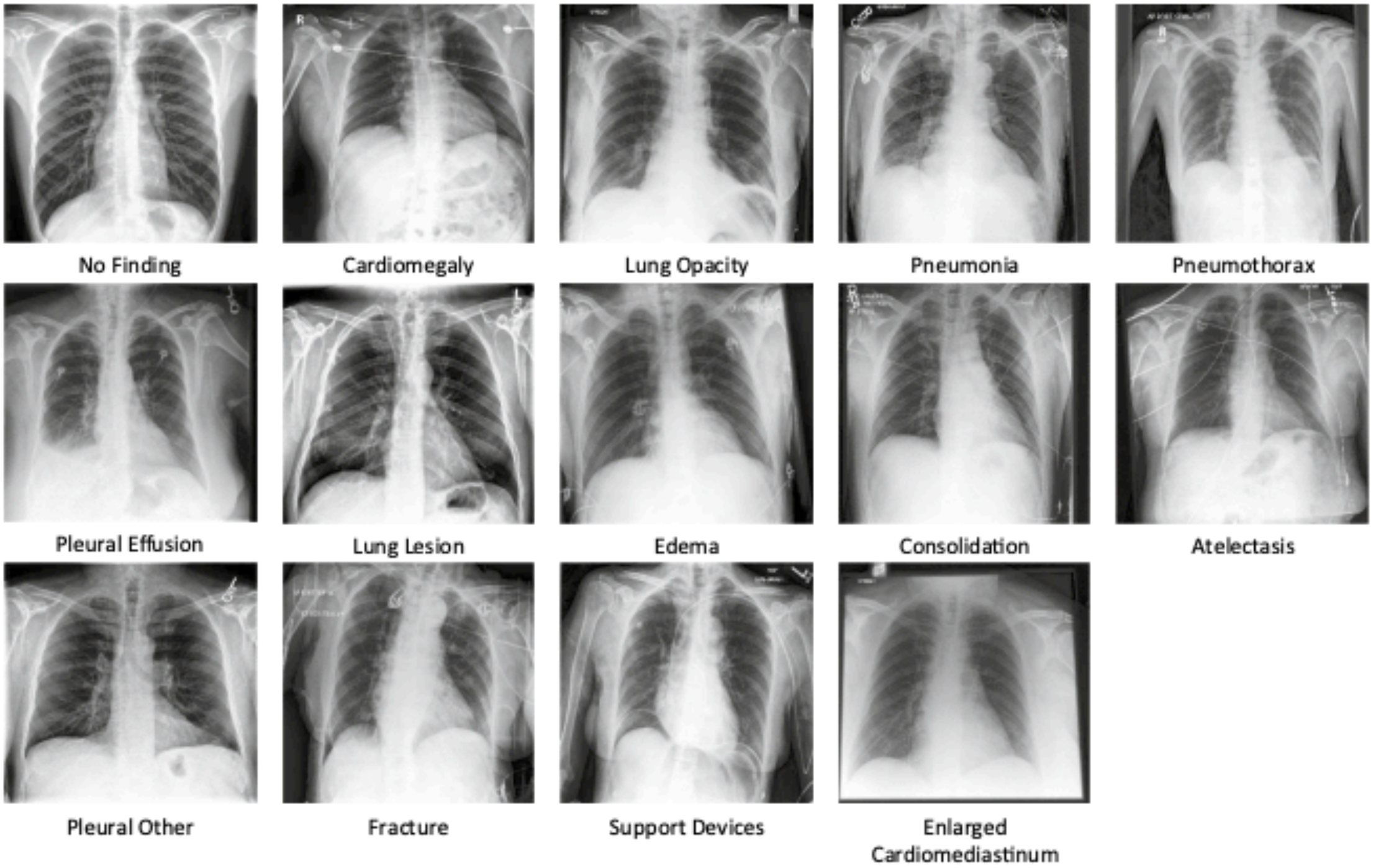
… in Neuroscience

- How to compare two brain activation maps?



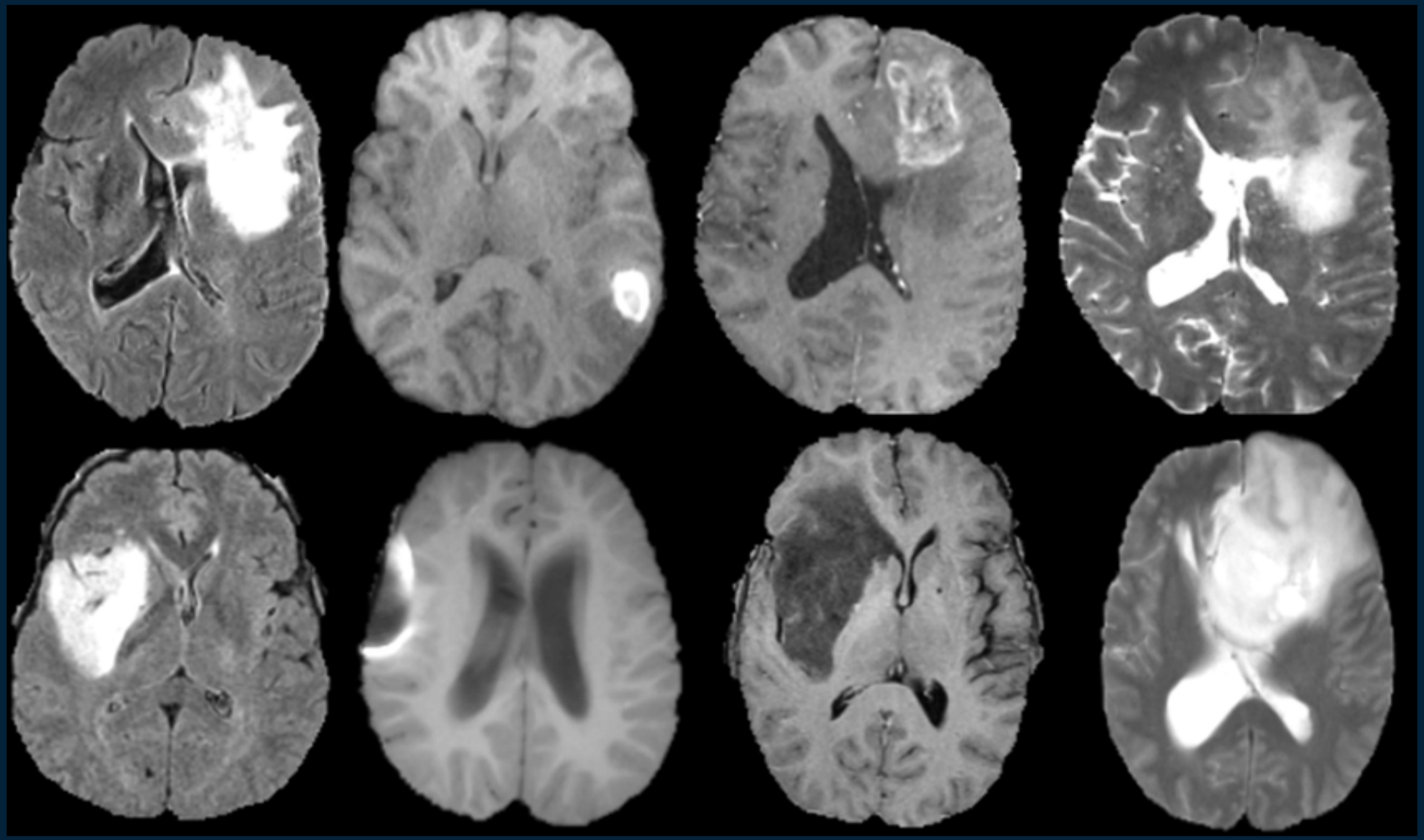
Source: Hu et al., 2008, Proceedings of the National Academy of Sciences

… in Classification: CheXpert data



Source: https://stanfordmlgroup.github.io/competitions/chexpert/

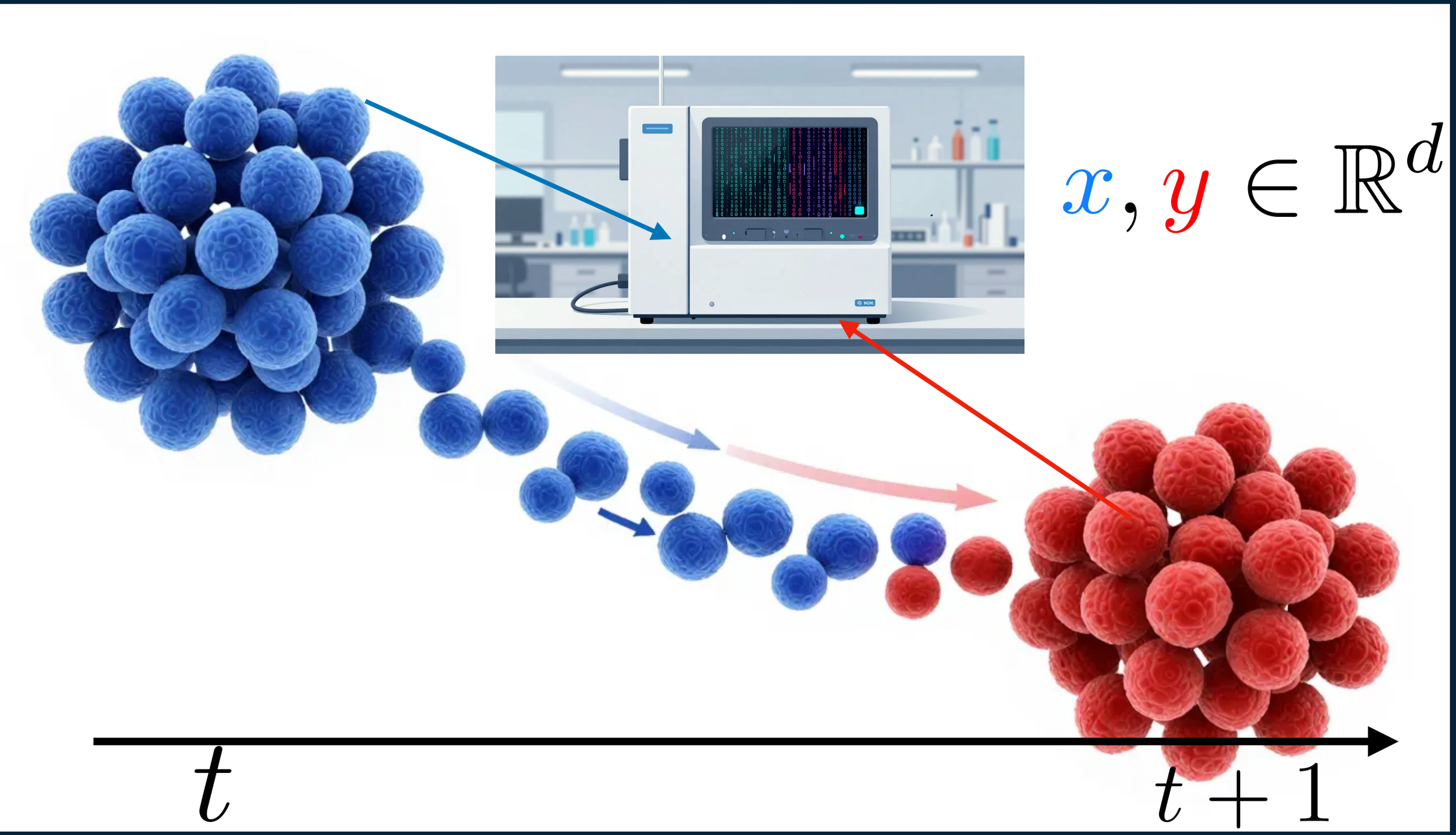
… in Anomaly detection: BraTS data



Source: https://www.med.upenn.edu/cbica/brats2020/registration.html

… in Genomics

- Understanding dynamics at individual cell level.



2. Machine Learning: Predictive Modeling

Training Set

$\mathcal{X}$ Feature Space

$\mathcal{Y}$ Label Space

$$(\vec{x}_i, y_i) \in \mathcal{X} \times \mathcal{Y}$$

$$\vec{x}_i = (x_{i1}, \ldots, x_{id})^\top \in \mathbb{R}^d$$

Sampling Data

$$\mathscr{D}_n = \{(\vec{x}_1, y_1), (\vec{x}_2, y_2), \ldots, (\vec{x}_n, y_n)\}$$

Learning Task

- The learning task consists of assuming that the labels have been calculated using a function.

$$h^\star : x \rightarrow y$$

- Find a hypothesis that better approximates the target function. Build a predictor model, classifier, or regression function.

$$\hat{h} \equiv h_{\hat{\theta}} : \mathcal{X} \rightarrow \mathcal{Y}$$

Learning Task: loss function

- A cost function, also known as a loss function, is a function

$$\ell : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}_+$$

used to quantify prediction quality

$$\ell(y, h(\vec{x}))$$

Real Risk

- Risk is defined as the expectation of a cost function (or expectation of prediction error), i.e.,

$$\mathcal{R}(h) = \mathbb{E}_{(\vec{x},y)\sim\mathbb{P}}\left[\ell(h(\vec{x}), y\right]$$

- Risk minimization is impossible in practice because the joint law $\mathbb{P}$ of observations is unknown.
- Idea: replace the theoretical probability measure $\mathbb{P}$ with the empirical probability measure $\mathbb{P}_n$:

$$d\mathbb{P}_n(x,y) = \frac{1}{n}\sum_{i=1}^{n}\delta_{(\vec{x}_i,y_i)}(\vec{x},y)$$

Empirical Risk Minimisation

- Empirical risk assesses the cumulative effect of errors

$$\mathcal{R}_n(h) = \frac{1}{n}\sum_{i=1}^{n} \ell(y_i, h(\vec{x}_i))$$

- Predictor by empirical risk minimization:

$$h_{\hat{\theta}} = \arg\min_{h \in \mathcal{H}} \mathcal{R}_n(h)$$

3. Optimal Transport

Origin: Monge Problem (1781)

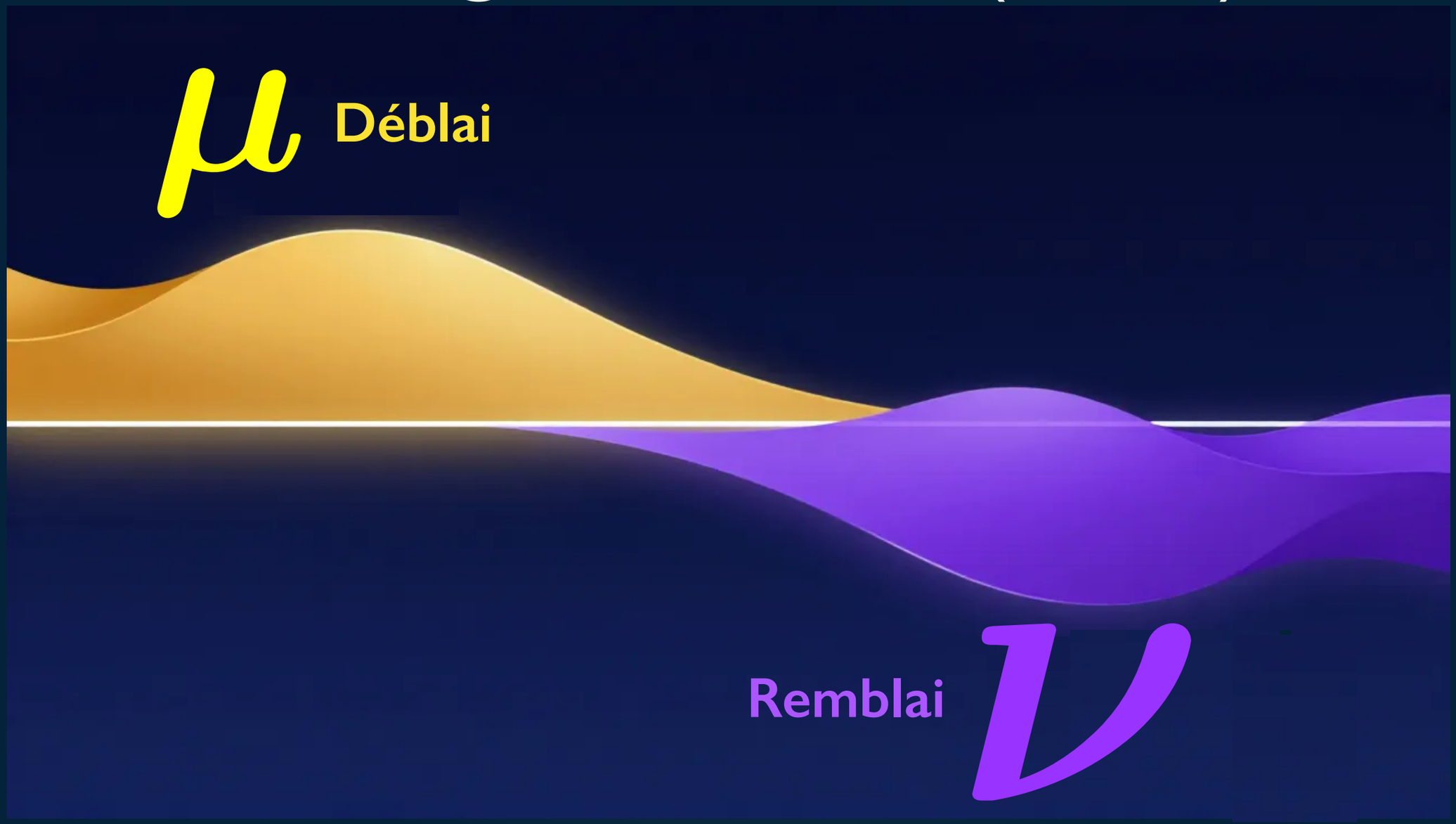
MÉMOIRE
SUR LA
THÉORIE DES DÉBLAIS
ET DES REMBLAIS.

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*.

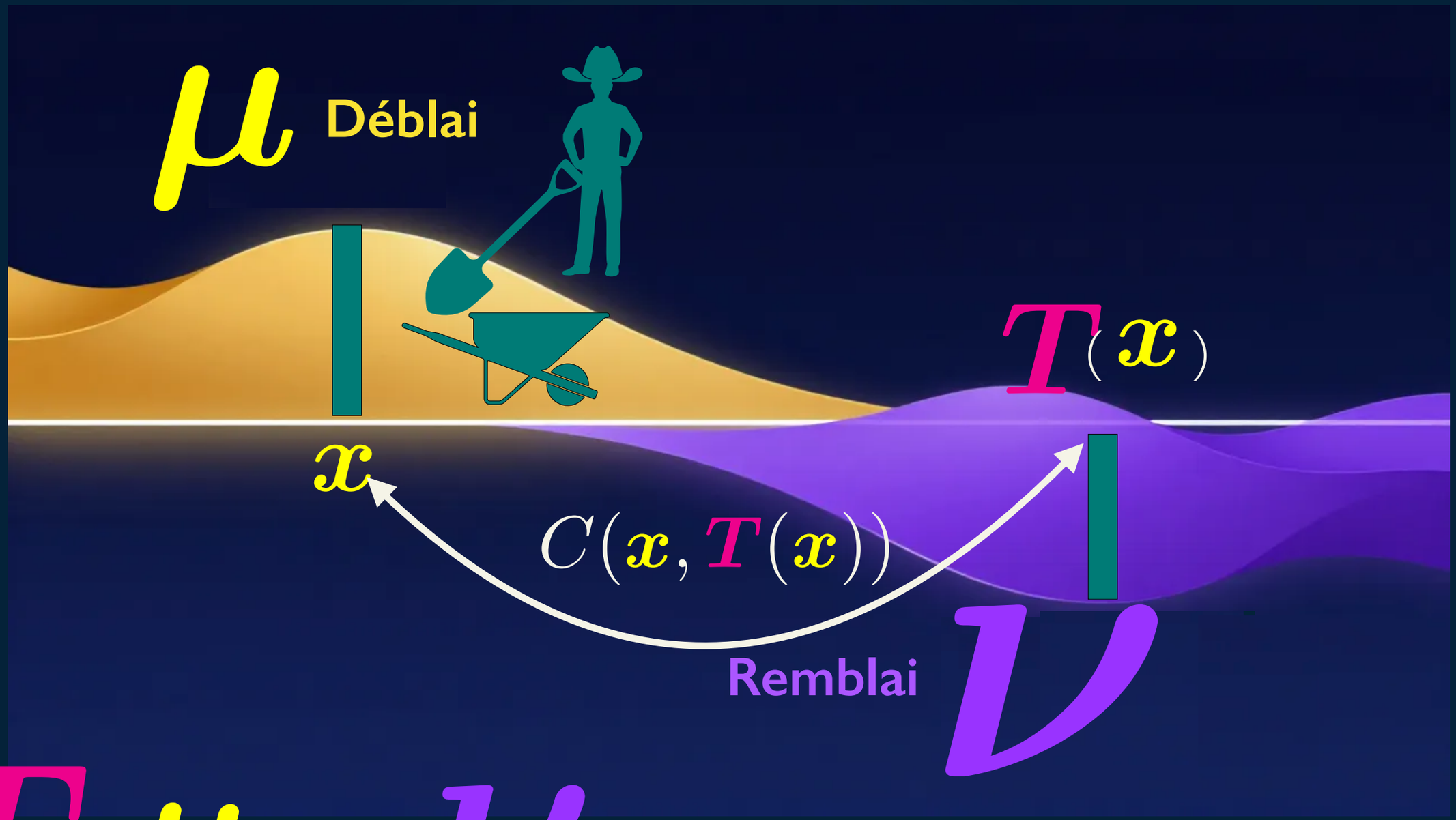
Monge Problem (1781)



- How to move dirt from one place (**déblai**) to another (**remblai**) while minimizing the effort?
- Find a mapping T between the two distributions of mass (**transport**).
- Optimize with respect to a displacement cost (**optimal**).

Monge Problem (1781)

- The mapping T must **push-forward** the **"déblai"** measure towards the **"remblai"**.



$$T_{\#}\mu = \nu$$

Monge Problem (1781)

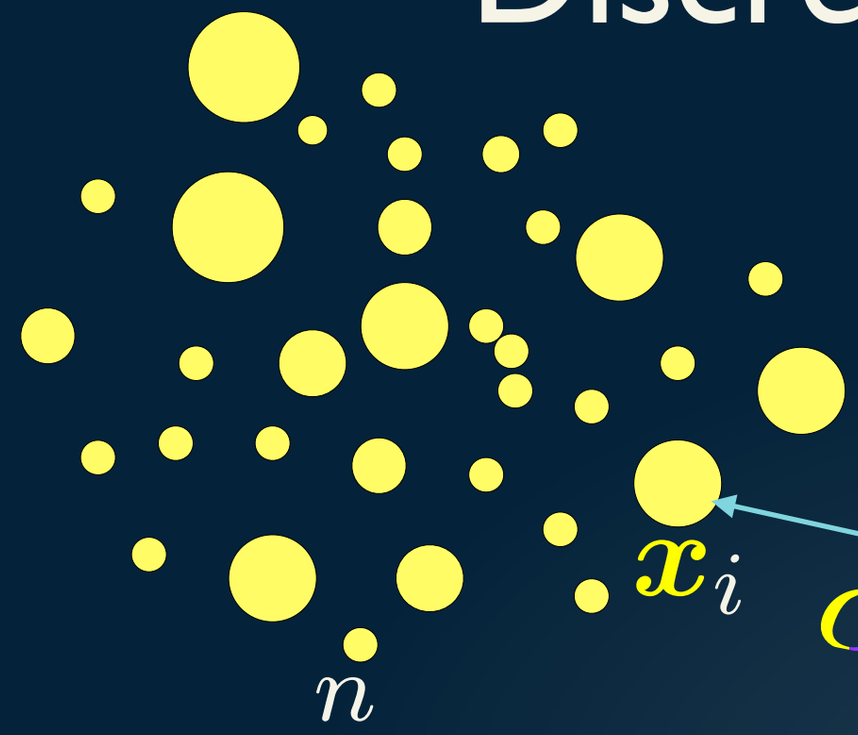
- Monge formulation aim at finding a mapping $\boldsymbol{T}$ such that:

$$\inf_{\boldsymbol{T}_{\#}\boldsymbol{\mu}=\boldsymbol{\nu}} \int \boldsymbol{C}(\boldsymbol{x}, \boldsymbol{T}(\boldsymbol{x}))\boldsymbol{\mu}(\boldsymbol{x})\mathrm{d}\boldsymbol{x}$$

- Mapping $\boldsymbol{T}$ does not exist in the general case.
- Brenier 1991, proved existence and unicity of the Monge map for Euclidean cost and distributions with densities.

Discrete OT Framework

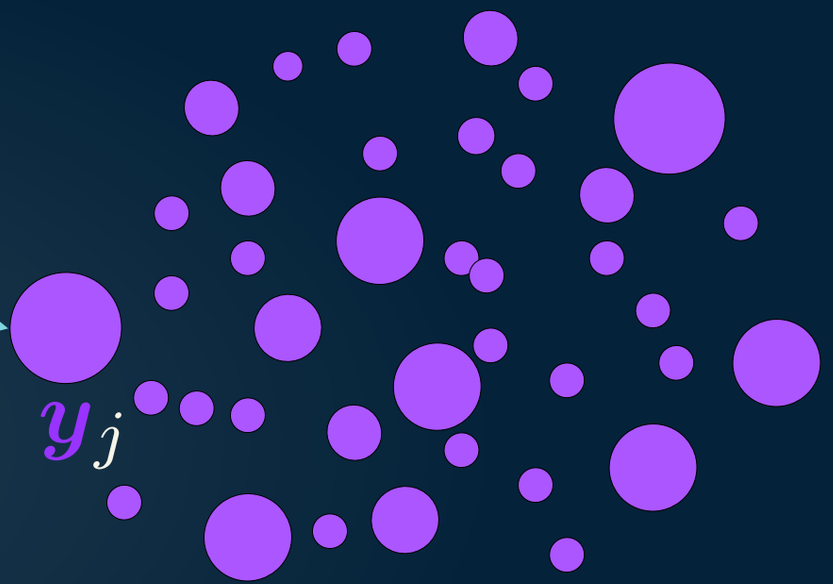
$$\boldsymbol{\nu} = \sum_{j=1}^{m} \boldsymbol{\nu}_j \delta_{\boldsymbol{y}_j}$$



n

$\boldsymbol{x}_i$

$\boldsymbol{C}_{ij} = (c(\boldsymbol{x}_i, \boldsymbol{y}_j))$

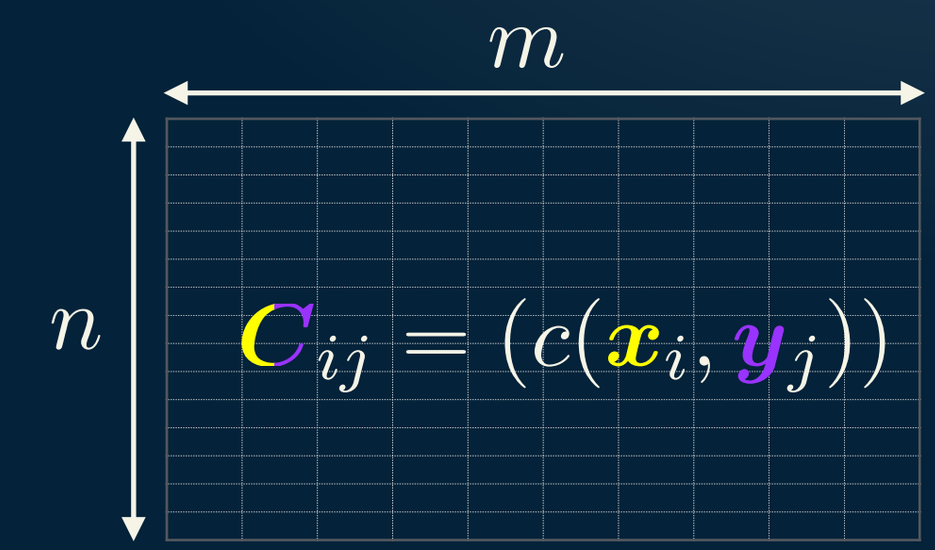


$\boldsymbol{y}_j$

$$\boldsymbol{\mu} = \sum_{i=1} \boldsymbol{\mu}_i \delta_{\boldsymbol{x}_i}$$

$\boldsymbol{C}$

Cost Matrix



$$\min_{\boldsymbol{T}_{\#}\boldsymbol{\mu}=\boldsymbol{\nu}} \sum_i \boldsymbol{C}(\boldsymbol{x}_i, \boldsymbol{T}(\boldsymbol{x}_i))\boldsymbol{\mu}_i$$

$$\forall j \in \{1, \ldots, m\}, \boldsymbol{\nu}_j = \sum_{i:\boldsymbol{T}(\boldsymbol{x}_i)=\boldsymbol{y}_j} \boldsymbol{\mu}_i$$

Discrete OT Framework: Monge's Formula

$$\min_{T_{\#}\mu=\nu} \sum_i C(\boldsymbol{x}_i, T(\boldsymbol{x}_i))\mu_i$$

$$\forall j \in \{1, \ldots, m\}, \nu_j = \sum_{i:T(\boldsymbol{x}_i)=\boldsymbol{y}_j} \mu_i$$

Strict: Deterministic Assignments

Discrete OT Framework: Monge's Formula

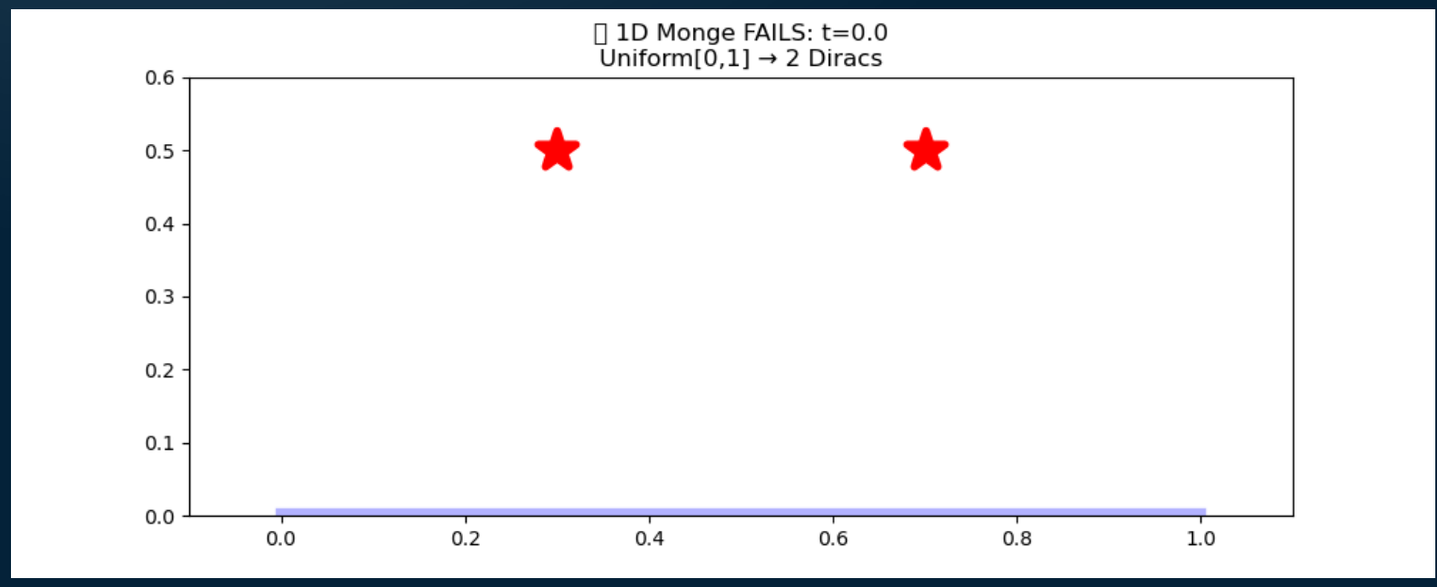
non-convex

combinatorial

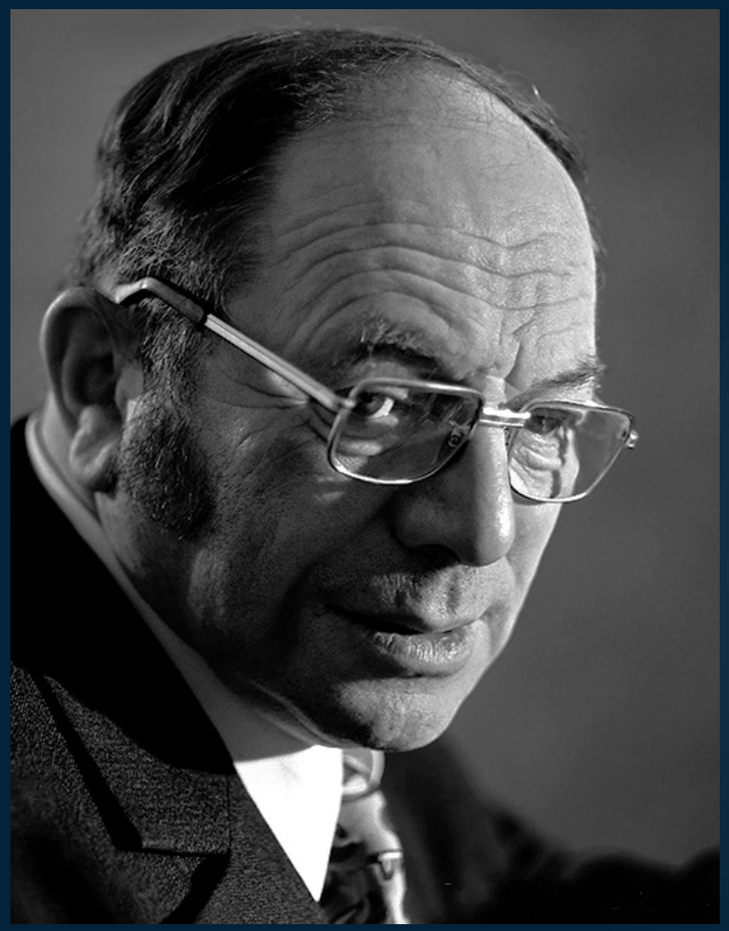
non-existant

Uniform weights

$$\min_{\sigma \in \mathfrak{S}_n} \sum_{i=1}^{n} C(x_i, y_{\sigma(i)})$$

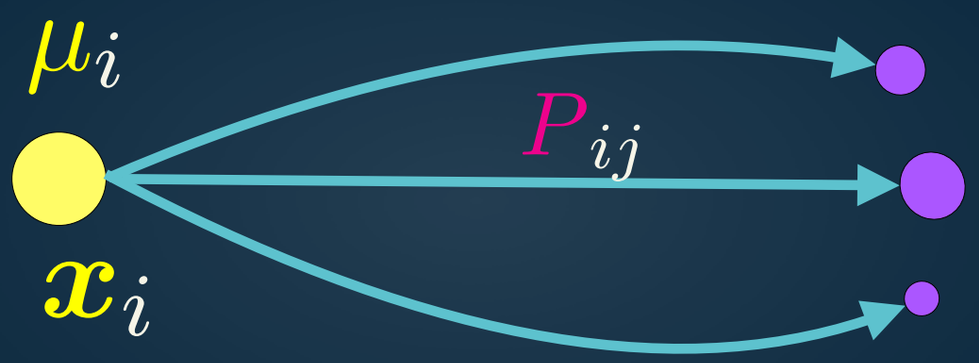


Discrete OT Framework: Kantorovich's Formula



Leonid Kantorovich
(1912-1986)

- Focus on where the mass goes, allow splitting.
- Applications mainly for resource allocation problems.



$$\mu_i = \sum_{i=1}^{m} P_{ij}$$

Relaxed: Fractional Assignments

Probabilistic couplings set (Transport Polytope)

$$\boldsymbol{\Pi}(\boldsymbol{\mu}, \boldsymbol{\nu}) = \{\boldsymbol{P} \in \mathbb{R}_+^{n \times m}, \boldsymbol{P}\mathbf{1}_m = \boldsymbol{\mu}, \boldsymbol{P}^\top \mathbf{1}_n = \boldsymbol{\nu}\}$$

Mass conservation constraints

Discrete OT Framework: Kantorovich's Formula

- Computing OT between μ and ν amounts to solving a linear problem:

Kantorovich 1942

$$\mathcal{S}(\mu,\nu) = \min_{P \in \Pi(\mu,\nu)} \{\langle C, P\rangle = \sum_{i=1}^{n}\sum_{j=1}^{m} C_{ij} P_{ij}\}$$

Distance

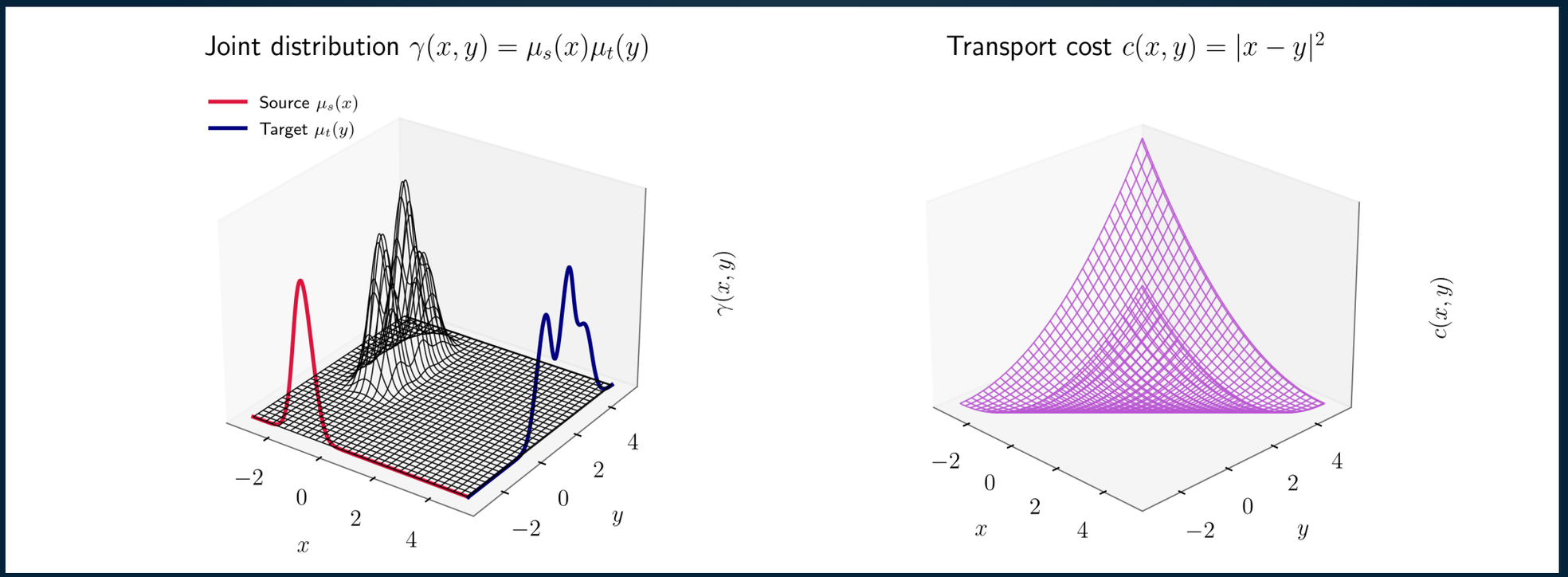
Monge-Kantorovich / Wasserstein Distance

Continuous OT Framework: Kantorovich's Formula

$$\min_{\boldsymbol{\gamma}\in\boldsymbol{\Pi}_{\mathrm{con}}(\boldsymbol{\mu},\boldsymbol{\nu})} \int_{\mathbb{R}^d\times\mathbb{R}^d} \boldsymbol{C}(\boldsymbol{x},\boldsymbol{y})\boldsymbol{\gamma}(\boldsymbol{x},\boldsymbol{y})\mathrm{d}\boldsymbol{x}\mathrm{d}\boldsymbol{y}$$

Probabilistic couplings set (Transport Polytope)

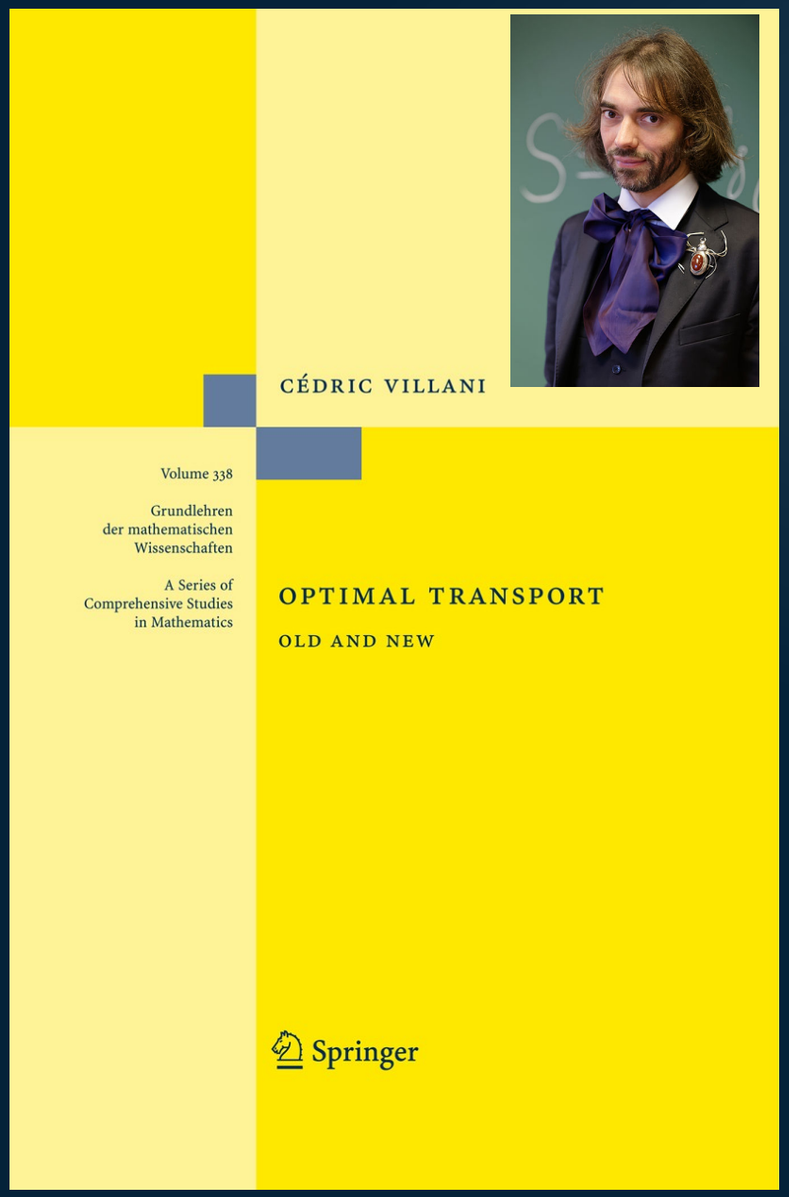
$$\boldsymbol{\Pi}_{\mathrm{con}}(\boldsymbol{\mu},\boldsymbol{\nu}) = \{\boldsymbol{\gamma}\geq 0, \int_{\mathbb{R}^d}\boldsymbol{\gamma}(\boldsymbol{x},\boldsymbol{y})\mathrm{d}\boldsymbol{y} = \boldsymbol{\mu}, \int_{\mathbb{R}^d}\boldsymbol{\gamma}(\boldsymbol{x},\boldsymbol{y})\mathrm{d}\boldsymbol{x} = \boldsymbol{\nu}\}$$

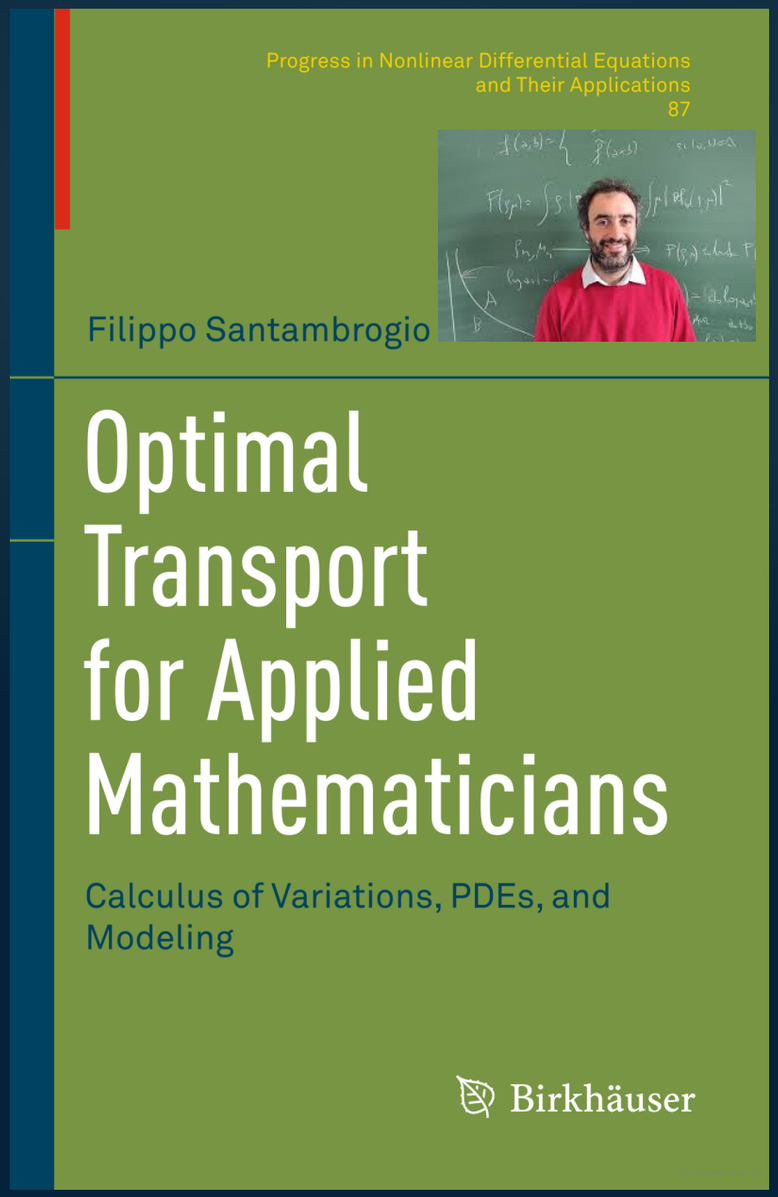


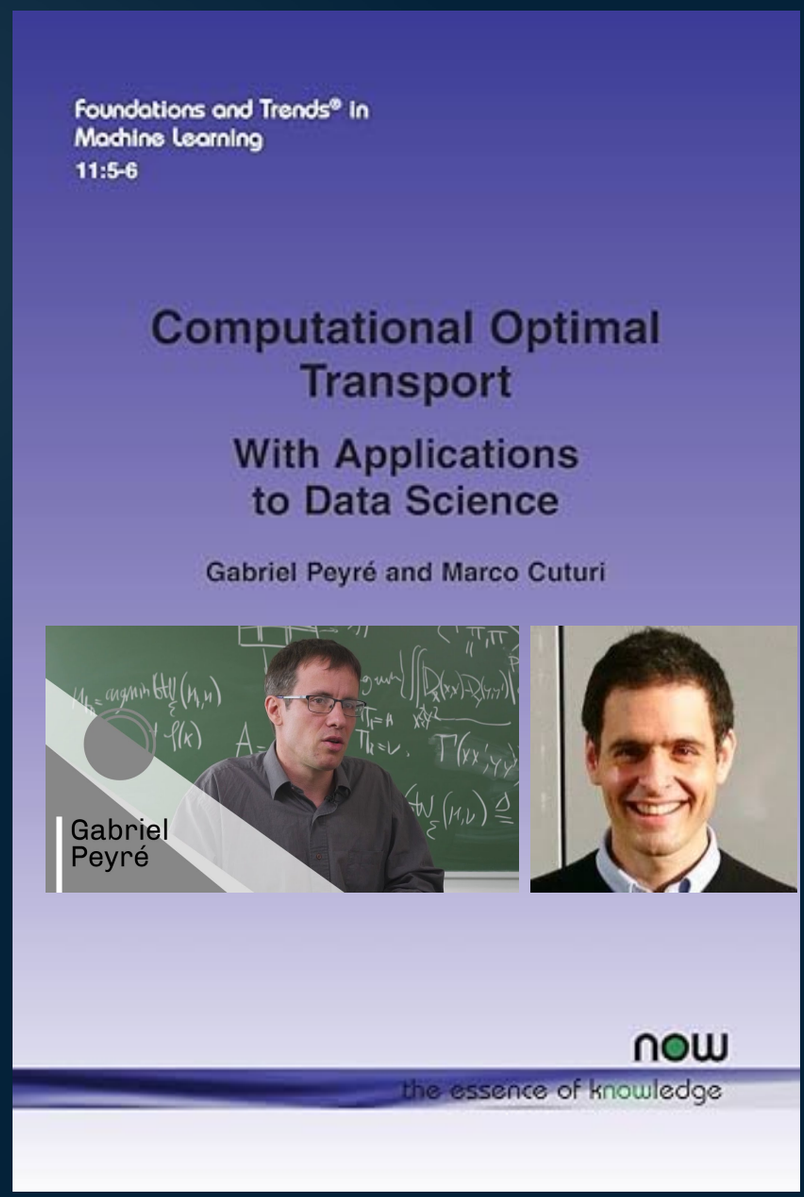
Continuous OT Framework: Wasserstein Distance

Wasserstein Distance

$$\mathrm{W}_p(\boldsymbol{\mu}, \boldsymbol{\nu}) = \left(\inf_{\boldsymbol{\gamma} \in \boldsymbol{\Pi}_{\mathrm{con}}(\boldsymbol{\mu}, \boldsymbol{\nu})} \int_{\mathbb{R}^d \times \mathbb{R}^d} D^p(\boldsymbol{x}, \boldsymbol{y}) \boldsymbol{\gamma}(\boldsymbol{x}, \boldsymbol{y}) \mathrm{d}\boldsymbol{x} \mathrm{d}\boldsymbol{y} \right)^{1/p} = \left(\mathbb{E}_{(\boldsymbol{x}, \boldsymbol{y}) \sim \boldsymbol{\gamma}} [D^p(\boldsymbol{x}, \boldsymbol{y})] \right)^{1/p}$$

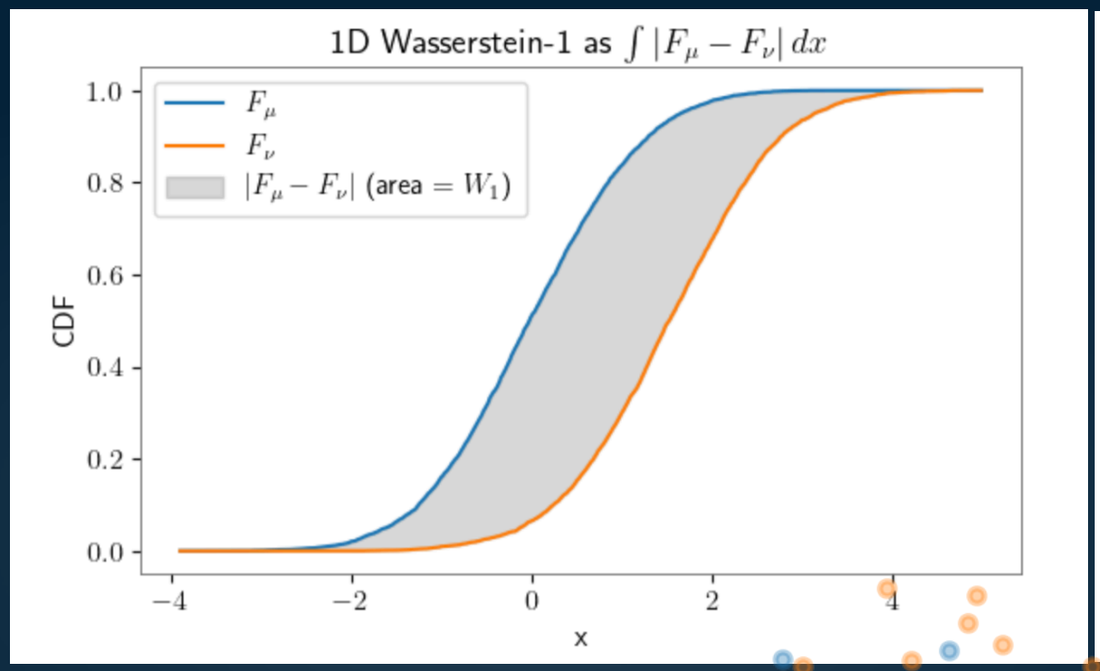


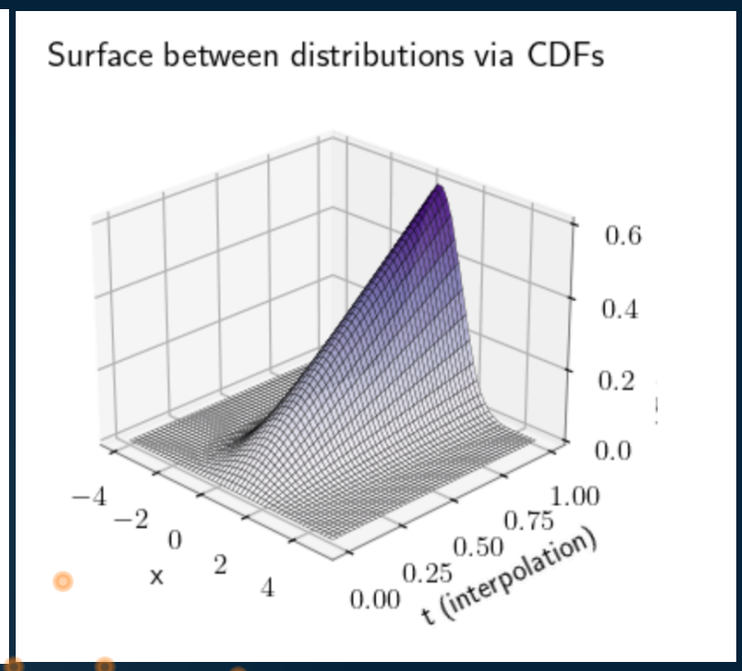




Continuous OT Framework: Wasserstein Distance

$$\mathrm{W}_1(\boldsymbol{\mu}, \boldsymbol{\nu})$$





Bures Distance

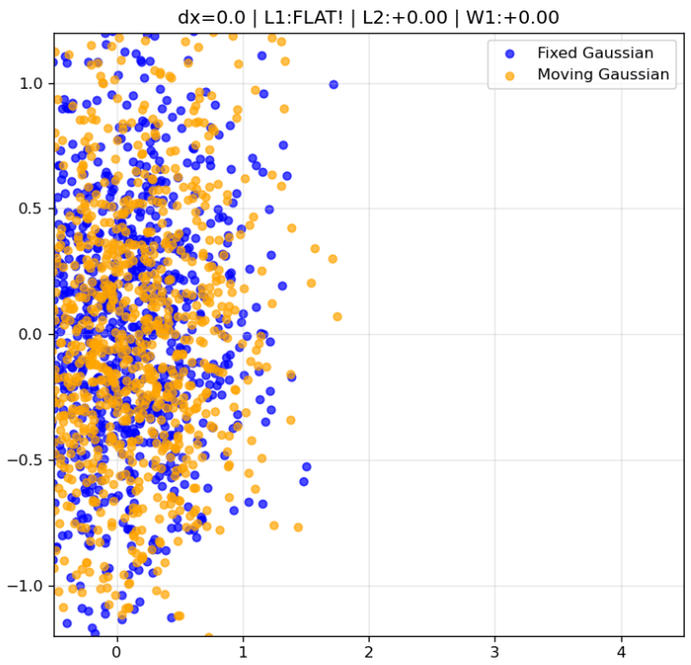
$$\mathrm{W}_2^2(\boldsymbol{\mu}, \boldsymbol{\nu})$$

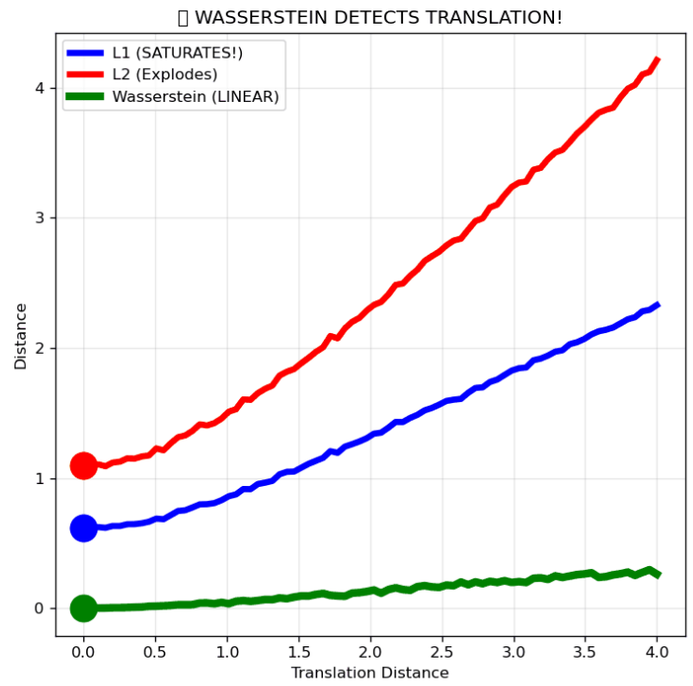
$$= \|m_0 - m_1\|^2 + \mathrm{Tr}\Big(\Sigma_0 + \Sigma_1 - 2\big(\Sigma_1^{1/2}\Sigma_0\Sigma_1^{1/2}\big)^{1/2}\Big).$$

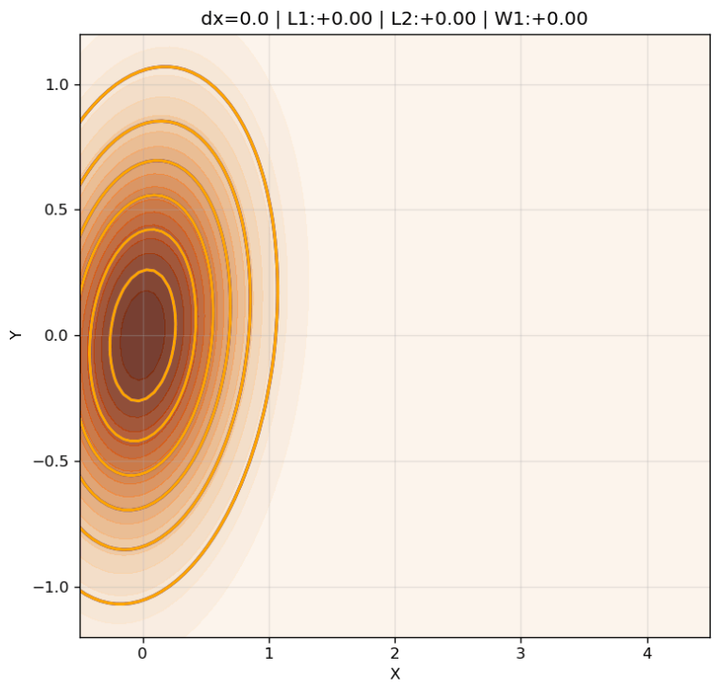
$\mathcal{N}(m_0, \Sigma_0)$

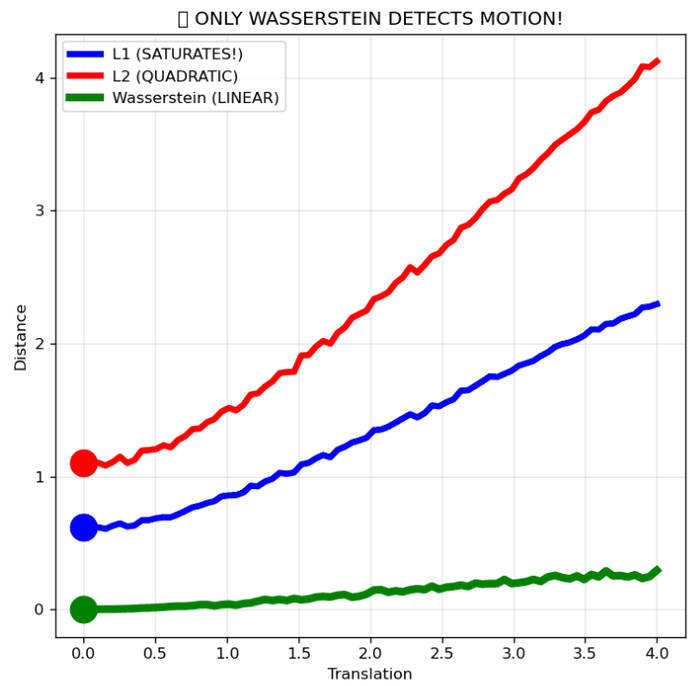
$\mathcal{N}(m_1, \Sigma_1)$

Benefit of Wasserstein Distance (1)

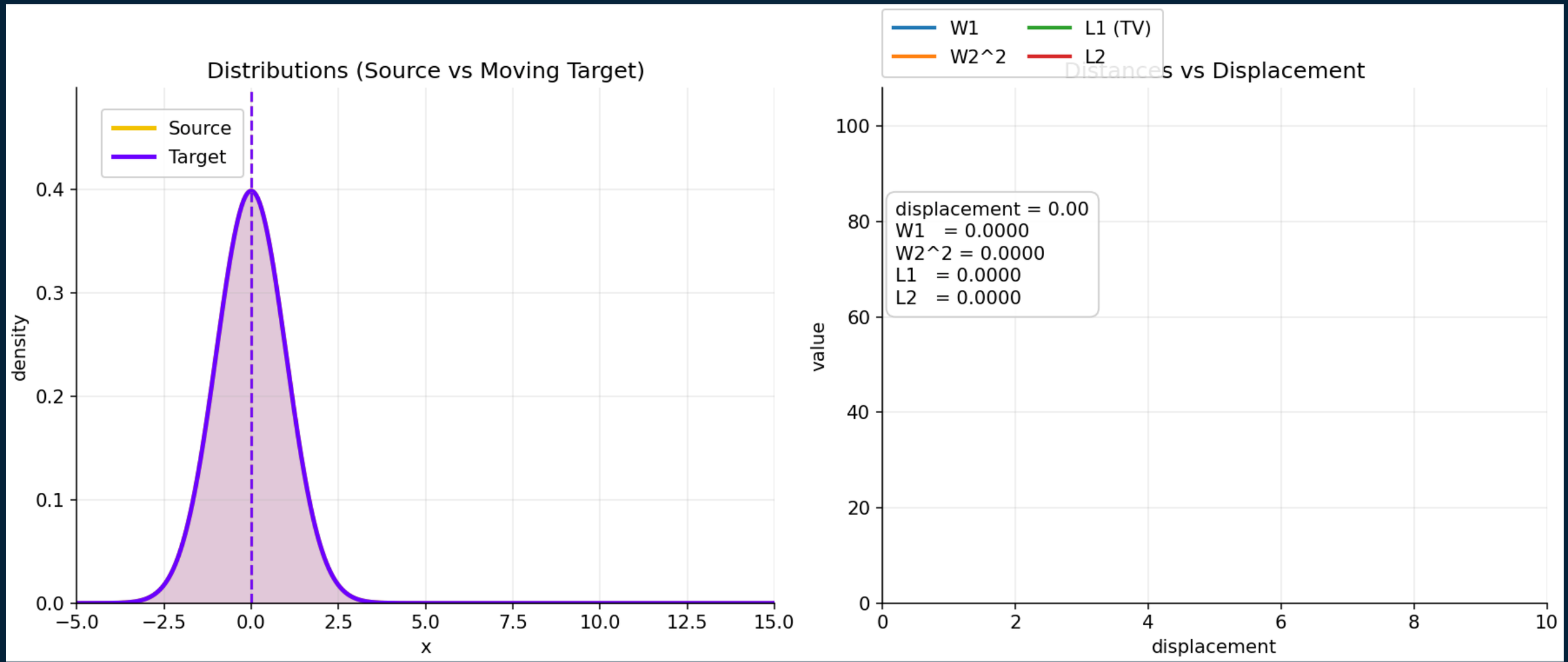




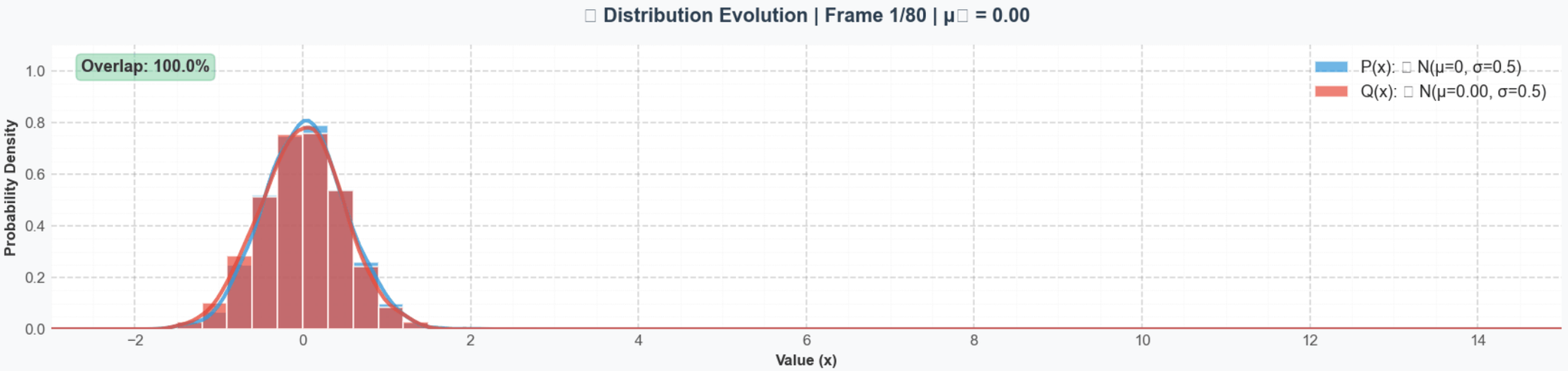


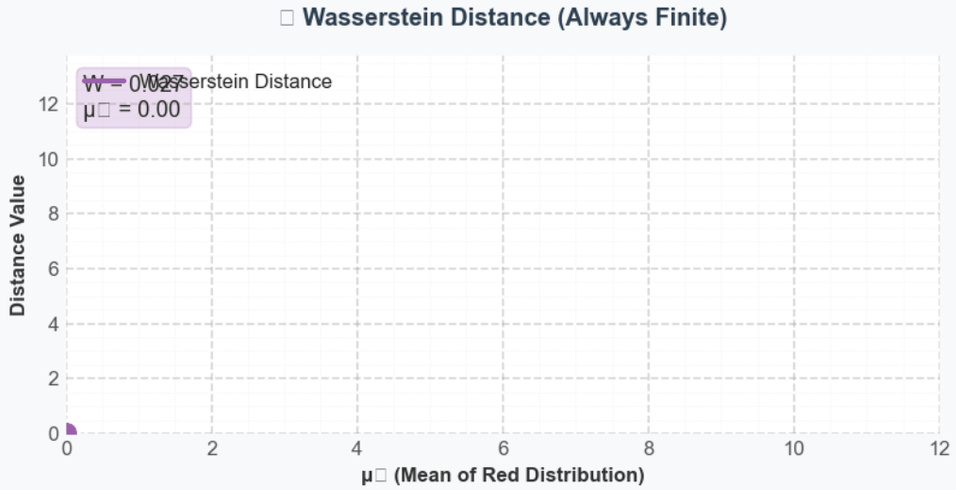


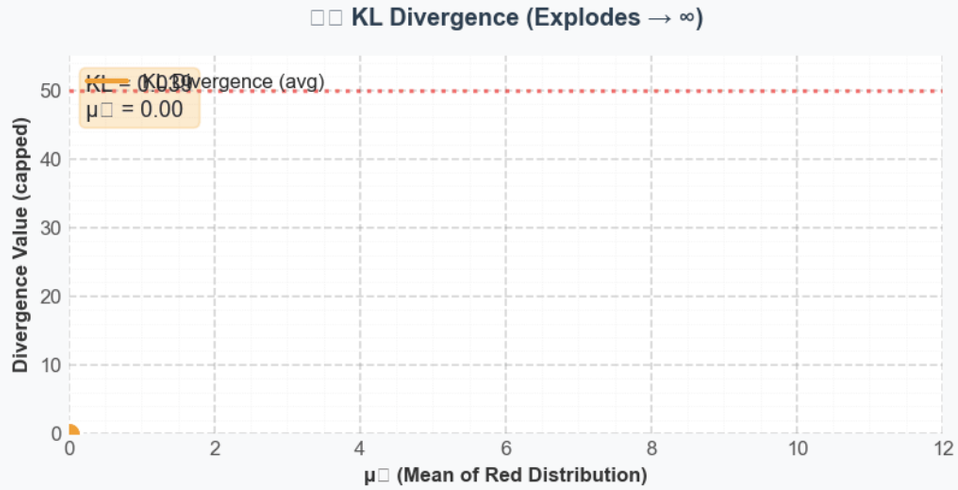
Benefit of Wasserstein Distance (2)

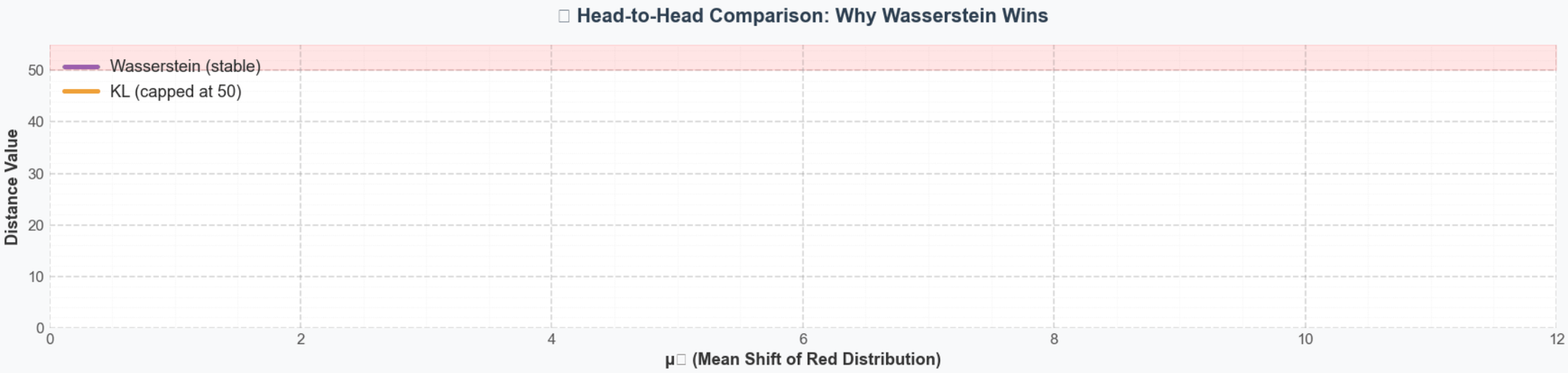


Benefit of Wasserstein Distance (3)



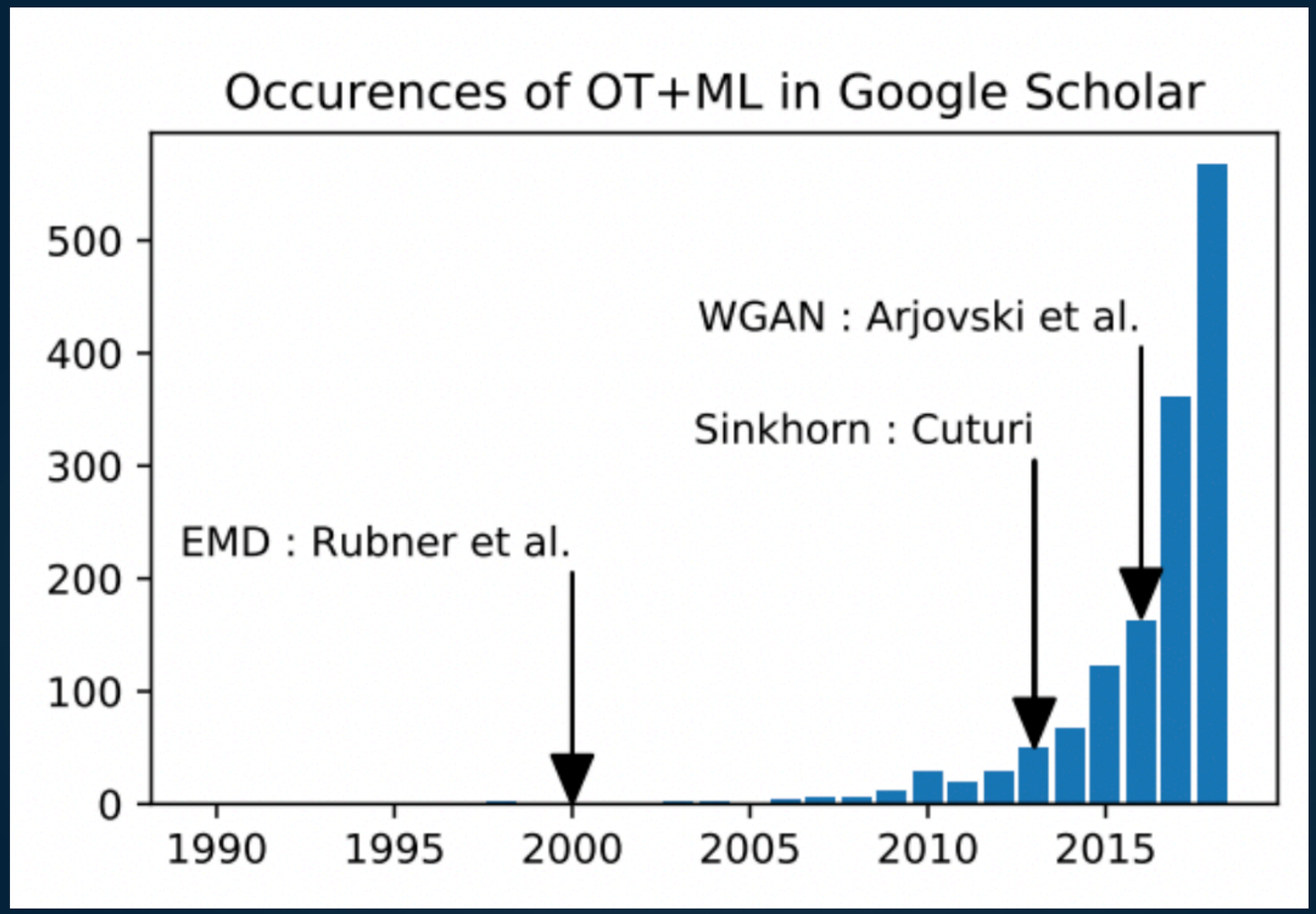






4. How can it be used in data science?

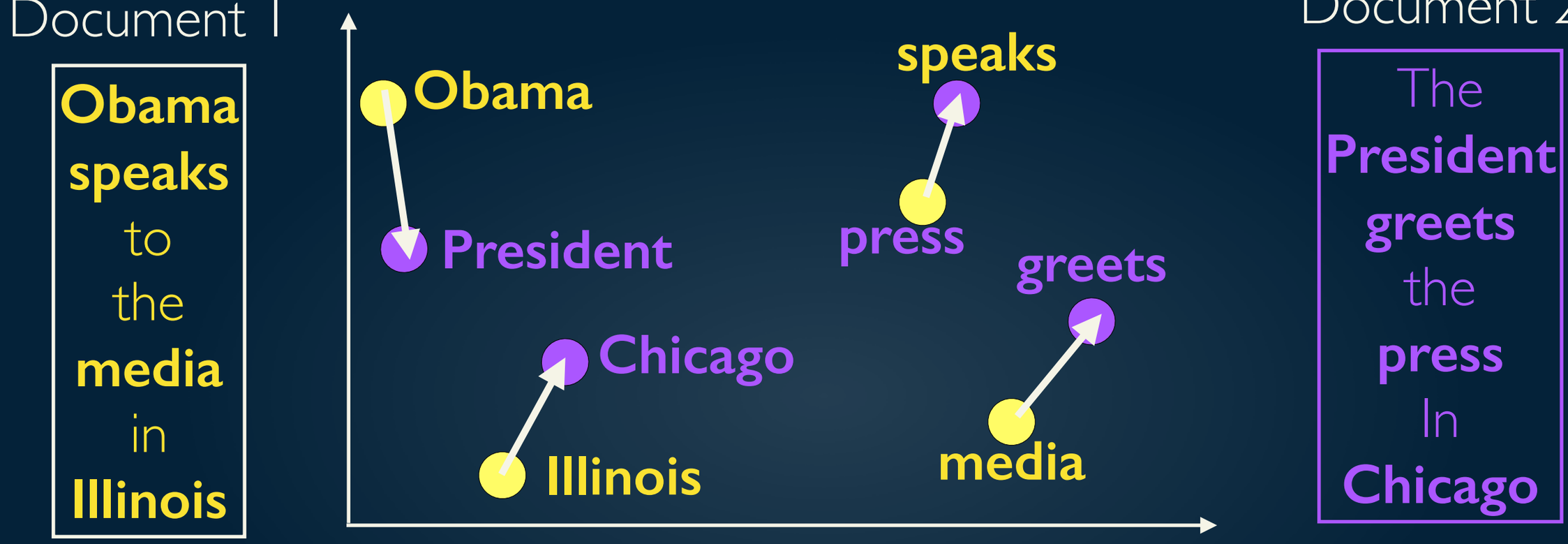
History of OT for machine learning



[R. Flamary, 2019 (HDR)]

- Recently introduced to ML (well know in image processing since 2000).
- Computational OT allows numerous applications (regularization).
- Deep learning boost (numerical optimisation and GAN).

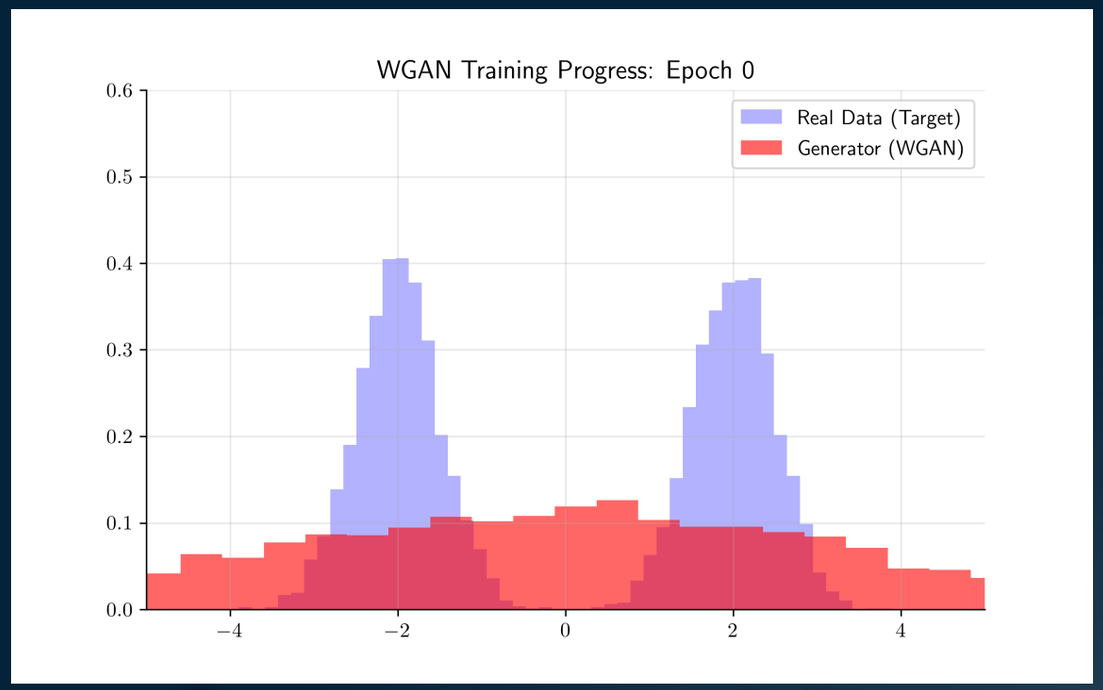
Matching words embeddings

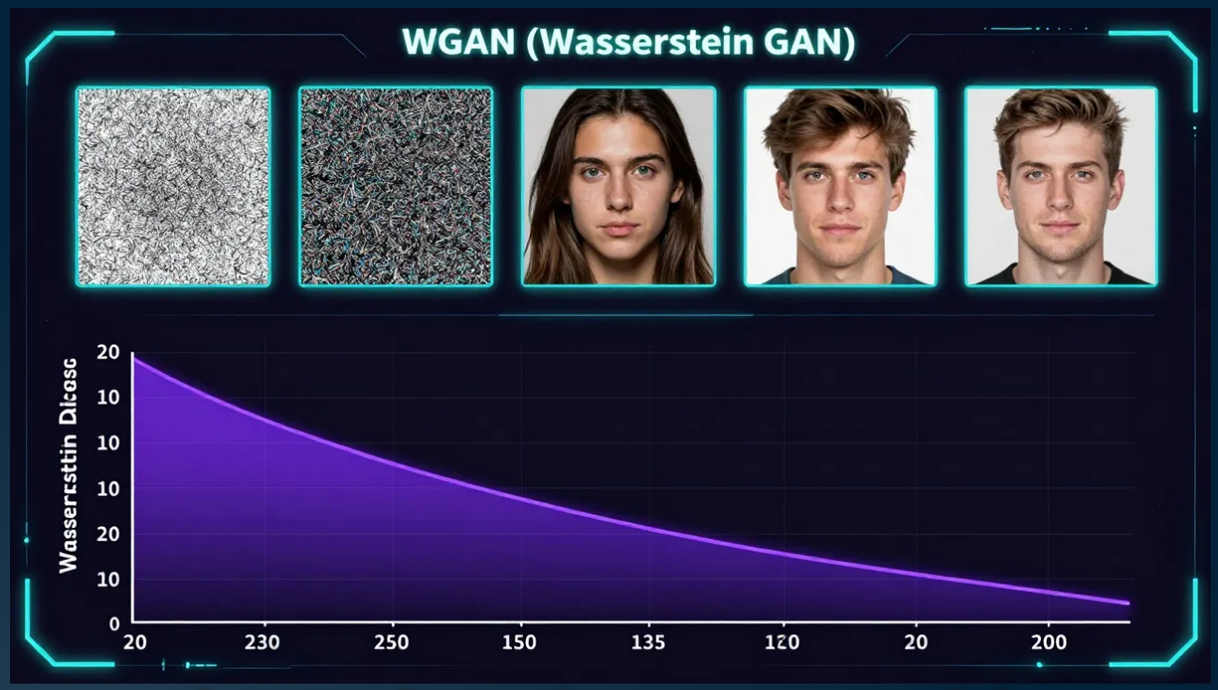


Word Mover's Distance avec Word2vec embeddings
[Kusner et al, 2015 (ICML)]

- Words are embedded in a high-dimensional space with deep neural networks.
- Matching two documents in an OT problem, with the Euclidean distance in the embedded space.

Wasserstein loss for generative modelling





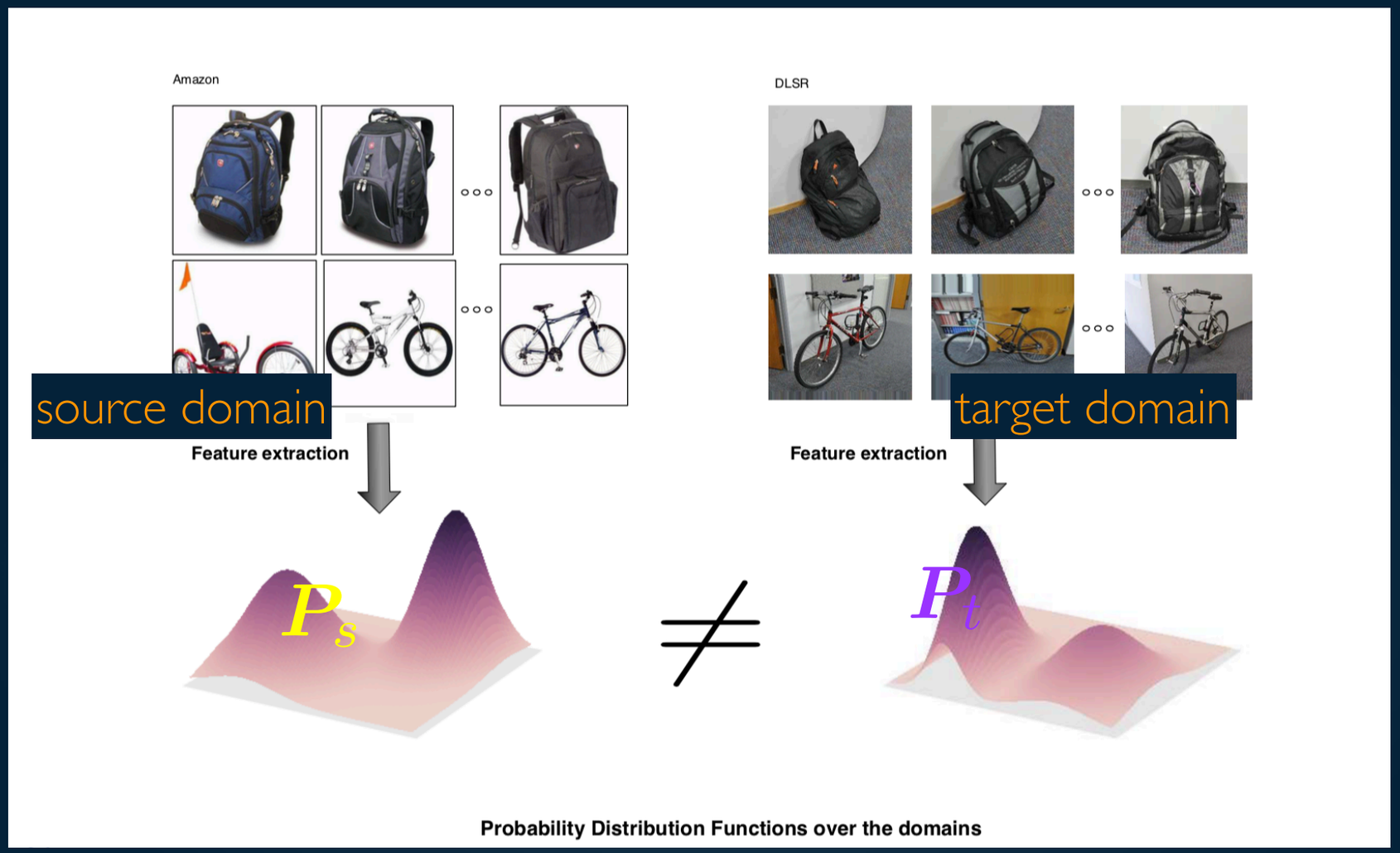
Generative modelling as a matching distribution problem

- Learn a model that maps random vector to target space.
- Distribution of the model is targeted to be similar to the learning samples.
- Similarity as Wasserstein sense [Arjovsky et al. 2017, Deshpande et al. 2018, Nguyen et al. 2020].

$$\min_{f_{\boldsymbol{\theta}}} W_p^p\left(\left\{f_{\boldsymbol{\theta}}(\boldsymbol{z}_i)\right\}_{i=1}^K, \left\{\boldsymbol{x}_j\right\}_{j=1}^K\right)$$

$\{\boldsymbol{z}_i\}$ some random vectors, $\{\boldsymbol{x}_j\}$ some samples from the target distribution.

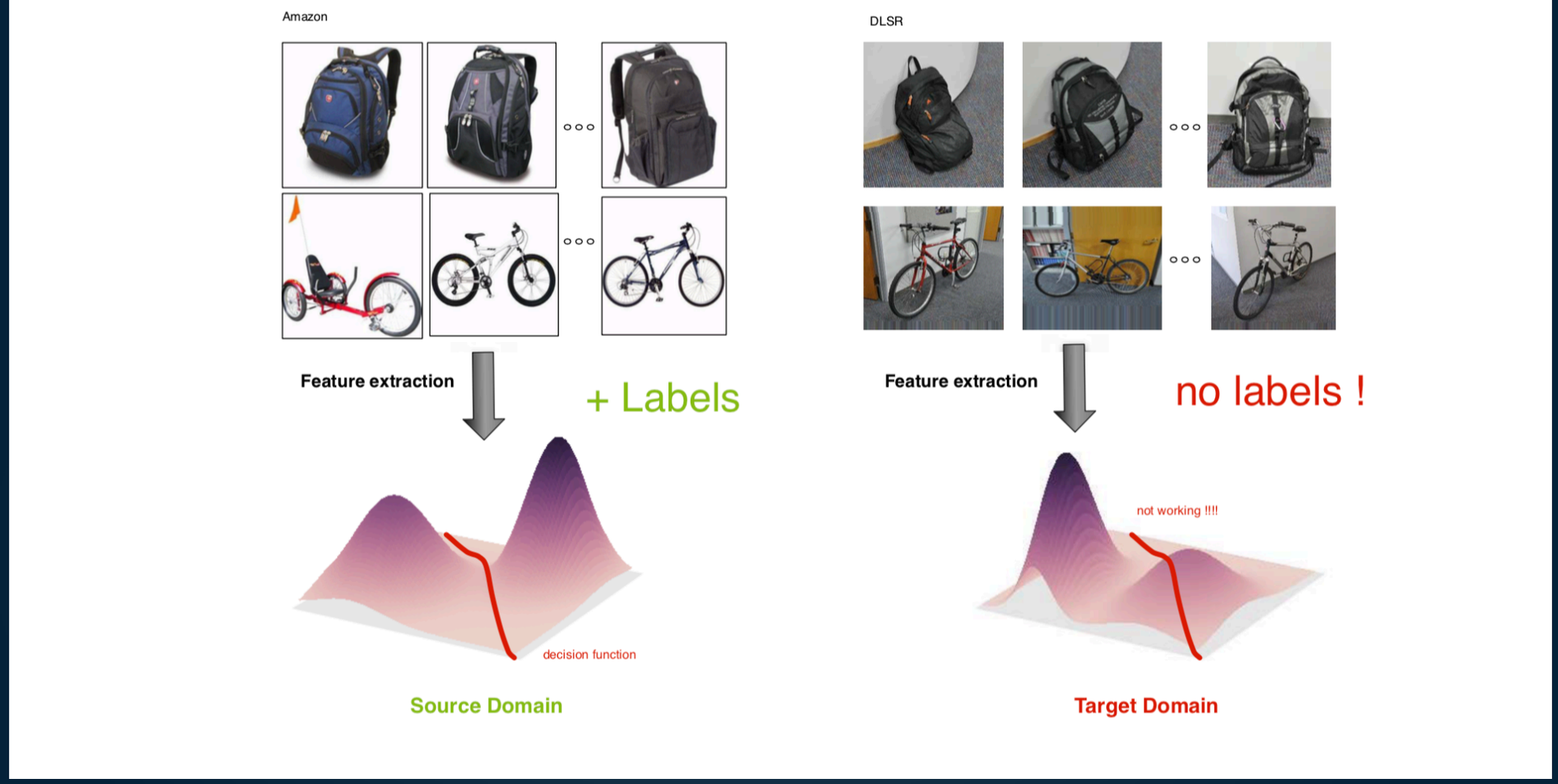
Unsupervised Domain Adaptation



- Traditional machine learning hypothesis:
  - We have access to training data. Probability distribution of the training set and the testing are the same.
  - We want to learn a classifier that generalizes to new data.

[Credit image: N. Courty]

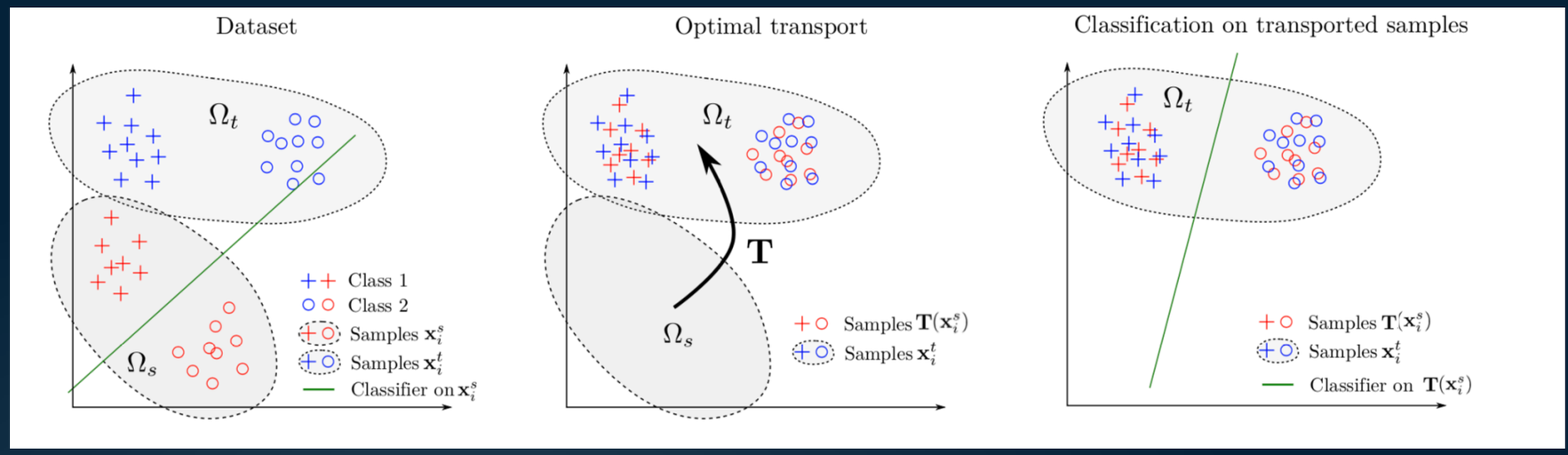
Unsupervised Domain Adaptation



- Domain adaptation: classification problem with data coming from different sources (domains).
- Labels only available in the source domain, and classification is conducted in the target domain.
- Classifier trained on the source domain data performs badly in the target domain.

[Credit image: N. Courty]

OTDA: Optimal Transport Domain Adaptation



Assumptions

- There exist a transport $\boldsymbol{T}$ in the feature space between the two domains.
- The transport preserves the conditional distributions:

$$\boldsymbol{P}_s[\boldsymbol{y}|\boldsymbol{x}_s] = \boldsymbol{P}_t[\boldsymbol{y}|\boldsymbol{T}(\boldsymbol{x}_s)]$$

3-step strategy

1. Estimate optimal transport between distributions.
2. Transport the training samples onto the target distribution using barycentric mapping [Ferradans et al., 2013].
3. Learn a classifier on the transported training samples.

[Source image: Courty et al., 2017]

5. (Smoothed, Sliced) OT

Wasserstein Distance: Curse of Dimensionality

$$\mathrm{W}_p(\boldsymbol{\mu}, \boldsymbol{\nu}) = \left(\inf_{\boldsymbol{\gamma} \in \boldsymbol{\Pi}_{\mathrm{con}}(\boldsymbol{\mu}, \boldsymbol{\nu})} \int_{\mathbb{R}^d \times \mathbb{R}^d} \|\boldsymbol{x} - \boldsymbol{y}\|^p \boldsymbol{\gamma}(\boldsymbol{x}, \boldsymbol{y}) \mathrm{d}\boldsymbol{x} \mathrm{d}\boldsymbol{y} \right)^{1/p}$$

- The Wasserstein distance is often estimated from samples.

$$\hat{\boldsymbol{\mu}}_n = \frac{1}{n} \sum_{i=1}^{n} \delta_{\boldsymbol{x}_i}$$

- The error of these empirical estimates suffers from an exponential dependence on dimension d that presents an obstacle to sample-efficient bounds.

$$\mathbb{E}[\mathrm{W}_p(\hat{\boldsymbol{\mu}}_n, \boldsymbol{\mu})] \lesssim n^{-1/d}$$

[Altschuler et al., 2017, Weed & Bach, 2019, Lei, 2020]

- Linear programming problem that requires generally $\mathcal{O}(n^3 \log(n)^2)$ arithmetic operations.

Wasserstein Distance in One-Dimension

- When $d = 1$, the Wasserstein distance can be calculated in closed-form owing to the cumulative distributions of $\boldsymbol{\mu}$ and $\boldsymbol{\nu}$.
- The Wasserstein distance admits the quantile representation

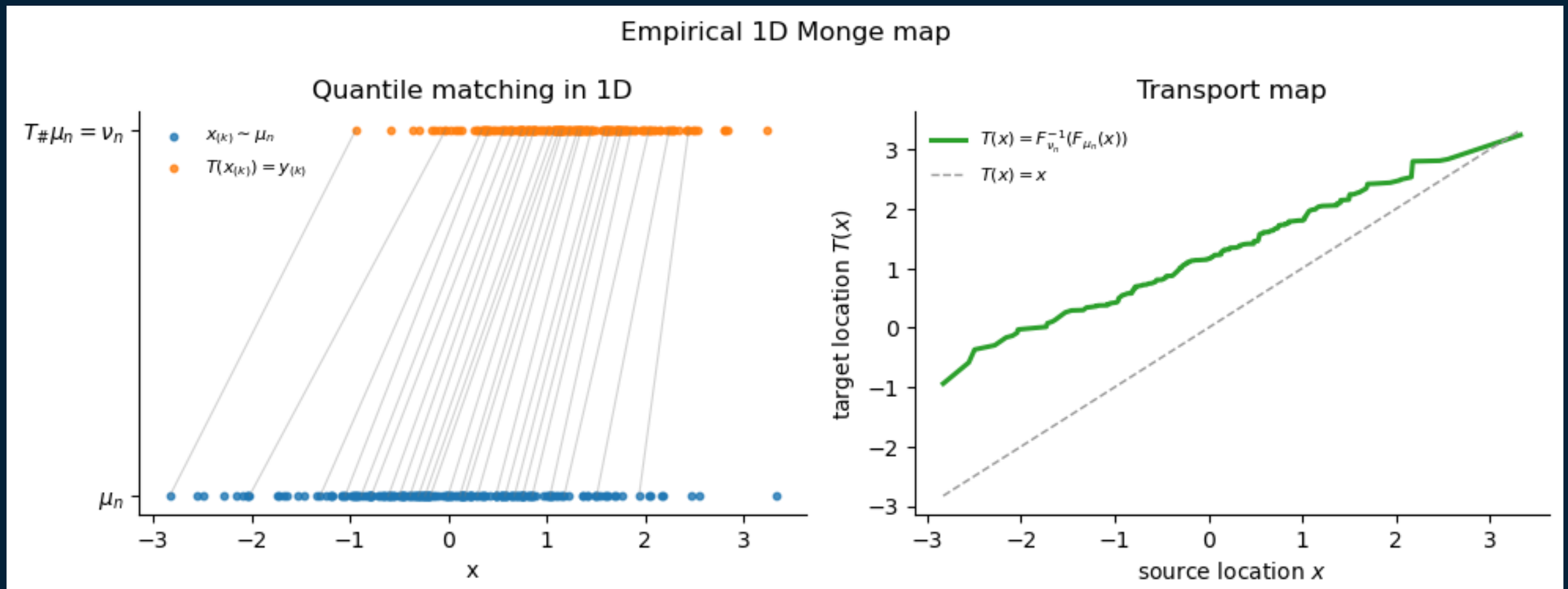
$$\mathrm{W}_p(\boldsymbol{\mu}, \boldsymbol{\nu}) = \left(\int_0^1 |F_{\boldsymbol{\mu}}^{-1}(q) - F_{\boldsymbol{\nu}}^{-1}(q)|^p \, dq \right)^{1/p}$$

- For empirical measures with equal weights, this reduces to matching order statistics

$$\mathrm{W}_p(\boldsymbol{\mu}_n, \boldsymbol{\nu}_n) = \left(\frac{1}{n} \sum_{k=1}^{n} |\boldsymbol{x}_{(k)} - \boldsymbol{y}_{(k)}|^p \right)^{1/p}$$

- Hence computing **1**D requires only the sorting of the samples, which yields a closed-form formula and an $\mathcal{O}(n \log(n))$.

Wasserstein Distance in One-Dimension



- To derive a metric for high-dimensional distributions based on one-dimensional Wasserstein distance.

- The main idea is to **project high-dimensional probability distributions onto a random one-dimensional space** and then to **compute the Wasserstein distance.**

Sliced-Wasserstein Distance

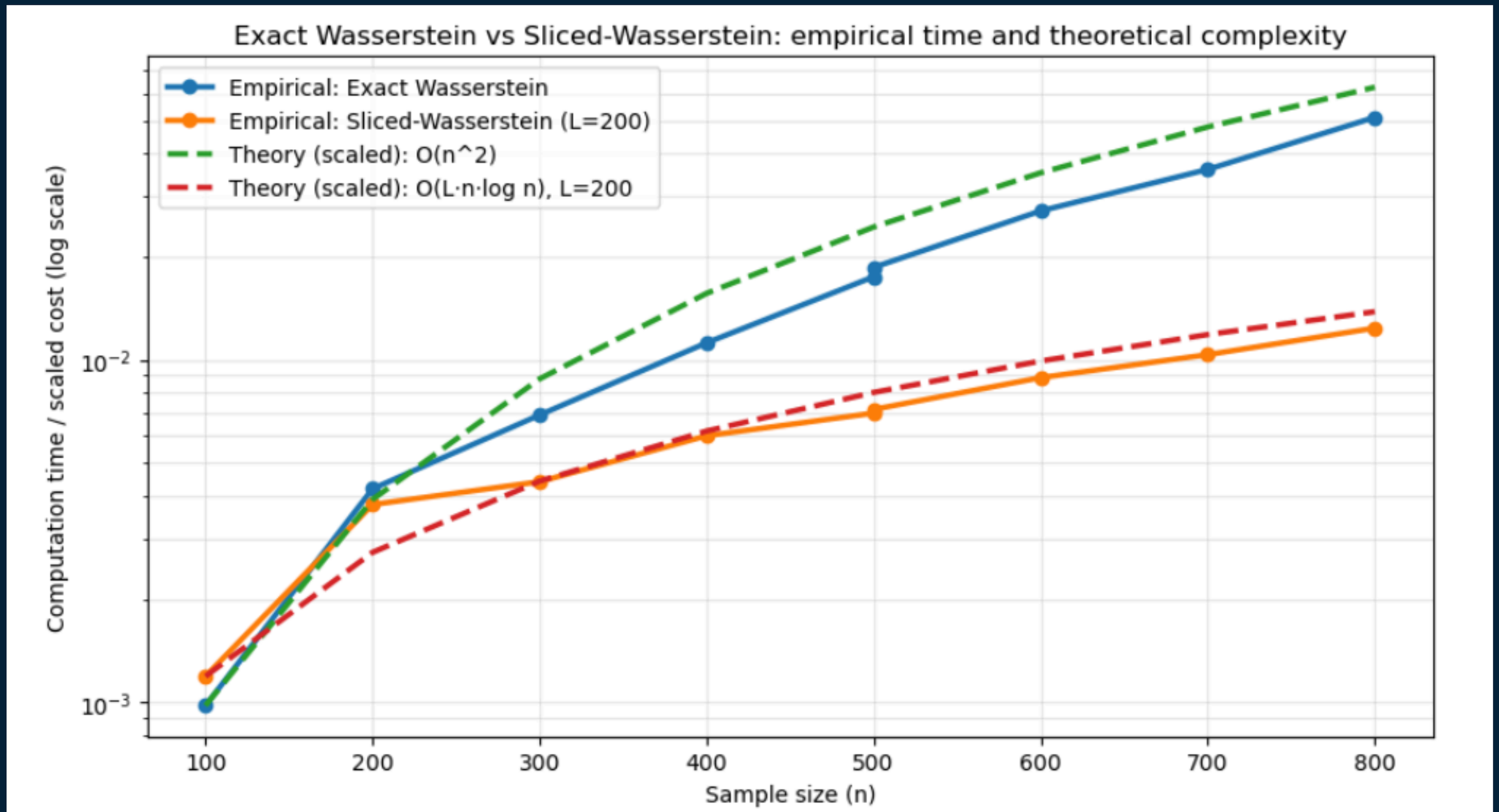
- The sliced Wasserstein distance (SW) reads as

$$\mathrm{SW}_p(\boldsymbol{\mu}, \boldsymbol{\nu}) = \left(\int_{\mathbb{S}^{d-1}} \mathrm{W}_p^p(\mathcal{R}_{\mathbf{u}}\boldsymbol{\mu}, \mathcal{R}_{\mathbf{u}}\boldsymbol{\nu}) u_d(\mathbf{u}) \mathrm{d}\mathbf{u} \right)^{1/p}.$$

Where $\mathcal{R}_{\mathbf{u}}$ the **Radon transform of a probability distribution**, i.e.,

$$\mathcal{R}_{\mathbf{u}}\boldsymbol{\mu}(\cdot) = \int_{\mathbb{R}^d} \boldsymbol{\mu}(\mathbf{s}) \delta(\cdot - \mathbf{s}^\top \mathbf{u}) \mathrm{d}\mathbf{s}$$

Sliced-Wasserstein Distance

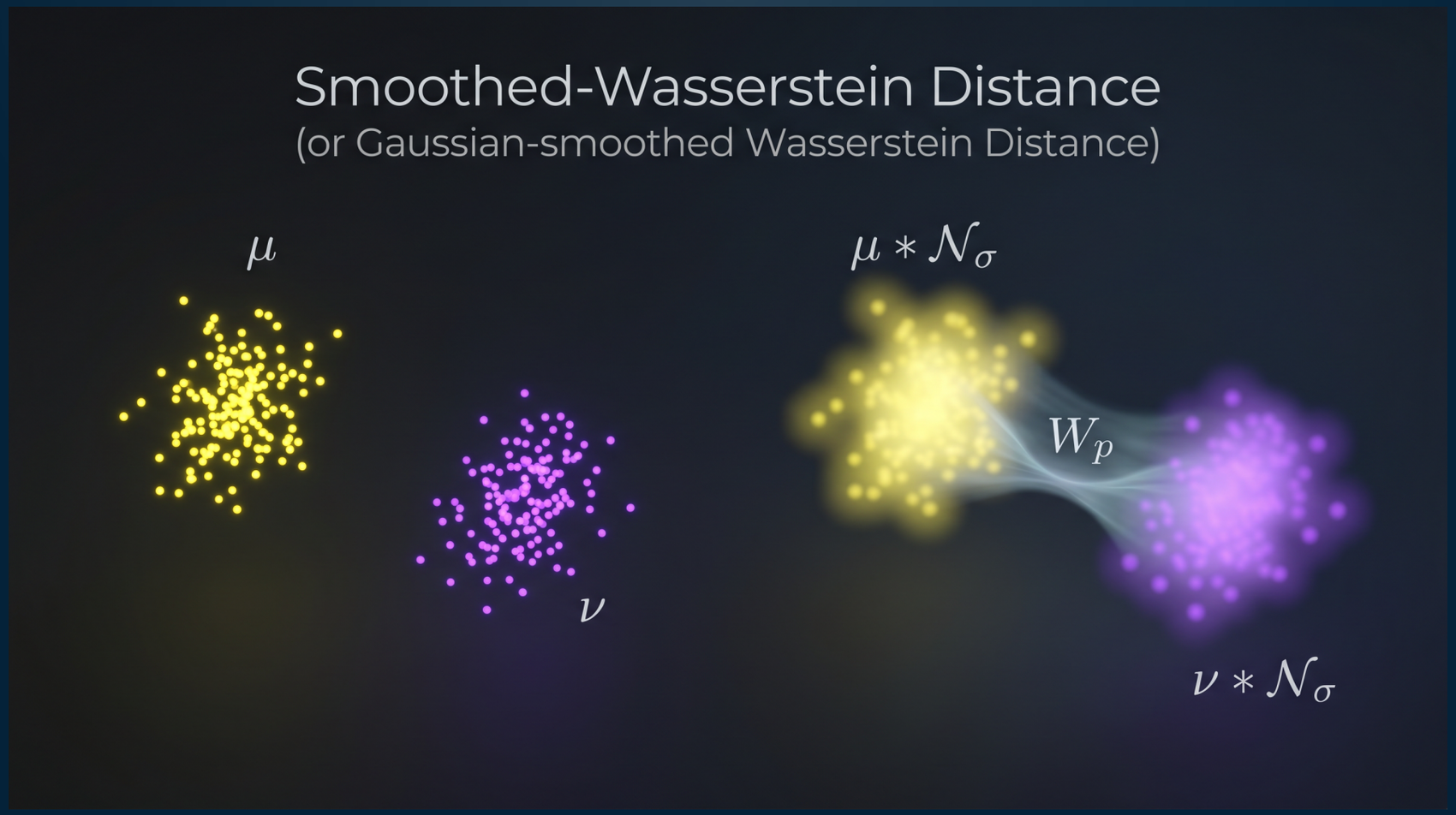


Complexity of SW

$$\mathcal{O}(Ldn + Ln\log n)$$

Wasserstein for Privacy-Sensitive Data: Smoothed-Wasserstein Distance

- We cannot expose raw samples (medical images, mobility traces, financial records) to define or optimize our objective.
- Instead, we convolve each empirical measure with a **Gaussian**: this hides individual points inside a local cloud of noise.
- We then compare these **blurred** distributions using a smoothed Wasserstein distance [Goldfeld et al., 2020; Goldfeld & Greenewald, 2020].



Smoothed-Wasserstein Distance

- The σ-smooth p-Wasserstein distance between probability measures is defined as

$$\mathrm{G}_\sigma \mathrm{W}_p(\boldsymbol{\mu}, \boldsymbol{\nu}) = \mathrm{W}_p(\boldsymbol{\mu} * \mathcal{N}_\sigma, \boldsymbol{\nu} * \mathcal{N}_\sigma)$$

- Fast rate of convergence [Nietertet al., 2021]

$$\mathbb{E}[\mathrm{G}_\sigma \mathrm{W}_p(\hat{\boldsymbol{\mu}}_n, \boldsymbol{\mu})] \lesssim n^{-1/2}$$

- We investigates the theoretical properties of the Gaussian smoothed sliced Wasserstein as well as those of generalized versions denoted as **Gaussian-Smoothed Sliced Divergences**.

$$\mathrm{G}_\sigma \mathrm{SD}_p(\boldsymbol{\mu}, \boldsymbol{\nu})$$

Gaussian-Smoothed Sliced Probability Divergences Distance

$$\mathrm{G}_\sigma \mathrm{SD}_p(\mu, \nu)$$

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TRANSACTIONS tmlr on ML RESEARCH

Gaussian-Smoothed Sliced Probability Divergences

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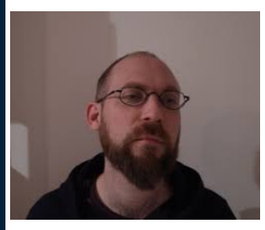

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Reviewed on OpenReview: *https://openreview.net/forum?id=weuALLWUV2*

$\mathrm{G}_\sigma\mathrm{SD}_p(\boldsymbol{\mu}, \boldsymbol{\nu})$

Gaussian-Smoothed Sliced Divergence

The σ-Gaussian-smooth p-Sliced Divergence between probability measures is defined as

$$\mathrm{G}_\sigma\mathrm{SD}_p(\boldsymbol{\mu}, \boldsymbol{\nu}) = \left(\int_{\mathbb{S}^{d-1}} \mathrm{D}^p(\mathcal{R}_{\mathbf{u}}\boldsymbol{\mu} * \mathcal{N}_\sigma, \mathcal{R}_{\mathbf{u}}\boldsymbol{\nu} * \mathcal{N}_\sigma) u_d(\mathbf{u}) \mathrm{d}\mathbf{u} \right)^{1/p}.$$

- Typical relevant divergences: Sinkhorn divergence or maximum mean discrepancy (MMD)

$\mathrm{G}_\sigma\mathrm{SD}_p(\boldsymbol{\mu}, \boldsymbol{\nu})$: Sinkhorn Divergence

- Entropic regularization of OT distances relies on the addition of a penalty term as follows:

Regularisation parameter

$$\mathcal{S}_\eta(\boldsymbol{\mu}, \boldsymbol{\nu}) = \min_{\boldsymbol{P} \in \boldsymbol{\Pi}(\boldsymbol{\mu}, \boldsymbol{\nu})} \{\langle \boldsymbol{C}, \boldsymbol{P} \rangle - \eta H(\boldsymbol{P})\} \quad \mathcal{O}(n^2)$$

$$H(\boldsymbol{P}) = -\sum_{i,j} \boldsymbol{P}_{ij} \log(\boldsymbol{P}_{ij})$$

Negative entropy

Marco Cuturi

Sinkhorn Distances:
Lightspeed Computation of Optimal Transport

Conference NeurIPS, 2013

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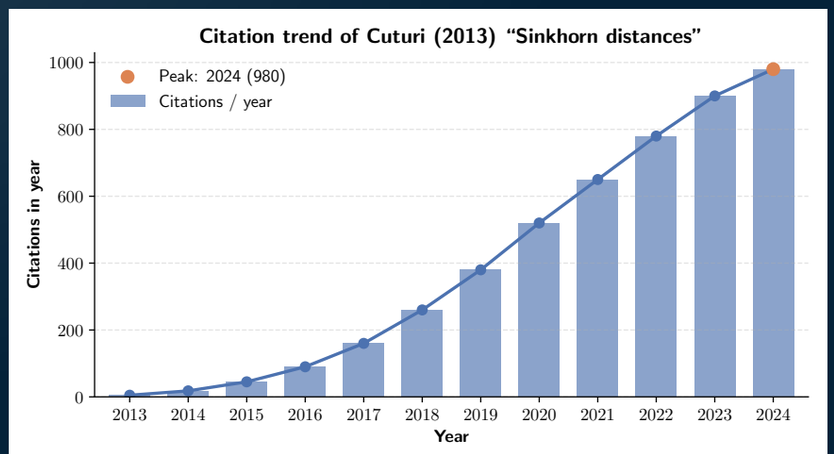


Sinkhorn divergence (Genevay et al., 2018; Peyré & Cuturi, 2019)

$$\mathcal{SKD}_\eta(\boldsymbol{\mu}, \boldsymbol{\nu}) = \mathcal{S}_\eta(\boldsymbol{\mu}, \boldsymbol{\nu}) - \frac{1}{2}\mathcal{S}_\eta(\boldsymbol{\mu}, \boldsymbol{\mu}) - \frac{1}{2}\mathcal{S}_\eta(\boldsymbol{\nu}, \boldsymbol{\nu})$$

$\mathrm{G}_\sigma\mathrm{SD}_p(\boldsymbol{\mu}, \boldsymbol{\nu})$: Maximum Mean Discrepancy

- Let $k : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ be a measurable bounded kernel on $\mathbb{R}$ and consider the reproducing kernel Hilbert space (RKHS) $\mathcal{H}_k$ associated with k and equipped with inner product $< \cdot, \cdot >_{\mathcal{H}_k}$ and norm $\| \cdot \|_{\mathcal{H}_k}$.

$$\forall t, k(t, \cdot) \in \mathcal{H}_k \text{ and } \forall f \in \mathcal{H}_k, f(t) =< f, k(t, \cdot) >_{\mathcal{H}_k}$$

- Let $\mathcal{P}_{\mathcal{H}_k}(\mathbb{R})$ be the set of probability measures η such that $\int_{\mathbb{R}} \sqrt{k(t,t)} d\eta(t) < \infty$.

- The **kernel mean embedding** is defined as

$$\Phi_k(\eta) = \int_{\mathbb{R}} k(\cdot, t) d\eta(t).$$

- The squared-maximum mean discrepancy (MMD) between $\boldsymbol{\mu}$ and $\boldsymbol{\nu}$

$$\mathrm{MMD}^2(\boldsymbol{\mu}, \boldsymbol{\nu}) = \|\Phi_k(\boldsymbol{\mu}) - \Phi_k(\boldsymbol{\nu})\|^2_{\mathcal{H}_k}$$

$$= \mathbb{E}_{T,T' \sim \boldsymbol{\mu}}[k(T, T')] - 2\mathbb{E}_{T \sim \boldsymbol{\mu}, R \sim \boldsymbol{\nu}}[k(T, R)] + \mathbb{E}_{R,R' \sim \boldsymbol{\nu}}[k(R, R')]$$

[Gretton et al. (2006)]

$\mathrm{G}_\sigma\mathrm{SD}_p(\boldsymbol{\mu}, \boldsymbol{\nu})$: Topological Properties

- $\mathrm{G}_\sigma\mathrm{SD}_p(\boldsymbol{\mu}, \boldsymbol{\nu})$ is a proper metric on $\mathcal{P}_p(\mathbb{R}^d) \times \mathcal{P}_p(\mathbb{R}^d)$.

Theorem *For any $\sigma > 0, p \geq 1$, the following properties hold:*

1. *if $\mathrm{D}(\cdot,\cdot)$ is non-negative (or symmetric), then $\mathrm{G}_\sigma\mathrm{SD}_p(\cdot,\cdot)$ is non-negative (or symmetric);*
2. *if $\mathrm{D}(\cdot,\cdot)$ satisfies the identity of indiscernibles, i.e. for $\mu', \nu' \in \mathcal{P}(\mathbb{R})$, $\mathrm{D}(\mu', \nu') = 0$ if and only if $\mu' = \nu'$, then this identity also holds for $\mathrm{G}_\sigma\mathrm{SD}_p(\cdot,\cdot)$ for any $\mu, \nu \in \mathcal{P}_p(\mathbb{R}^d)$;*
3. *if $\mathrm{D}(\cdot,\cdot)$ satisfies the triangle inequality then $\mathrm{G}_\sigma\mathrm{SD}_p(\cdot,\cdot)$ satisfies the triangle inequality.*

- $\mathrm{G}_\sigma\mathrm{SD}_p(\boldsymbol{\mu}, \boldsymbol{\nu})$ metrizes the weak topology.

Theorem *Let $\sigma > 0, p \geq 1$, $\mu \in \mathcal{P}_p(\mathbb{R}^d)$, and $\{\mu_k \in \mathcal{P}_p(\mathbb{R}^d)\}_{k\in\mathbb{N}}$ a sequence of distributions. Assume that the divergence D is bounded and metrizes the weak topology on $\mathcal{P}(\mathbb{R})$. Then, $\lim_{k\to\infty} \mathrm{G}_\sigma\mathrm{SD}_p(\mu_k, \mu) = 0$ if and only if $\mu_k \Rightarrow \mu$.*

- $\mathrm{G}_\sigma\mathrm{SD}_p(\boldsymbol{\mu}, \boldsymbol{\nu})$ is lower semi-continuous.

Proposition *Let $\sigma > 0, p \geq 1$ and assume that the base divergence D is lower semi-continuous w.r.t. the weak topology in $\mathcal{P}(\mathbb{R})$. Then, $\mathrm{G}_\sigma\mathrm{SD}_p$ is lower semi-continuous with respect to the weak topology in $\mathcal{P}_p(\mathbb{R}^d)$.*

$\mathrm{G}_\sigma\mathrm{SD}_p(\boldsymbol{\mu}, \boldsymbol{\nu})$: Statistical Properties (I)

- The smoothed Gaussian sliced divergence between the empirical probability measures $\hat{\boldsymbol{\mu}}_n$ and $\hat{\boldsymbol{\nu}}_n$

$$\mathrm{G}_\sigma\mathrm{SD}_p(\hat{\boldsymbol{\mu}}_n, \hat{\boldsymbol{\nu}}_n) = \left(\int_{\mathbb{S}^{d-1}} \mathrm{D}^p(\mathcal{R}_{\mathbf{u}}\hat{\boldsymbol{\mu}}_n * \mathcal{N}_\sigma, \mathcal{R}_{\mathbf{u}}\hat{\boldsymbol{\nu}}_n * \mathcal{N}_\sigma) \mathcal{U}_d(\mathbf{u}) \mathrm{d}\mathbf{u} \right)^{1/p}.$$

- Remark that for fixed direction $\boldsymbol{u} \in \mathbb{S}^{d-1}$, the distributions $\mathcal{R}_{\boldsymbol{u}}\hat{\boldsymbol{\mu}}_n * \mathcal{N}_\sigma$ and $\mathcal{R}_{\boldsymbol{u}}\hat{\boldsymbol{\nu}}_n * \mathcal{N}_\sigma$ are **continuous**, in particular they are a mixture of Gaussian distributions centered on the projected samples with variance σ^2.

Lemma

Conditionally on the samples $\{X_i\}_{i=1,\dots,n}$ and $\{Y_i\}_{i=1,\dots,n}$ one has:

$$\mathcal{R}_{\boldsymbol{u}}\hat{\boldsymbol{\mu}}_n * \mathcal{N}_\sigma = \frac{1}{n}\sum_{i=1}^{n} \mathcal{N}(\boldsymbol{u}^\top X_i, \sigma^2) \quad \mathcal{R}_{\boldsymbol{u}}\hat{\boldsymbol{\nu}}_n * \mathcal{N}_\sigma = \frac{1}{n}\sum_{i=1}^{n} \mathcal{N}(\boldsymbol{u}^\top Y_i, \sigma^2)$$

$\mathrm{G}_\sigma\mathrm{SD}_p(\boldsymbol{\mu}, \boldsymbol{\nu})$: Statistical Properties (II)

- We further need to sample with respect to the continuous mixture Gaussian measures in order to get a **fully** empirical measure version of $\mathrm{G}_\sigma\mathrm{SD}_p(\boldsymbol{\mu}, \boldsymbol{\nu})$.

- Let $T_1^x, \ldots, T_n^x$ and $T_1^y, \ldots, T_n^y$ be i.i.d. observations of $\mathcal{R}_{\boldsymbol{u}}\hat{\mu}_n * \mathcal{N}_\sigma$ and $\mathcal{R}_{\boldsymbol{u}}\hat{\nu}_n * \mathcal{N}_\sigma$ respectively.

- Sampling i.i.d. $\{T_i^x\}_{i=1,\ldots,n}$ is given by the following scheme: we first choose the component $\mathcal{N}(\boldsymbol{u}^\top X_i, \sigma^2)$ then we generate $T_i^x = \boldsymbol{u}^\top X_i + Z_i^x$, where $Z_i^x \sim \mathcal{N}_\sigma$.

$\mathrm{G}_\sigma\mathrm{SD}_p(\boldsymbol{\mu}, \boldsymbol{\nu})$: Statistical Properties (II)

- Hence, we set, for a given direction $\boldsymbol{u}$

$$\hat{\hat{\boldsymbol{\mu}}}_n = \frac{1}{n}\sum_{i=1}^{n} \delta_{T_i^x} = \frac{1}{n}\sum_{i=1}^{n} \delta_{\boldsymbol{u}^\top X_i + Z_i^x}$$

- The measure $\hat{\hat{\boldsymbol{\mu}}}_n \in \mathcal{P}(\mathbb{R})$ defines an empirical version of the continuous $\mathcal{R}_{\boldsymbol{u}}\hat{\boldsymbol{\mu}}_n * \mathcal{N}_\sigma$.
- We define the **double empirical smoothed Gaussian sliced divergence** as:

Double Empirical Divergence

The double empirical smoothed Gaussian sliced divergence reads as

$$\hat{\mathrm{G}}_\sigma\mathrm{SD}_p(\hat{\boldsymbol{\mu}}_n, \hat{\boldsymbol{\nu}}_n) = \left(\int_{\mathbb{S}^{d-1}} \mathrm{D}^p(\hat{\hat{\boldsymbol{\mu}}}_n, \hat{\hat{\boldsymbol{\nu}}}_n) u_d(\mathbf{u}) \mathrm{d}\mathbf{u}\right)^{1/p}$$

$\mathrm{G}_\sigma\mathrm{SD}_p(\mu,\nu)$: Statistical Properties (III)

- The empirical distributions are derived from a **double sampling process**, which leads to consider a double expectations, wrt the origin distribution $\mathbb{E}_{\mu^{\otimes n}}$ and wrt the sampling from the Gaussian smoothing $\mathbb{E}_{\mathcal{N}_\sigma^{\otimes n}}$.

- We first consider the conditional expectation given the samples $\mathbb{E}_{\mathcal{N}_\sigma^{\otimes n}}[\cdot|X_1,\ldots,X_n]$ then apply $\mathbb{E}_{\mu^{\otimes n}}$. We denote by

$$\mathbb{E}_{\mu^{\otimes n}|\mathcal{N}_\sigma^{\otimes n}}[\cdot] = \mathbb{E}_{\mu^{\otimes n}}\left[\mathbb{E}_{\mathcal{N}_\sigma^{\otimes n}}[\cdot|X_1,\ldots,X_n]\right].$$

Proposition *Fix $\sigma>0, p\geq 1$ and $\vartheta>\sqrt{2}$. For $X\sim\mu$, assume that $\int_0^\infty e^{\frac{2\xi^2}{\sigma^2\vartheta^2}}\mathbf{P}\left[\|X\|>\xi\right]d\xi<\infty$. Then,*

Convergence with a rate $\mathcal{O}(n^{-1/2p})$

$$\mathbf{E}_{\mu^{\otimes n}|\mathcal{N}_\sigma^{\otimes n}}[\hat{\mathrm{G}}_\sigma\mathrm{SW}_p(\hat{\mu}_n,\mu)] \leq \Xi_{p,\sigma,\vartheta}\frac{1}{n^{1/2p}} + \Upsilon_{p,\sigma,\mu}\frac{(\log n)^{1/p}}{n^{1/p}},$$

where $\Xi_{p,\sigma,\vartheta} = \frac{2^{\frac{5}{2}-\frac{5}{4p}}}{\pi^{1/2p}}\sigma^{1-\frac{1}{4p}}\vartheta^{1+\frac{1}{p}}\left(\Gamma\left(p+\frac{1}{2}\right)\left(\sqrt{\frac{4\pi\sigma^2\vartheta^2}{\vartheta^2-2}}+4\int_0^\infty e^{\frac{2\xi^2}{\sigma^2\vartheta^2}}\mathbf{P}[\|X\|>\xi]d\xi\right)\right)^{1/2p}$ *and* $\Upsilon_{p,\sigma,\mu} = \frac{2^{2-\frac{1}{2p}}C_p}{\pi^{1/2p}}\sigma^2\left(\Gamma(p+\frac{1}{2})\sum_{k=0}^\infty\frac{(-p)_k}{(\frac{1}{2})_k}\frac{(-1)^k}{(2\sigma^2)^k k!}M_{2k}(\mu)\right)^{1/p}$ *with C_p is a positive constant depending only on p.*

Domain adaptation with $\mathrm{G}_\sigma\mathrm{SW}$

$$\min_{g,h} \left\{ \mathcal{L}_c(h(g(\mathbf{X}_s)), \mathbf{y}_s) + \mathcal{D}(g(\mathbf{X}_s), g(\mathbf{X}_t)) \right\}$$

- $\mathcal{L}_c$ can be the **cross-entropy loss or a quadratic loss** and $\mathcal{D}$ a **divergence between empirical distributions** (Gaussian-smoothed sliced divergence). We solve this problem through stochastic gradient descent.

- When performing such model adaptation, a **privacy/utility trade-off** that has to be handled. In practice, one would prefer the most private model while not hurting its performance. Hence, one would seek the largest noise level $\sigma > 0$ to use while preserving accuracy on target domain.
- We have considered two datasets: a handwritten digit recognition (USPS/MNIST) and Office 31 datasets.

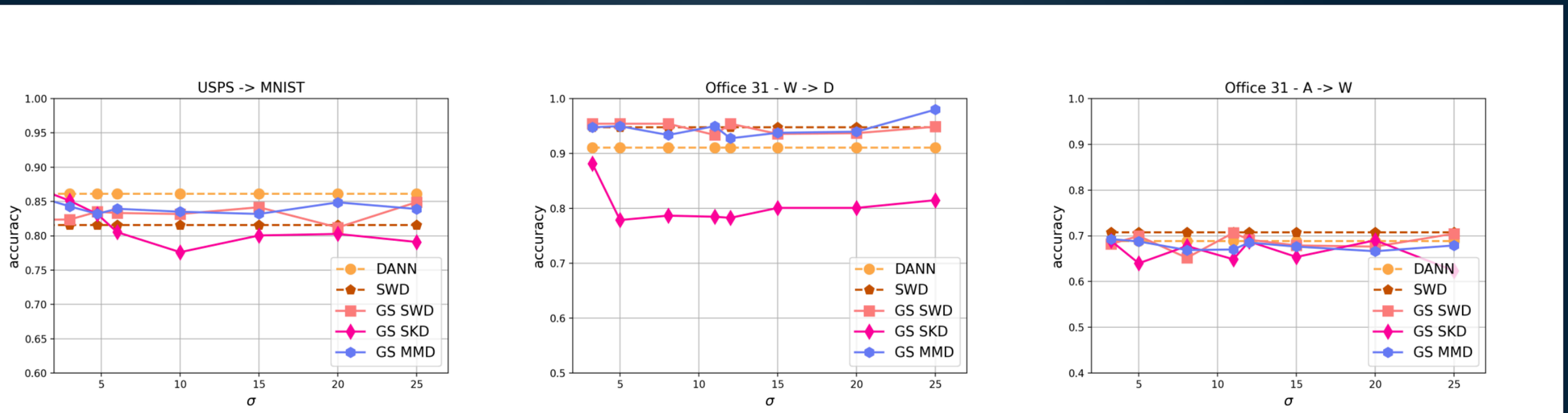
Domain adaptation with $\mathrm{G}_\sigma\mathrm{SW}$: MNIST(source) to USPS (target)

MNIST

USPS

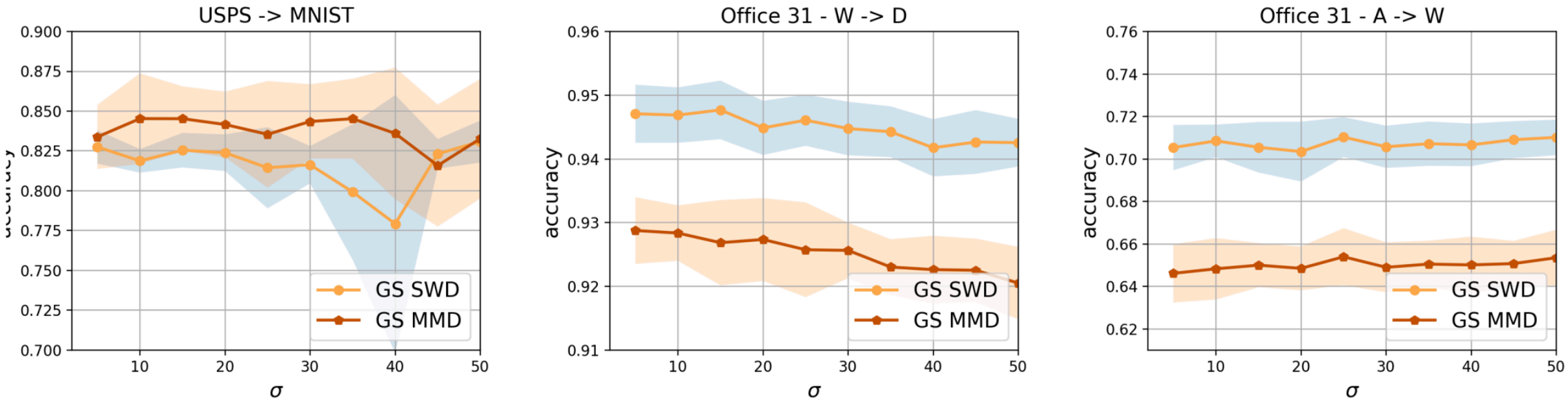
Domain adaptation with $\mathrm{G}_\sigma\mathrm{SW}$

$$\min_{g,h} \left\{ \mathcal{L}_c(h(g(\mathbf{X}_s)), \mathbf{y}_s) + \mathcal{D}(g(\mathbf{X}_s), g(\mathbf{X}_t)) \right\}$$



Domain adaptation performances using different divergences on distributions with respect to the Gaussian smoothing. (Left) USPS to MNIST. (Middle) Office-31 Webcam to DSLR. (Right) Office-31 Amazon to Webcam.

Domain adaptation with $\mathrm{G}_\sigma\mathrm{SW}$



Domain adaptation performances using different divergences on distributions with respect to the Gaussian smoothing using one-epoch-fine-tuned models. (Left) USPS to MNIST. (Middle) Office-31 Webcam to DSLR. (Right) Office-31 Amazon to Webcam.

Take Home Message

- A powerful tool, well theoretically grounded, for manipulating distributions in machine learning.

- Despite its initial computational complexity, a lot of applications, even in large scale/deep learning settings.

- Others OT aspects (out the scope of the presentation): Gromov-Wasserstein distance (working with structured data), Sliced Wasserstein, Multimarginal Optimal Transport (MOT) and many more !

- We provide properties of Gaussian-smoothed sliced divergences for comparing distributions.

- An important direction for future research is considering non Gaussian smoothing distribution enjoying this property.

Some References

- G. Peyré and M. Cuturi,
  Computational Optimal Transport with Applications to Data Sciences, 2019
- N. country, R. Flamary, D. Tuia and A. Rakotomamonjy.
  Optimal Transport for Domain Adaptation, *PAMI 2017*
- R. Flamary et al. POT: Python Optimal Transport Library, *JMLR 2021*.

POT: Python Optimal Transport

Contents

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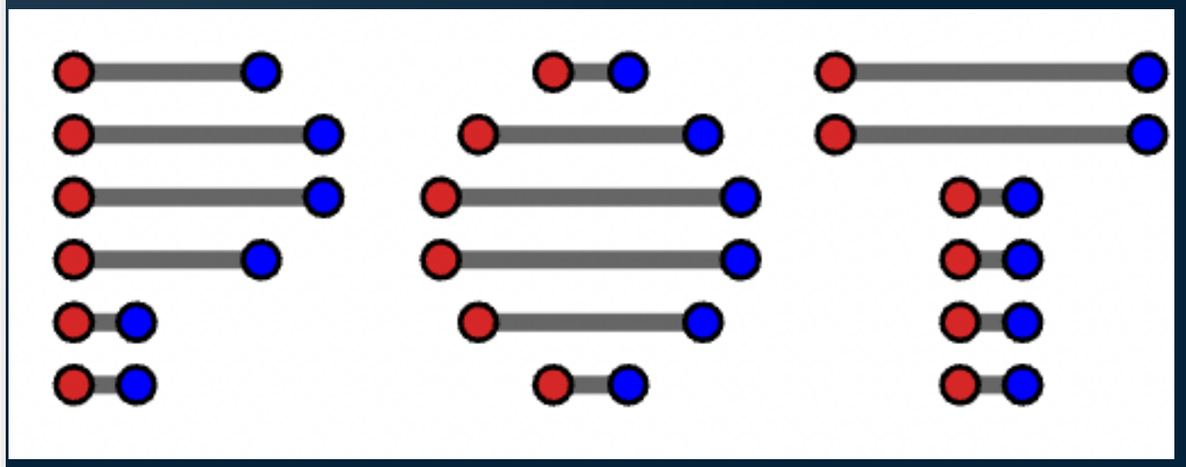
This open source Python library provide several solvers for optimization problems related to Optimal Transport for signal, image processing and machine learning.

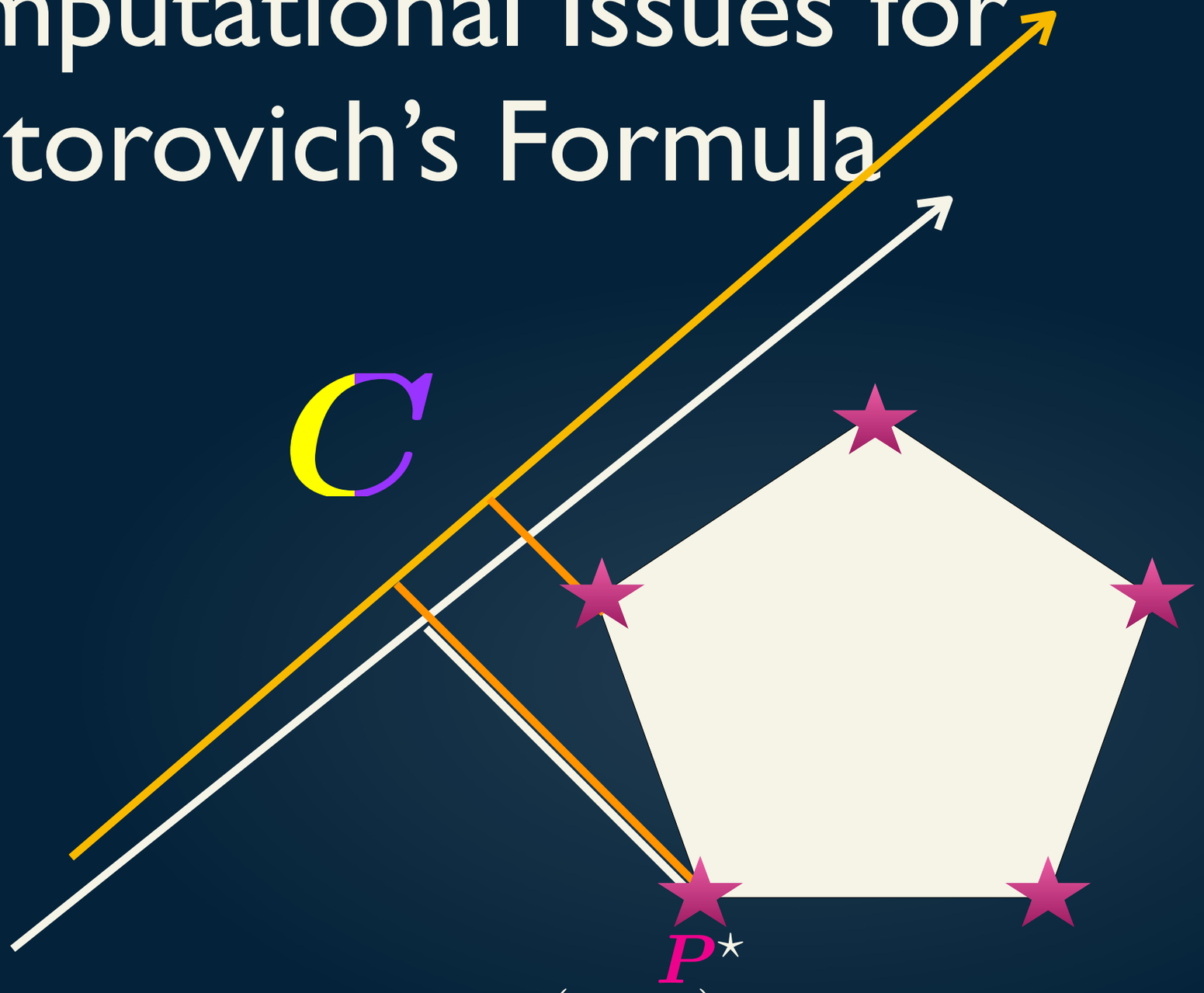
Website and documentation: https://PythonOT.github.io/

Source Code (MIT): https://github.com/PythonOT/POT



Thank You for your attention!

Computational Issues for Kantorovich's Formula



$\Pi(\mu, \nu)$ is the Birkhoff polytope

- No unique solution in some cases, numerical instabilities.
- Linear programming problem that requires generally $\mathcal{O}(n^3 \log(n)^2)$ arithmetic operations.

Regularized Discrete OT Framework: Sinkhorn Divergence

- Entropic regularization of OT distances relies on the addition of a penalty term as follows:

Regularisation parameter

$$\mathcal{S}_\eta(\boldsymbol{\mu}, \boldsymbol{\nu}) = \min_{\boldsymbol{P} \in \boldsymbol{\Pi}(\boldsymbol{\mu}, \boldsymbol{\nu})} \{\langle \boldsymbol{C}, \boldsymbol{P} \rangle - \eta H(\boldsymbol{P})\}$$

Sinkhorn divergence

Negative entropy

$$H(\boldsymbol{P}) = -\sum_{i,j} \boldsymbol{P}_{ij} \log(\boldsymbol{P}_{ij})$$

Marco Cuturi

Conference NeurIPS, 2013

Sinkhorn Distances:
Lightspeed Computation of Optimal Transport

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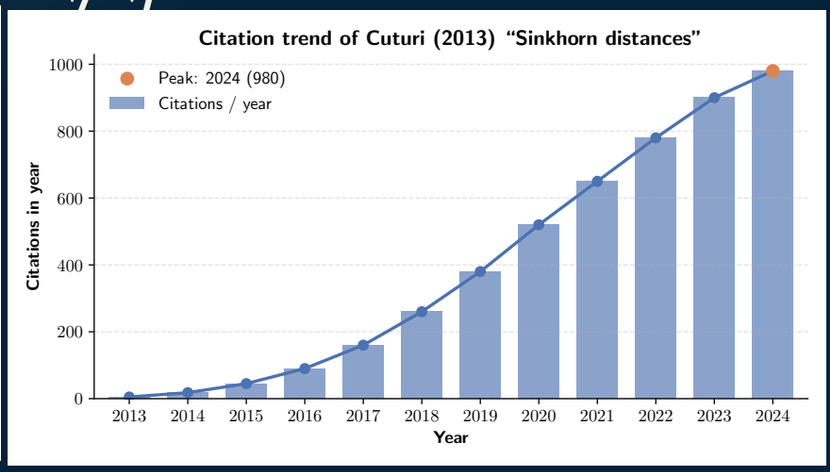

Regularized Discrete OT Framework: Dual of $\mathcal{S}_\eta(\boldsymbol{\mu}, \boldsymbol{\nu})$

Dual of Sinkhorn divergence

$$\mathcal{S}_\eta^{\mathrm{d}}(\boldsymbol{\mu}, \boldsymbol{\nu}) = \min_{\boldsymbol{u}\in\mathbb{R}^n, \boldsymbol{v}\in\mathbb{R}^m} \left\{ \Psi(\boldsymbol{u}, \boldsymbol{v}) := \mathbf{1}_n^\top B(\boldsymbol{u}, \boldsymbol{v}) \mathbf{1}_m - \langle \boldsymbol{u}, \boldsymbol{\mu} \rangle - \langle \boldsymbol{v}, \boldsymbol{\nu} \rangle \right\}$$

where

$$B(\boldsymbol{u}, \boldsymbol{v}) := \mathrm{diag}(e^{\boldsymbol{u}}) \; \boldsymbol{K} \, \mathrm{diag}(e^{\boldsymbol{v}})$$

$$\boldsymbol{K} = e^{-\boldsymbol{C}/\eta}$$

Gibbs Kernel

- The primal optimal solution $\boldsymbol{P}^\star$ takes the form:

$$\boldsymbol{P}^\star = \mathrm{diag}(e^{\boldsymbol{u}^\star}) \; \boldsymbol{K} \, \mathrm{diag}(e^{\boldsymbol{v}^\star})$$

Optimal Transportation Plan

with $(\boldsymbol{u}^\star, \boldsymbol{v}^\star) = \underset{\boldsymbol{u}\in\mathbb{R}^n, \boldsymbol{v}\in\mathbb{R}^m}{\mathrm{argmin}} \; \{\Psi(\boldsymbol{u}, \boldsymbol{v})\}$

Dual Optimal Variables

Regularized Discrete OT Framework: Sinkhorn Algorithm

- $\boldsymbol{P}^\star$ can be solved efficiently by Sinkhorn iterations (near- $\mathcal{O}(n^2)$ complexity [Altschuler et al., 2017]).

SINKHORN($\boldsymbol{C}, \boldsymbol{\mu}, \boldsymbol{\nu}$) Matrix-Scaling Problem

1. $\boldsymbol{a}^{(0)} \leftarrow \mathbf{1}_n/n, \boldsymbol{b}^{(0)} \leftarrow \mathbf{1}_m/m;$
2. $\boldsymbol{K} \leftarrow e^{-\boldsymbol{C}/\eta};$
3. For $k = 1, 2, 3, \ldots$
   - $\boldsymbol{a}^{(k)} \leftarrow \boldsymbol{\mu} \oslash \boldsymbol{K}\boldsymbol{b}^{(k-1)};$
   - $\boldsymbol{b}^{(k)} \leftarrow \boldsymbol{\nu} \oslash \boldsymbol{K}^\top \boldsymbol{a}^{(k-1)};$
4. Return $\mathrm{diag}(\boldsymbol{a}^{(k)})\ \boldsymbol{K}\,\mathrm{diag}(\boldsymbol{b}^{(k)})$

python POT

(Flamary et al. 2017)

```
from ot import sinkhorn
P_star = sinkhorn(mu, nu, C, eta)
```

Sparsity of Transport Plan