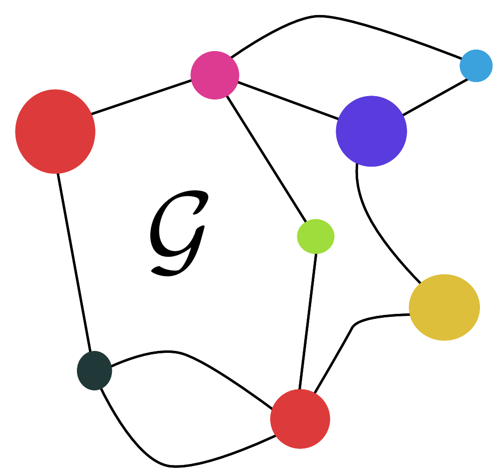
The optimal transportation problem for structured data (and heterogeneous?)

Titouan Vayer

Post-Doc



Seminar

11/01/2021

Nicolas Courty

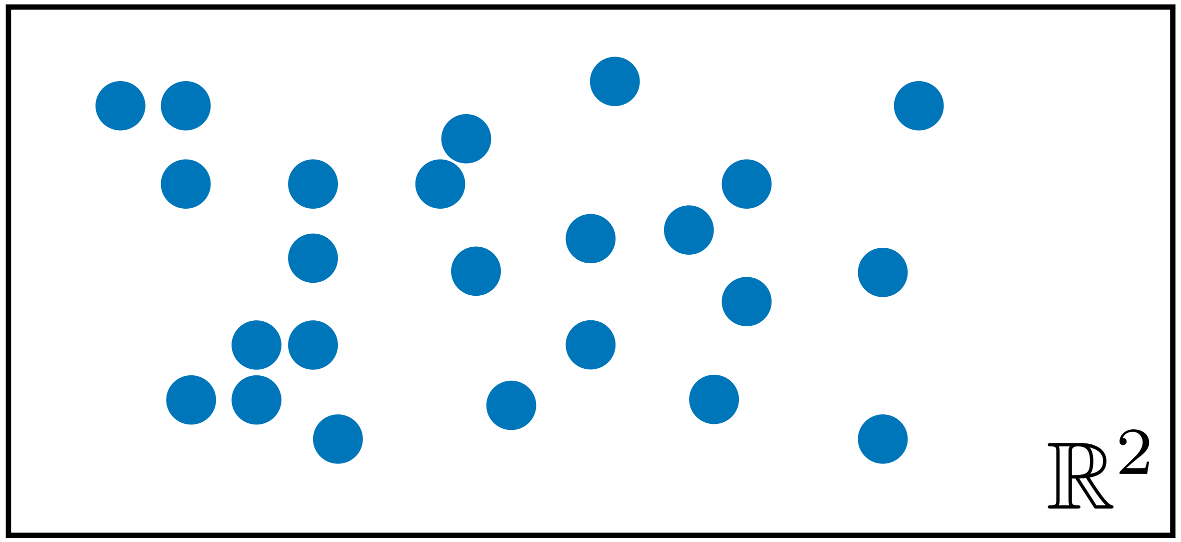
Laetitia Chapel

Romain Tavenard

Rémi Flamary

In short:

Machine Learning: Learn to make decision from **data**



In short:

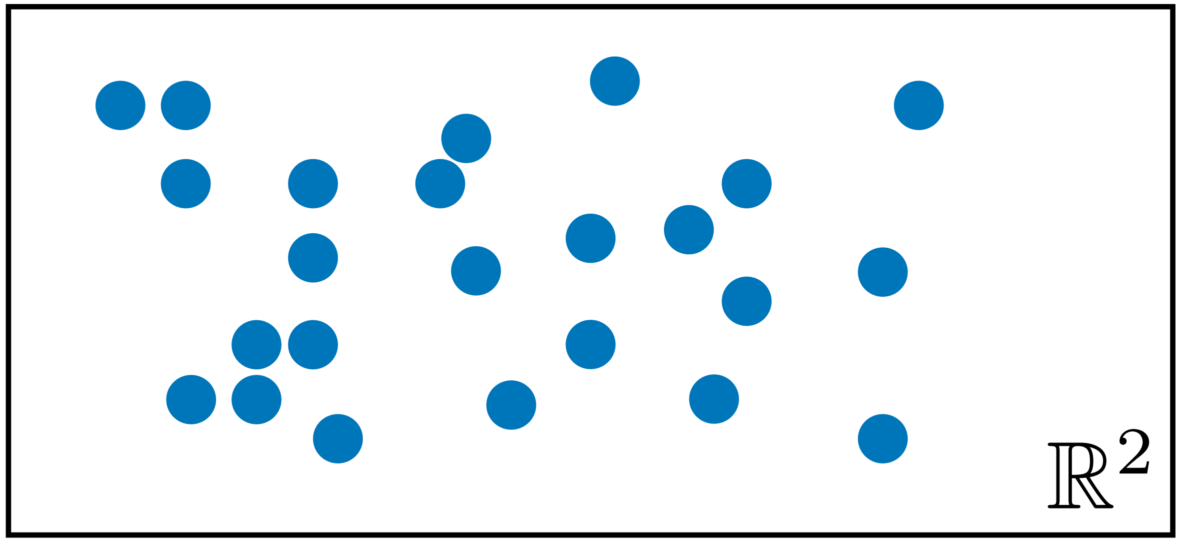
Machine Learning: Learn to make decision from **data**

How to represent data?

How to operate on them?

Mathematical representation

Tools which build upon this representation



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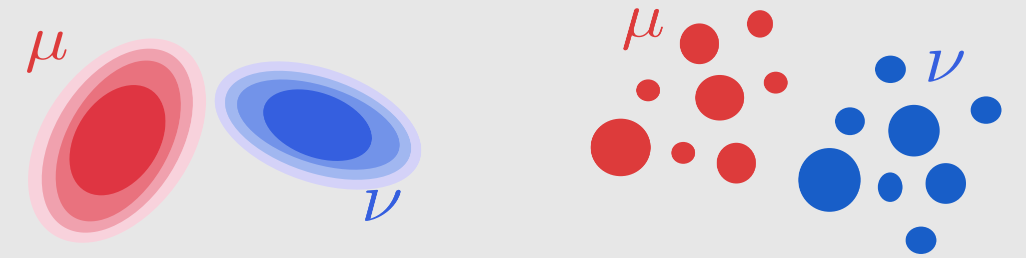
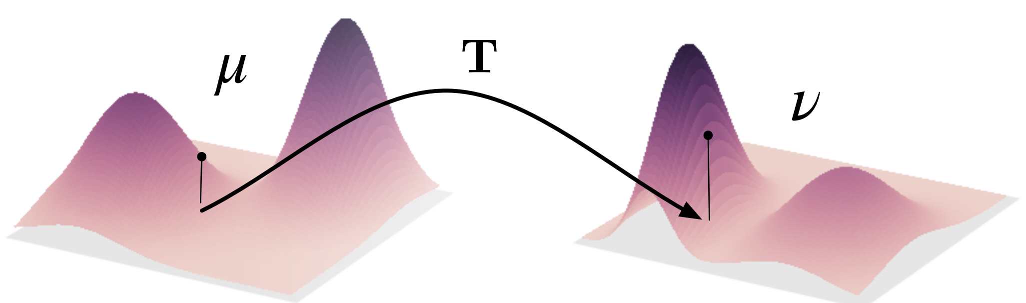
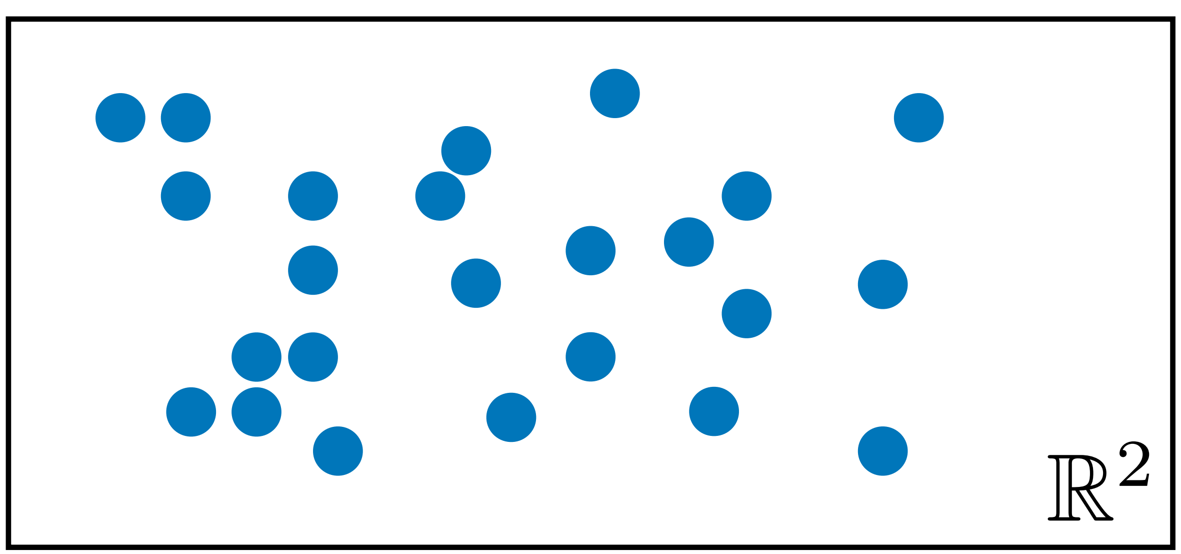
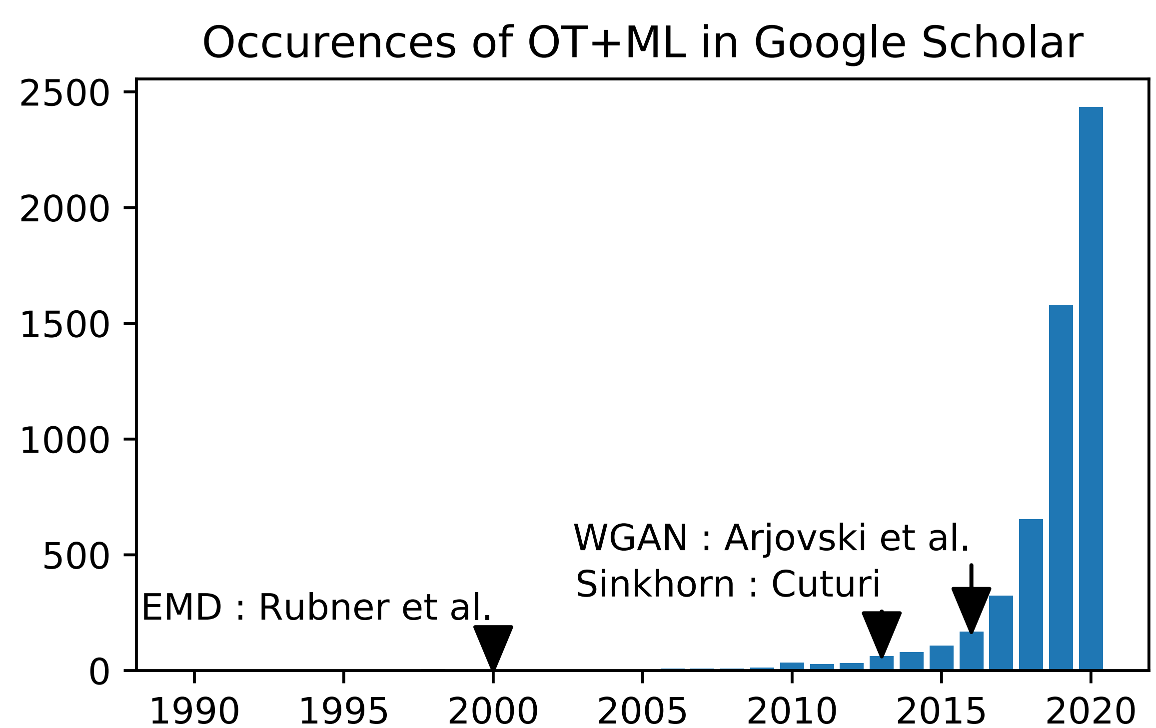


Tools which build upon this representation

Optimal Transport theory







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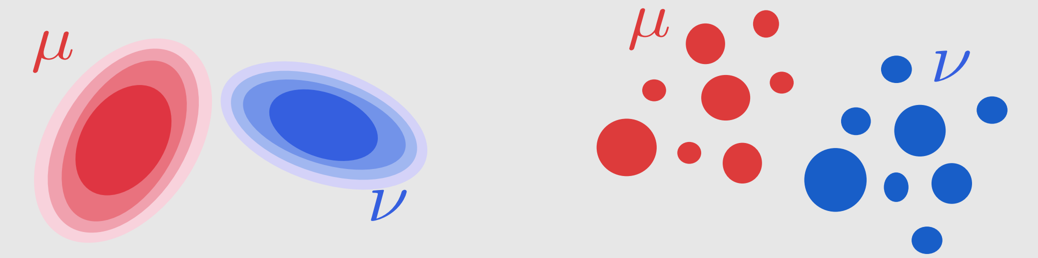
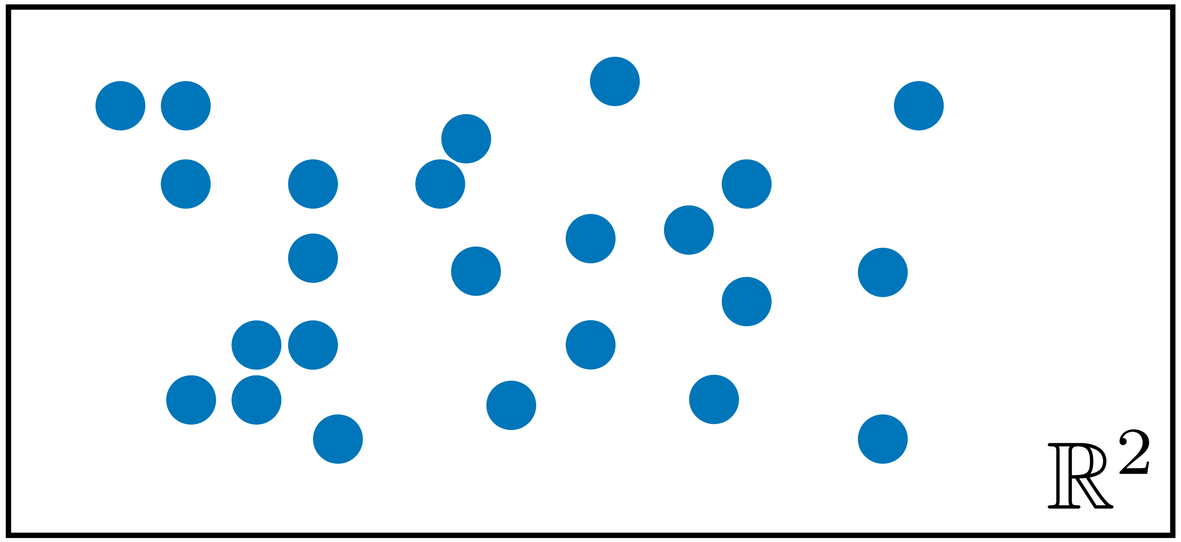


Tools which build upon this representation

Optimal Transport theory

Particularly challenging: highly structured data, heterogeneous spaces



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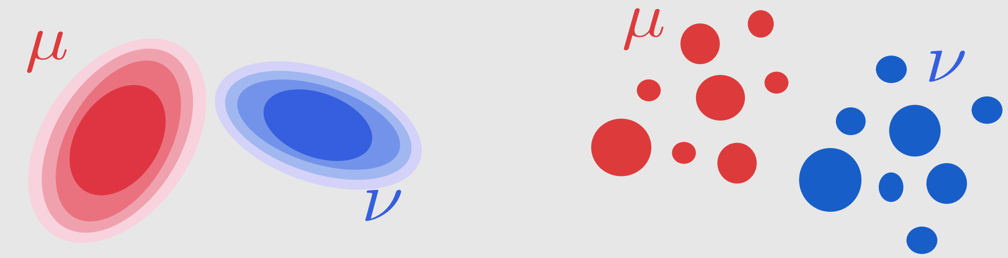

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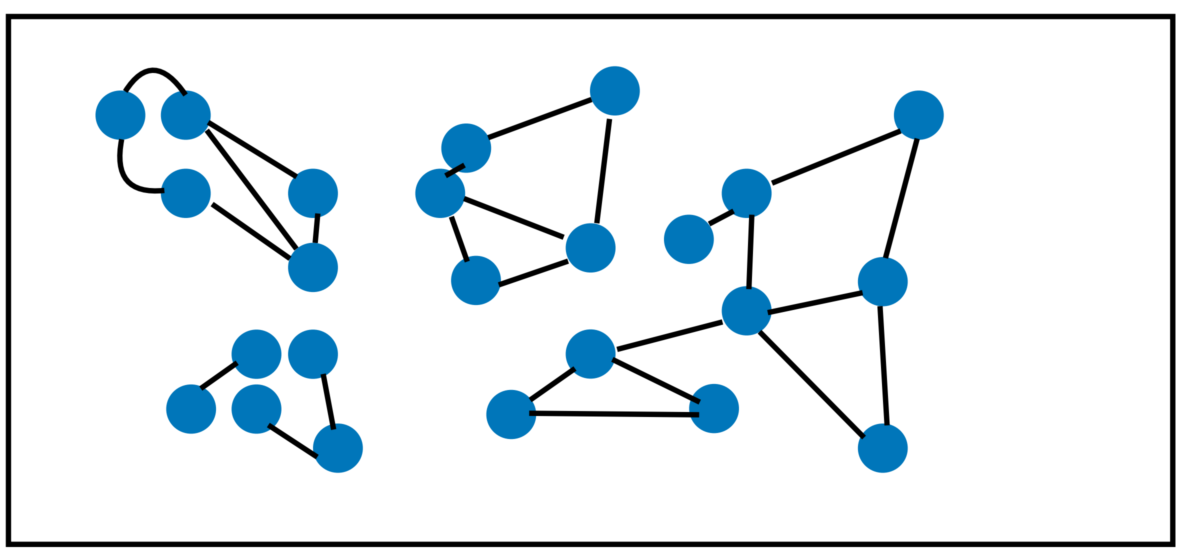
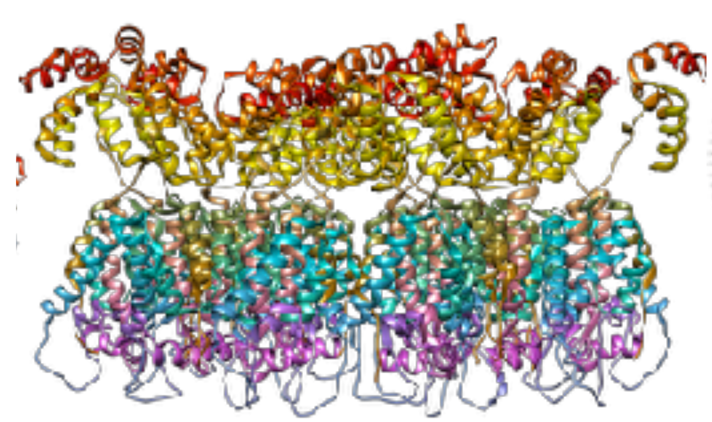
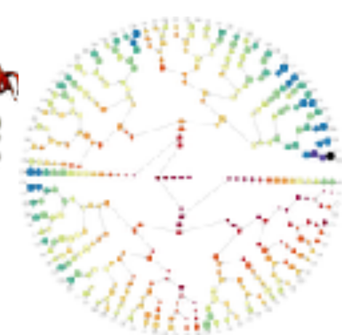




molecules, sequences..

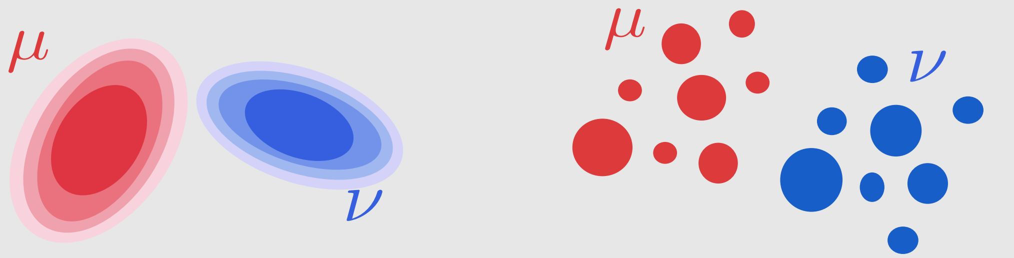


graphs

In short:

Mathematical representation

As probability distributions



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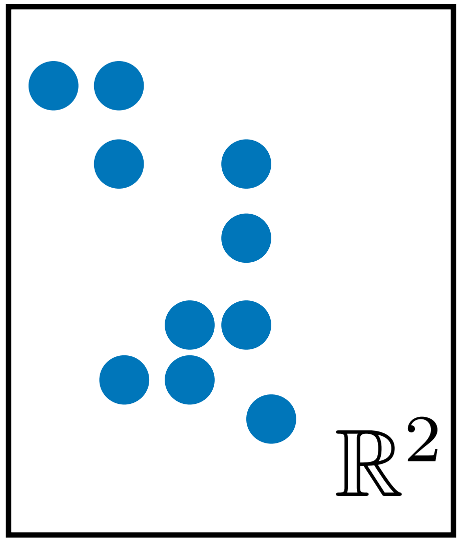
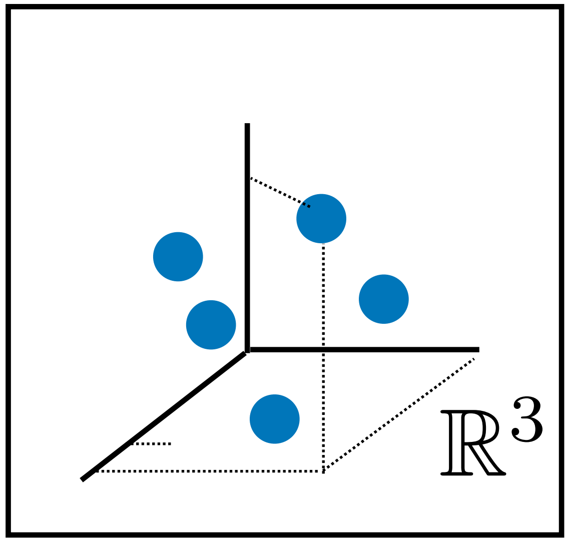
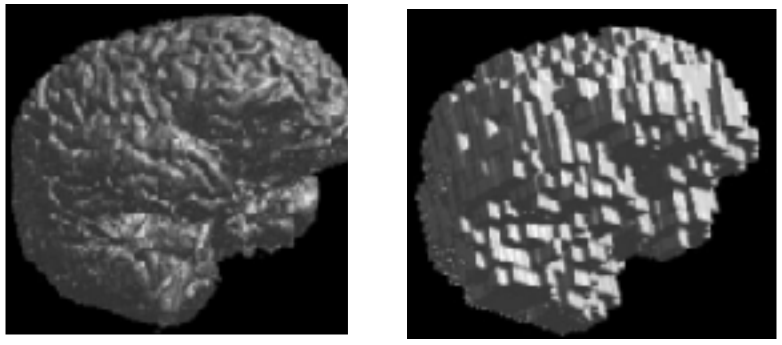
Particularly challenging: highly structured data, **heterogeneous spaces**







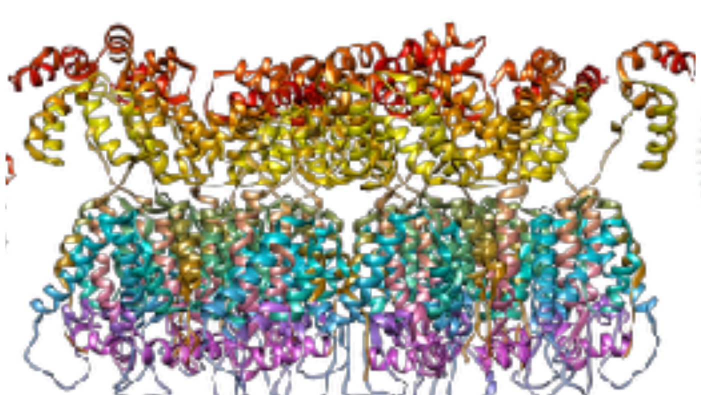
high & low resolution images

In short:

Machine Learning: Learn to make decision from **data**

- **How to represent data?**
- **How to operate on them?**

Particularly challenging: highly structured data, heterogeneous spaces



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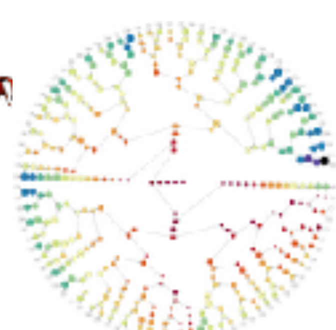

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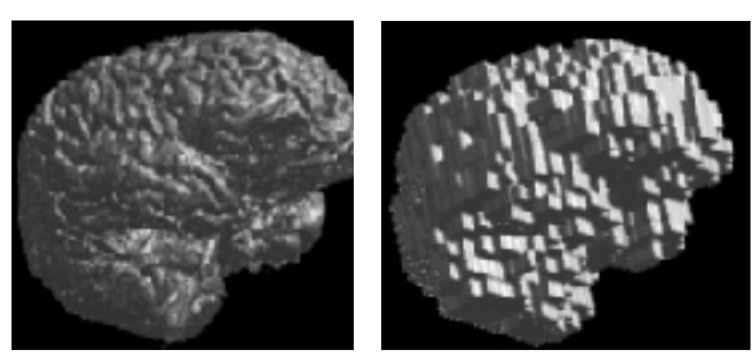

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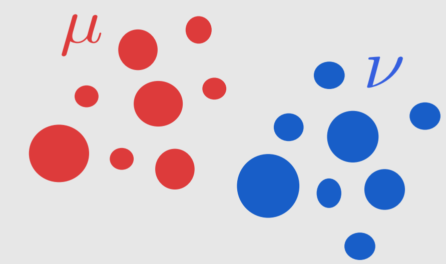
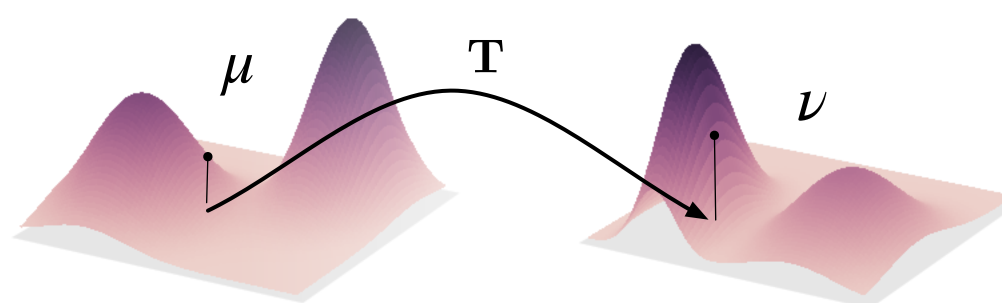


Tools which build upon this representation

Optimal Transport theory

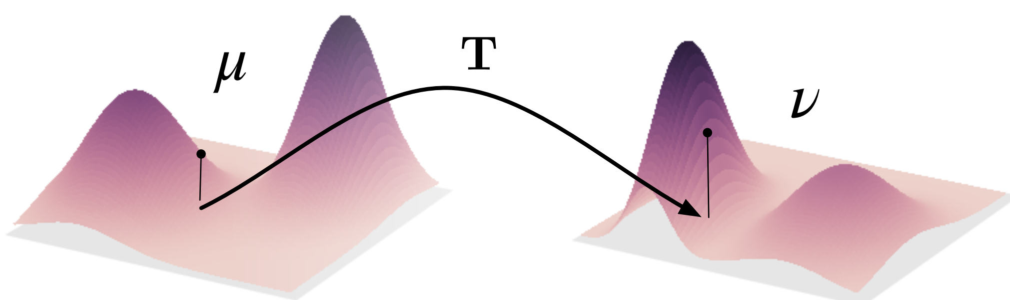


Use + Develop the Optimal transport theory in this challenging scenario

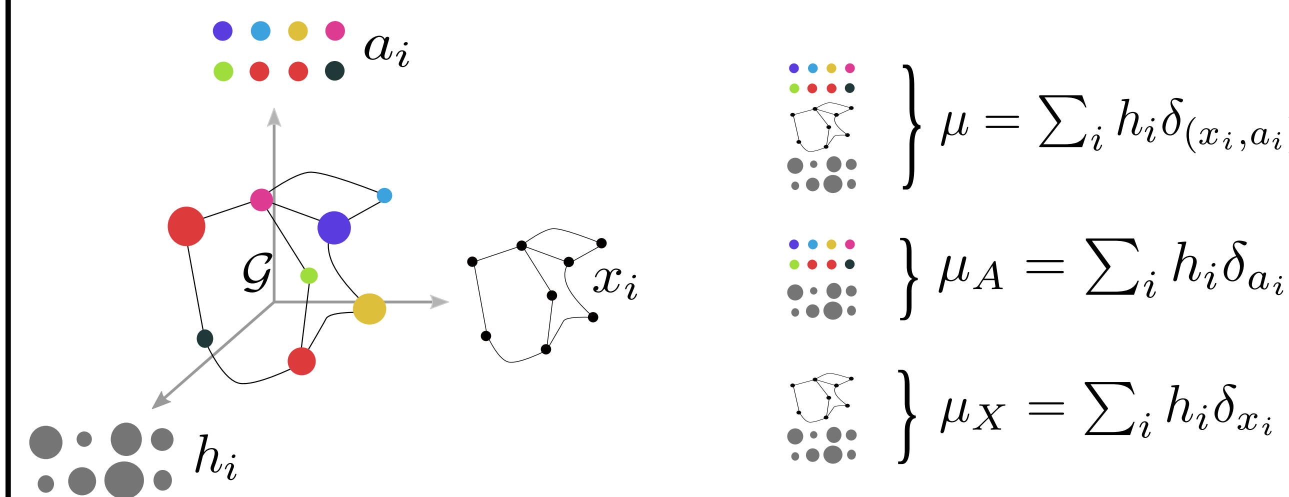
- **Applicability**
- **Mathematical foundations**

Overview of the talk

Part I: Optimal Transport « in short »

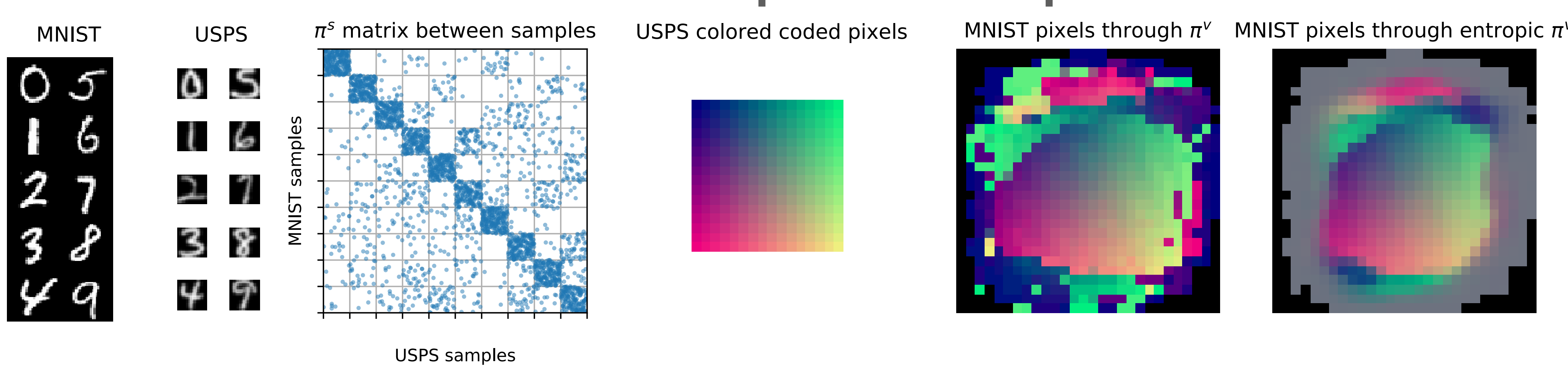


Part II: Optimal Transport for structured data



ICML' 2019

Part III: CO-Optimal Transport



NeurIPS' 2020

From linear Optimal Transport to Gromov-Wasserstein

From linear Optimal Transport…

What is it?

Input:

$$\mu \in \mathcal{P}(\mathcal{X}), \nu \in \mathcal{P}(\mathcal{Y})$$

Two probability distributions

From linear Optimal Transport…

What is it?

Input:

$$\color{red}{\mu} \in \mathcal{P}(\mathcal{X}), \color{blue}{\nu} \in \mathcal{P}(\mathcal{Y})$$

Two probability distributions

Output:

Geometric notion of distance between these distributions

Find correspondences/relations between the samples

From linear Optimal Transport…

Why do we care about probability distributions?

Measure and probability distributions are at the core of Machine learning

From linear Optimal Transport…

Why do we care about probability distributions?

Measure and probability distributions are at the core of Machine learning

A point of view on the data

Data: $(\mathbf{x}_i)_{i \in [\![n]\!]}$; $\mathbf{x}_i \in \mathbb{R}^d$ ⟶ A probability distribution describing the data

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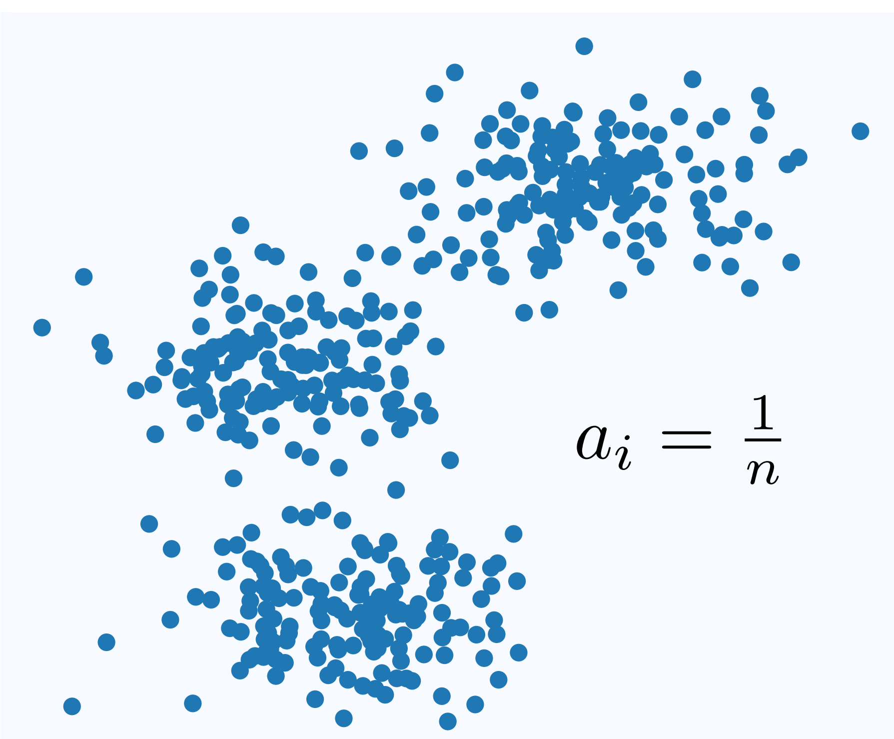
Lagrangian: $\sum_{i=1}^n a_i \delta_{x_i}$



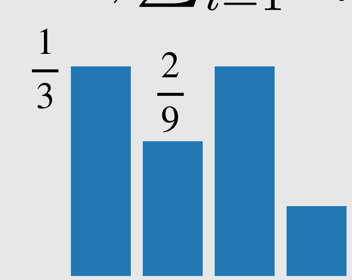
(point clouds)

$\delta_{\mathbf{x}_i}(\mathbf{x}) = 1$ if $\mathbf{x} = \mathbf{x}_i$ else 0

Probability simplex

$\mathbf{a} = (a_i)_{i \in [\![n]\!]} \in \Sigma_n$

$a_i \geq 0, \sum_{i=1}^n a_i = 1$



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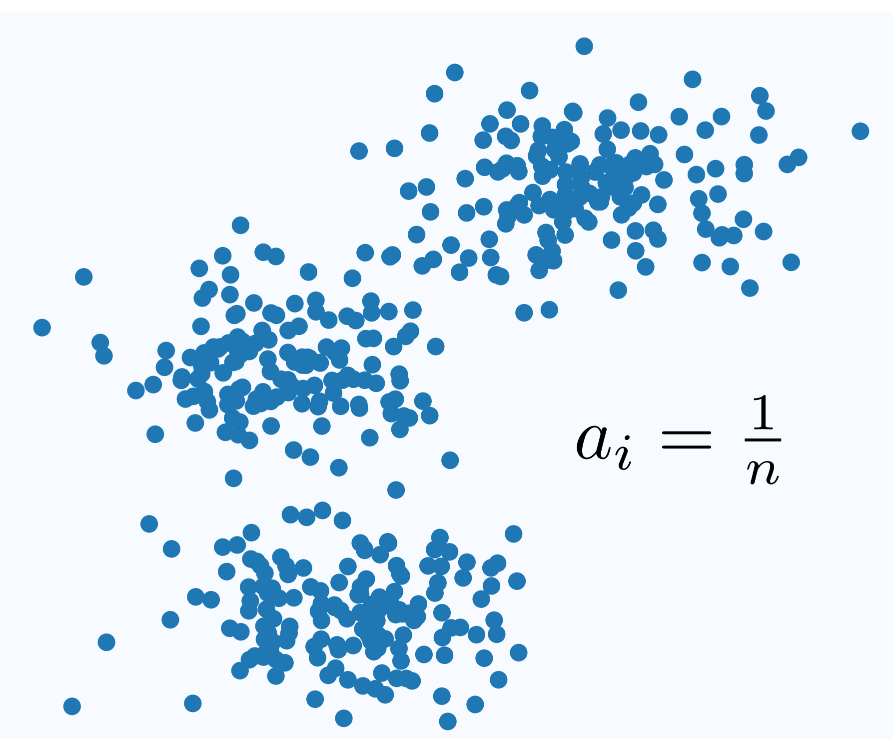
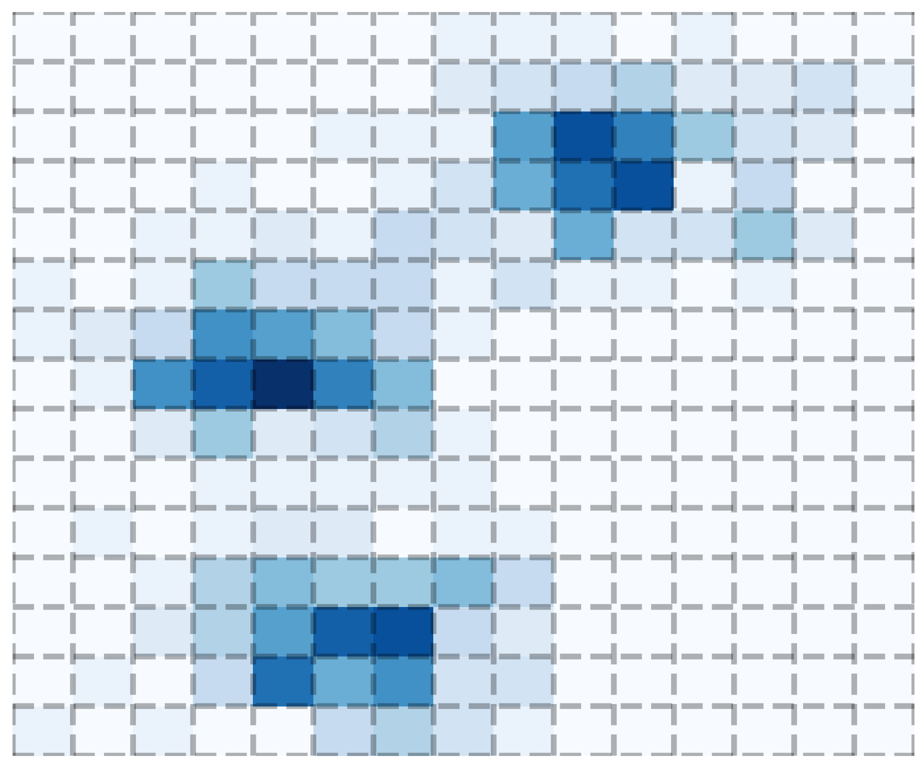


(point clouds)

$\delta_{\mathbf{x}_i}(\mathbf{x}) = 1 \text{ if } \mathbf{x} = \mathbf{x}_i \text{ else } 0$

Eulerian: $\sum_{i=1}^{N} a_i \delta_{\hat{x}_i}$



(histograms)

$\hat{x}_i$ fixed position (grid)

Probability simplex

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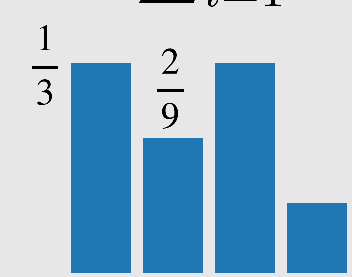

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Data: $(\mathbf{x}_i)_{i \in [\![n]\!]}$; $\mathbf{x}_i \in \mathbb{R}^d$ $\longrightarrow$ A probability distribution describing the data

A formalism for many machine learning paradigms

(ERM) $\min_f \mathbb{E}_{(x,y)\sim\mu} [L(f(x), y)]$ $\longrightarrow$ (follow the law given by the prob.) $\mu = \frac{1}{n} \sum_{i=1}^n \delta_{(\mathbf{x}_i, y_i)}$

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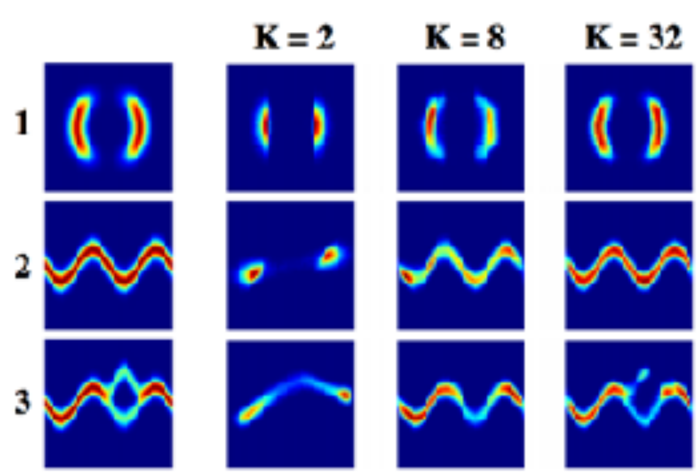
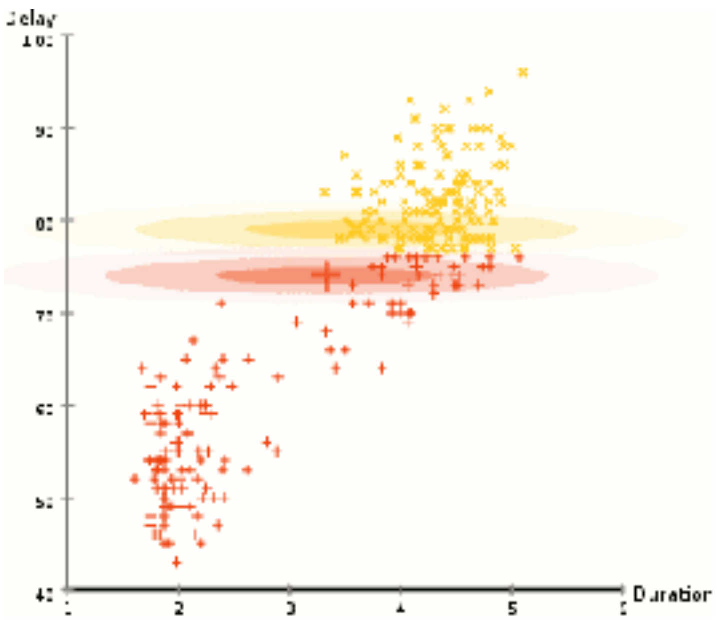


[Rezende 2016]



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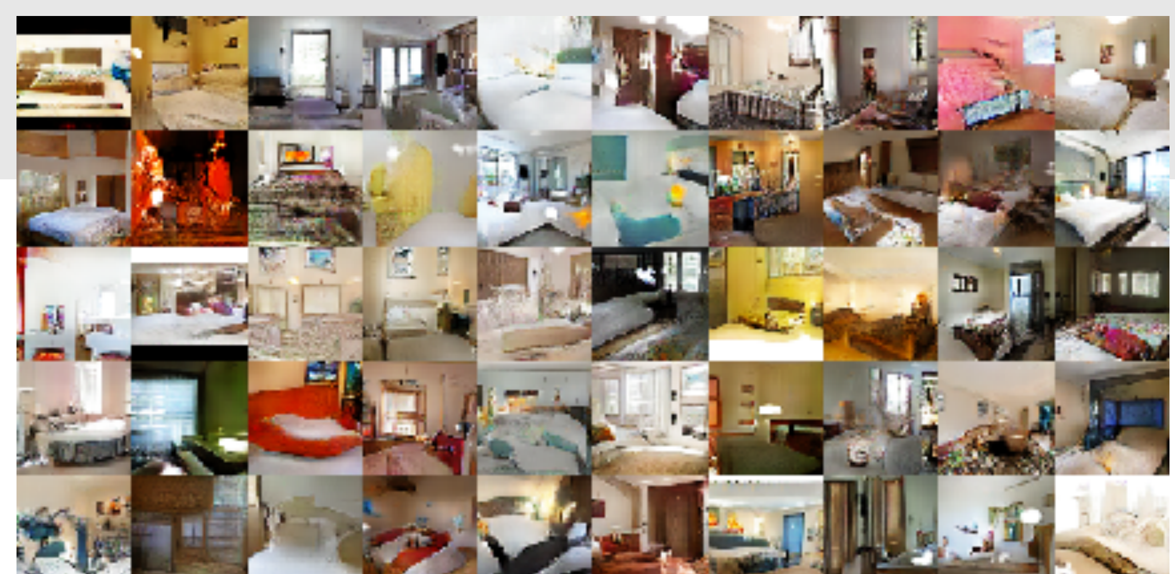
(GAN) $\min_{\boldsymbol{\theta}\in\Theta} D(\mu_{\boldsymbol{\theta}}, \nu)$



[Radford 2015]

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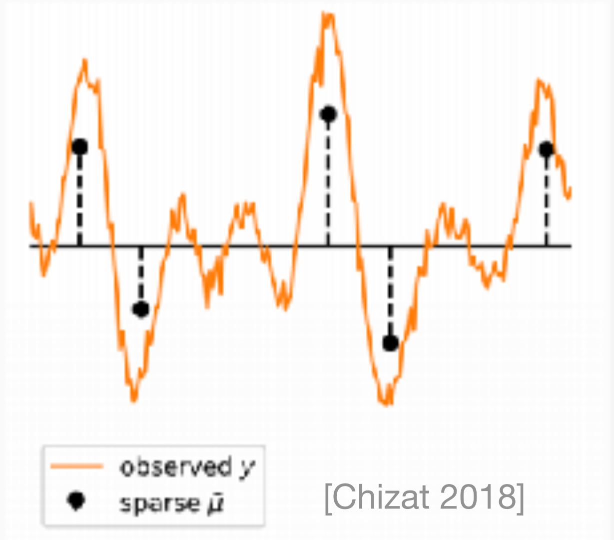
(GAN) $\min_{\boldsymbol{\theta}\in\Theta} D(\mu_{\boldsymbol{\theta}}, \nu)$

(Signal processing) Recover a sparse signal

$$\min_{\mu\in\mathcal{M}(\Theta)} \frac{1}{2}\|\mathbf{y} - \phi * \mu\|_{L^2}^2 + R(\mu) \qquad \overline{\mu} = \sum_i w_i \delta_{\boldsymbol{\theta}_i}$$



[Chizat 2018]

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(GAN) $\min_{\boldsymbol{\theta}\in\Theta} D(\mu_{\boldsymbol{\theta}}, \nu)$

(Signal processing) $\min_{\mu\in\mathcal{M}(\Theta)} \frac{1}{2}\|\mathbf{y} - \phi * \mu\|_{L^2}^2 + R(\mu)$

Advocates for finding an appropriate way of comparing probability distributions

From linear Optimal Transport…

Formulation


Two probability distributions

$\mu \in \mathcal{P}(\mathcal{X}), \nu \in \mathcal{P}(\mathcal{Y})$

A cost function

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

Optimal Transport

From linear Optimal Transport…

Kantorovitch Formulation

Two probability distributions

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Optimal Transport

All the mass of μ is **transported** to ν by a **transport plan** $\pi \in \mathcal{P}(\mathcal{X} \times \mathcal{Y})$

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Optimal Transport

All the mass of μ is **transported** to ν by a **transport plan** $\pi \in \mathcal{P}(\mathcal{X} \times \mathcal{Y})$

We want to find the plan that **minimizes the overall cost** of moving all the points

From linear Optimal Transport…

Kantorovitch Formulation: an example

Two probability distributions

$$\mu = \sum_{i=1}^{n} a_i \delta_{x_i} \qquad \nu = \sum_{j=1}^{m} b_j \delta_{y_j}$$

A cost function

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

Bakeries = quantity of breads

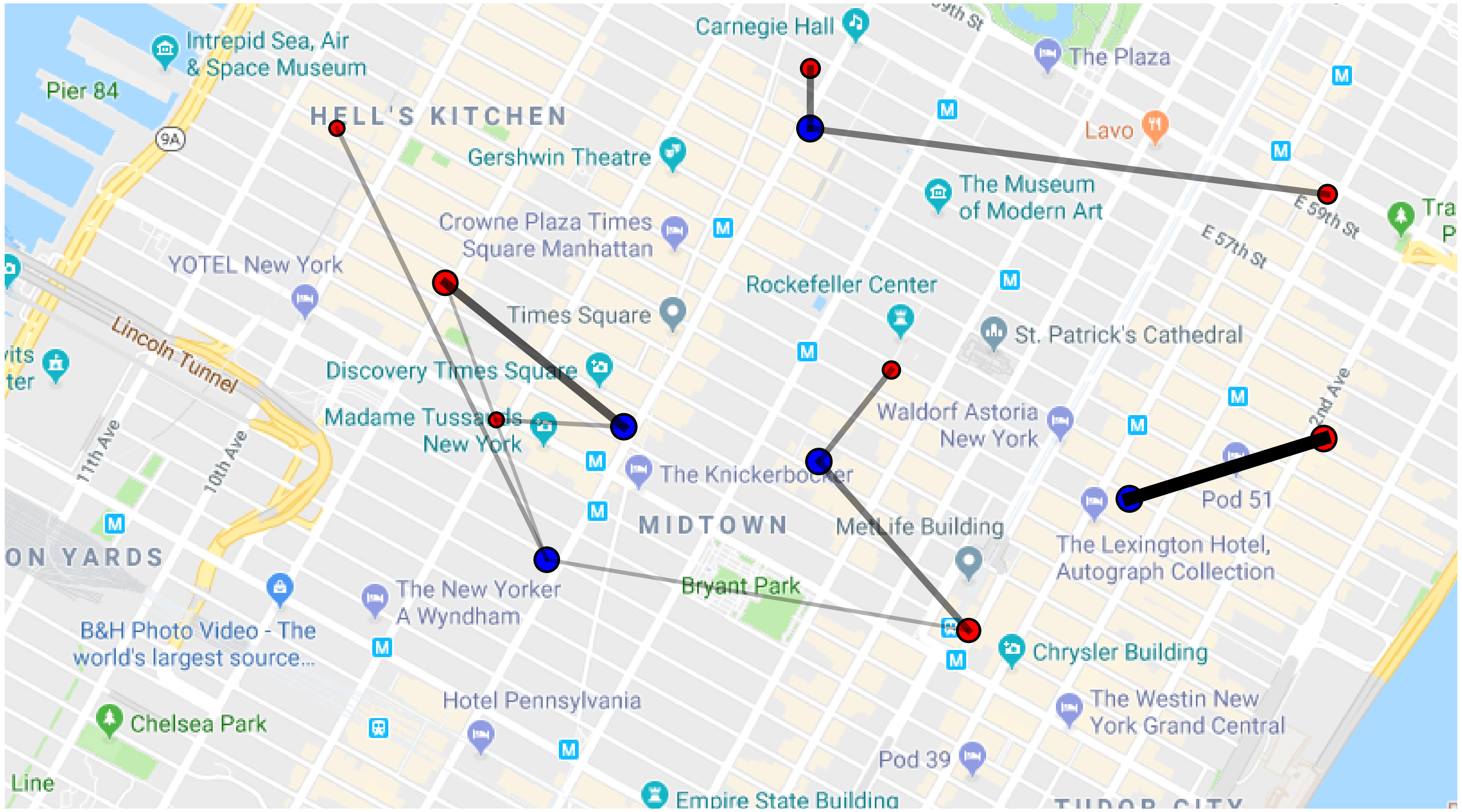
loc: x_i quantity: a_i

Cafés = demand of breads

loc: y_j demand: b_j

Distance between bakeries and cafés

$$c(x_i, y_j)$$



We want to route all the breads from bakeries to cafés the cheapest way

From linear Optimal Transport…

Kantorovitch Formulation: an example

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A cost function

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

Kantorovitch formulation

$$\min_{\boldsymbol{\pi} \in \Pi(\mathbf{a}, \mathbf{b})} \sum_{i,j=1}^{m,n} c(x_i, y_j) \pi_{ij}$$

From linear Optimal Transport…

Kantorovich Formulation: an example

Two probability distributions

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A cost function

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

Kantorovich formulation

$$\min_{\boldsymbol{\pi} \in \Pi(\mathbf{a}, \mathbf{b})} \sum_{i,j=1}^{m,n} c(x_i, y_j) \pi_{ij}$$

Set of couplings/ transport plans

$$\Pi(\mathbf{a}, \mathbf{b})$$

From linear Optimal Transport…

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A cost function

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

Kantorovitch formulation

$$\min_{\boldsymbol{\pi} \in \Pi(\mathbf{a}, \mathbf{b})} \sum_{i,j=1}^{m,n} c(x_i, y_j) \pi_{ij}$$

How much is shifted from x_i to y_j

From linear Optimal Transport…

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

A cost function

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

Kantorovitch formulation

$$\min_{\boldsymbol{\pi} \in \Pi(\mathbf{a}, \mathbf{b})} \sum_{i,j=1}^{m,n} c(x_i, y_j) \pi_{ij}$$

Cost of moving masses from x_i to y_j

From linear Optimal Transport…

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Total cost

From linear Optimal Transport…

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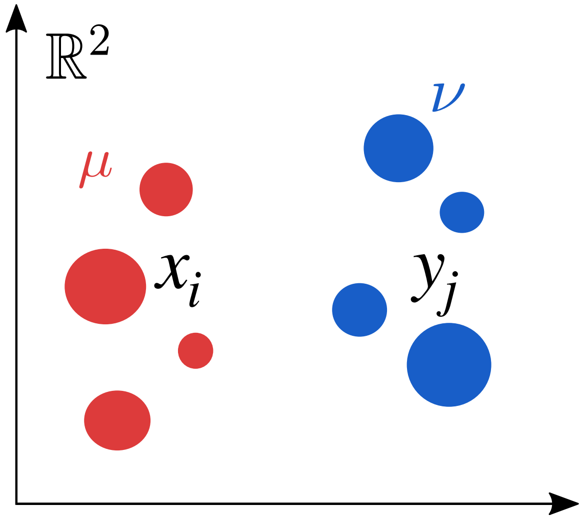
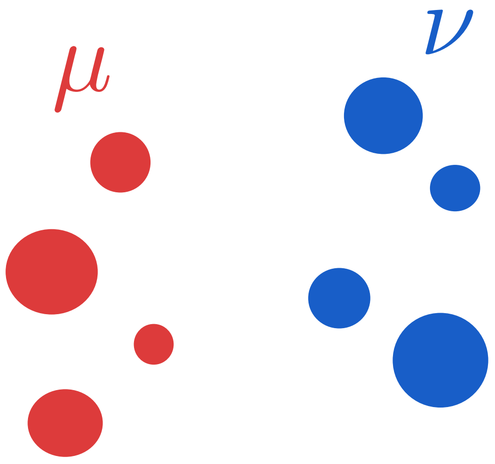


$$\Pi(\mathbf{a},\mathbf{b}) = \{\boldsymbol{\pi} \in \mathbb{R}_+^{n\times m} \mid \forall (i,j), \sum_{j=1}^{m} \pi_{ij} = a_i, \ \sum_{i=1}^{n} \pi_{ij} = b_j\}$$



From linear Optimal Transport…

Kantorovitch Formulation: an example

Two probability distributions

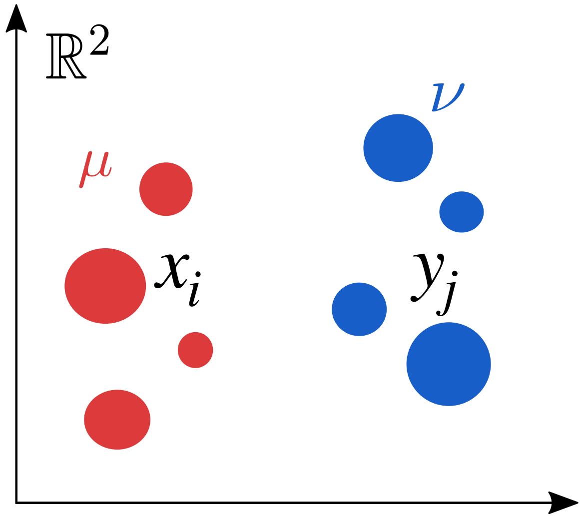
$\mu = \sum_{i=1}^{n} a_i \delta_{x_i} \qquad \nu = \sum_{j=1}^{m} b_j \delta_{y_j}$

A cost function

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

Kantorovitch formulation

$$\min_{\boldsymbol{\pi} \in \Pi(\mathbf{a}, \mathbf{b})} \sum_{i,j=1}^{m,n} c(x_i, y_j) \pi_{ij}$$



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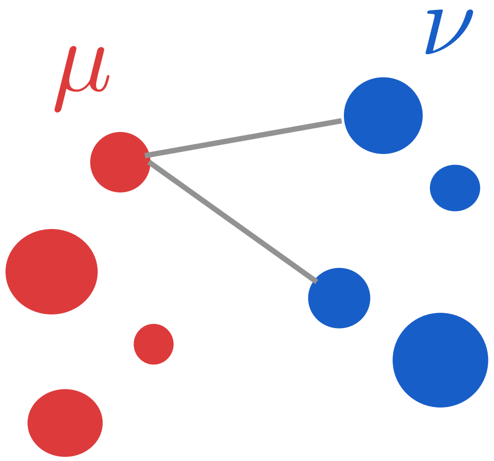

From linear Optimal Transport…

Kantorovich Formulation: an example

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Kantorovich formulation

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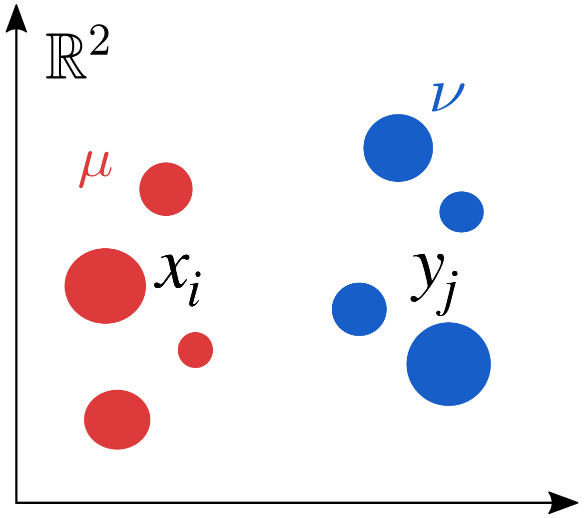

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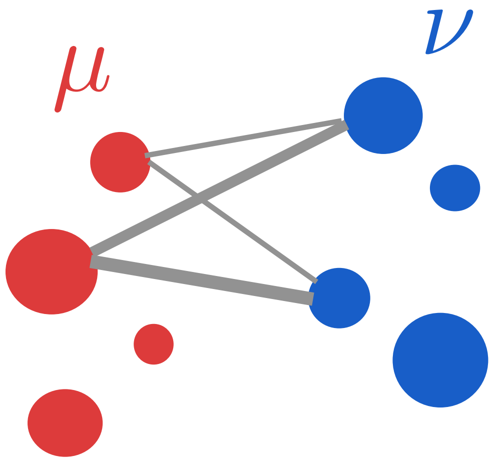

From linear Optimal Transport…

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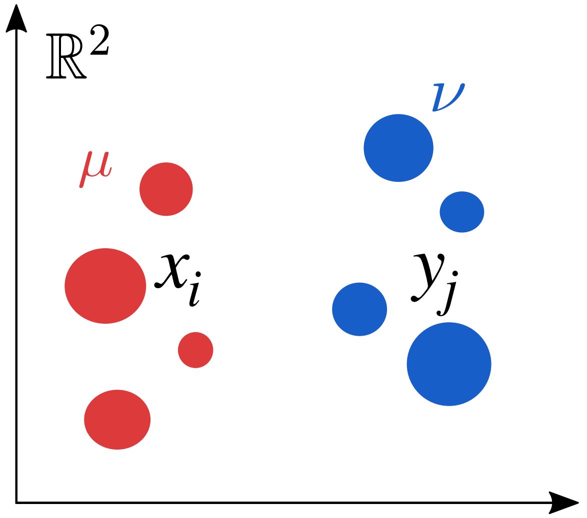

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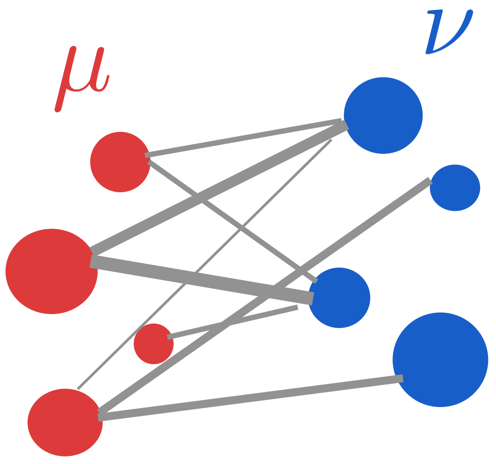

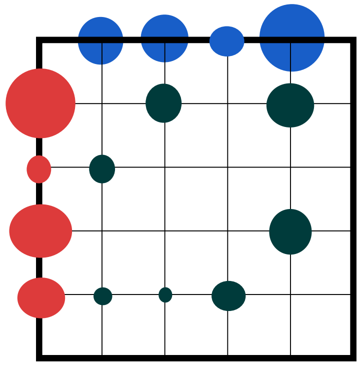

$\pi \in \mathbb{R}_+^{n\times m}$

From linear Optimal Transport…

Kantorovitch Formulation: general case

Two probability distributions

$\mu \in \mathcal{P}(\mathcal{X}), \nu \in \mathcal{P}(\mathcal{Y})$

A cost function

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

Kantorovitch formulation

$$\mathcal{T}_c(\mu, \nu) = \inf_{\pi \in \Pi(\mu, \nu)} \int_{\mathcal{X} \times \mathcal{Y}} c(x, y) \mathrm{d}\pi(x, y)$$

From linear Optimal Transport...

Wasserstein distance

Two probability distributions

$\mu \in \mathcal{P}(\Omega), \nu \in \mathcal{P}(\Omega)$

A distance

$d : \Omega \times \Omega \to \mathbb{R}_+$

Example: $\Omega = \mathbb{R}^d$

Wasserstein distance

$$W_p^p(\mu, \nu) = \inf_{\pi \in \Pi(\mu, \nu)} \int_{\Omega \times \Omega} d^p(x, y) \mathrm{d}\pi(x, y)$$

$\mathcal{P}(\Omega)$ is a metric space

$W_p(\mu, \nu) = 0 \iff \mu = \nu$

From linear Optimal Transport…

Wasserstein distance

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$\mathcal{P}(\Omega)$ is a metric space

$W_p(\mu, \nu) = 0 \iff \mu = \nu$

Powerful tool for comparing probability distributions on the same space

...to Gromov-Wasserstein

What if ?

Data are in Incomparable spaces

Two probability distributions

$$\mu \in \mathcal{P}(\mathcal{X}), \nu \in \mathcal{P}(\mathcal{Y}) \text{ with } \mathcal{X}, \mathcal{Y} \nsubseteq \Omega$$

A cost function ?????

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

⇨ Not straightforward to find a suitable cost (e.g. no distance available)

...to Gromov-Wasserstein

What if ?

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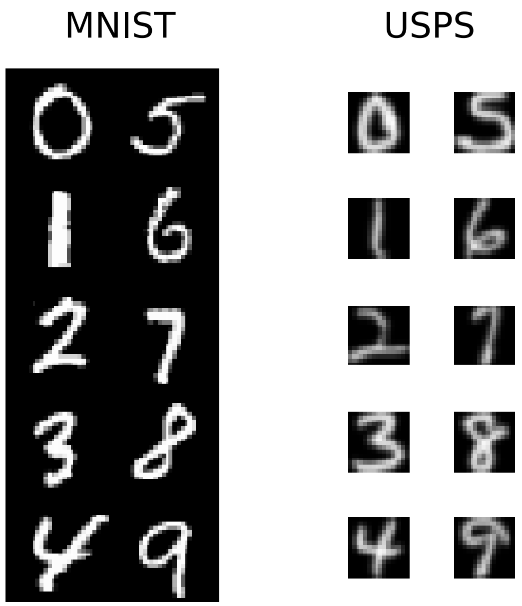
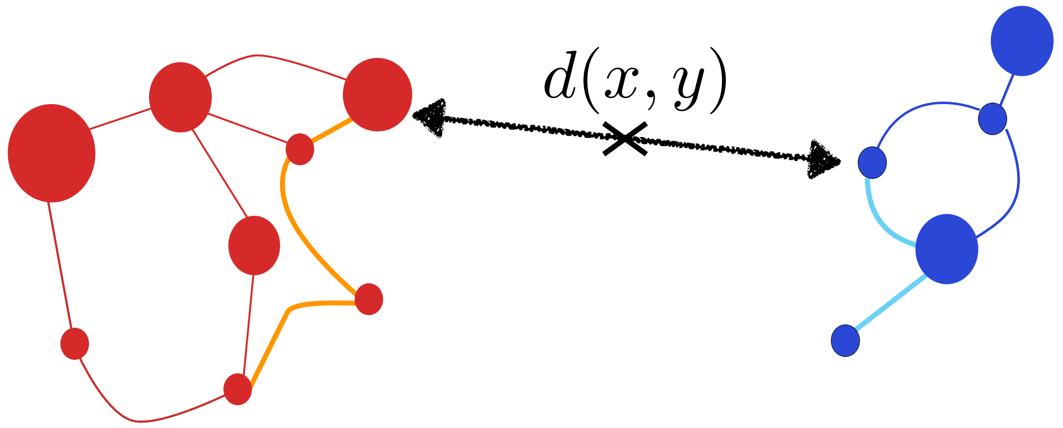
Different Euclidean spaces



Example: $\mathcal{X} = \mathbb{R}^{28*28}, \mathcal{Y} = \mathbb{R}^{16*16}$

Samples = nodes of different graphs



Example: $\mathcal{X} = \text{Graph 1}, \mathcal{Y} = \text{Graph 2}$

...to Gromov-Wasserstein

Gromov-Wasserstein distance

Two probability distributions

$$\mu \in \mathcal{P}(\mathcal{X}), \nu \in \mathcal{P}(\mathcal{Y})$$

Two « intra-domain » costs

$$c_{\mathcal{X}} : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$$
$$c_{\mathcal{Y}} : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$$

Gromov-Wasserstein distance

$$GW_p^p(c_{\mathcal{X}}, c_{\mathcal{Y}}, \mu, \nu) = \inf_{\pi \in \Pi(\mu,\nu)} \int_{\mathcal{X}\times\mathcal{Y}} \int_{\mathcal{X}\times\mathcal{Y}} \left| c_{\mathcal{X}}(x,x') - c_{\mathcal{Y}}(y,y') \right|^p \mathrm{d}\pi(x,y)\mathrm{d}\pi(x',y')$$

...to Gromov-Wasserstein

Gromov-Wasserstein distance

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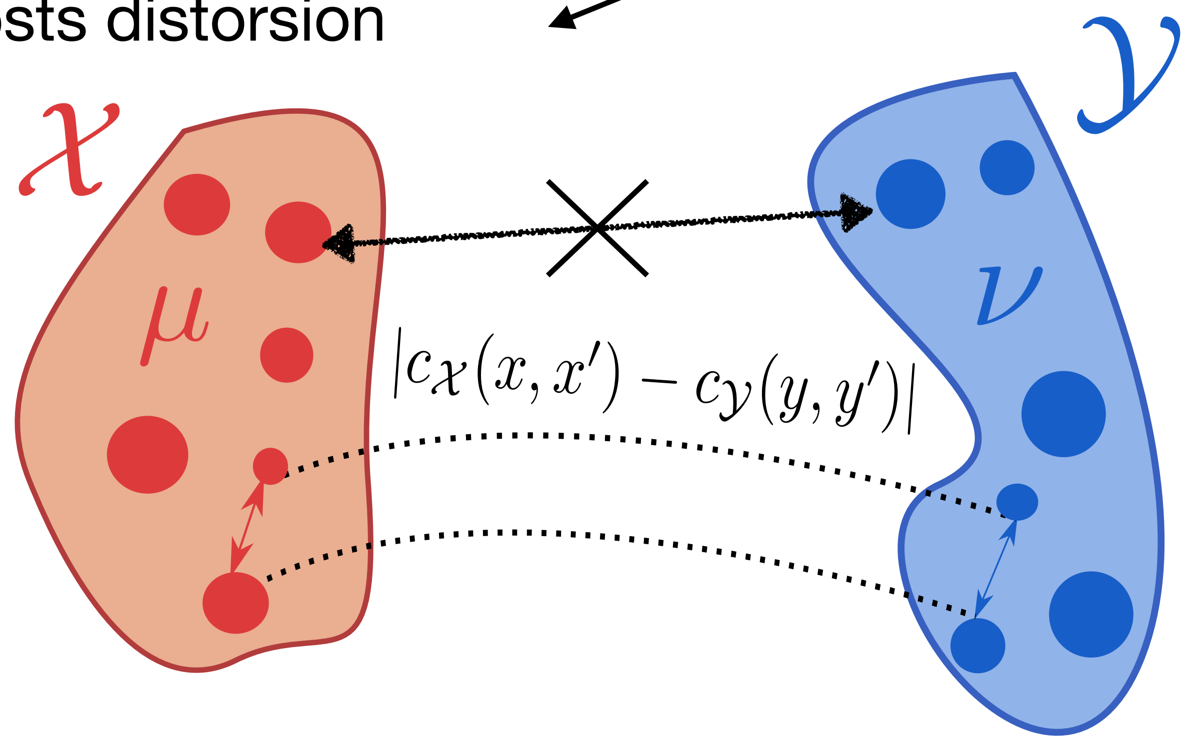
Measure the costs distortion



...to Gromov-Wasserstein

Gromov-Wasserstein distance

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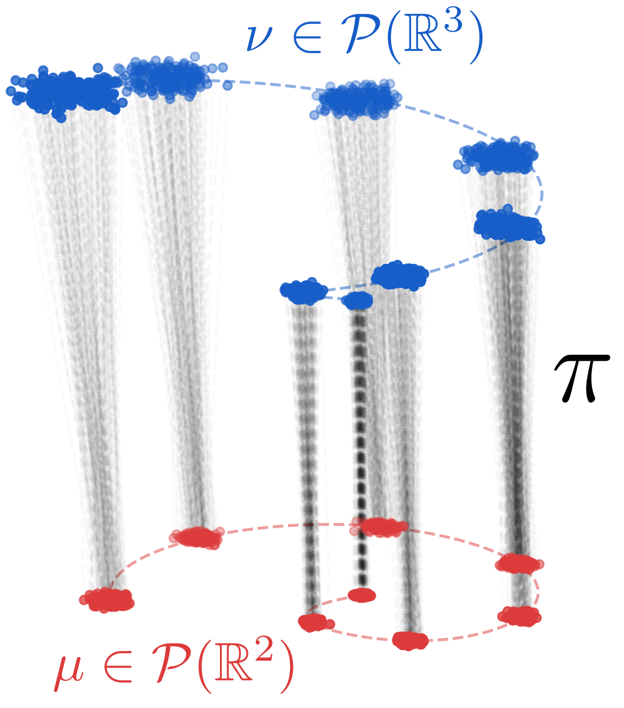
The transportation problem is not linear anymore but **quadratic**

Associate pair of points with similar costs in each space



...to Gromov-Wasserstein

Gromov-Wasserstein distance

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A distance w.r.t isomorphism

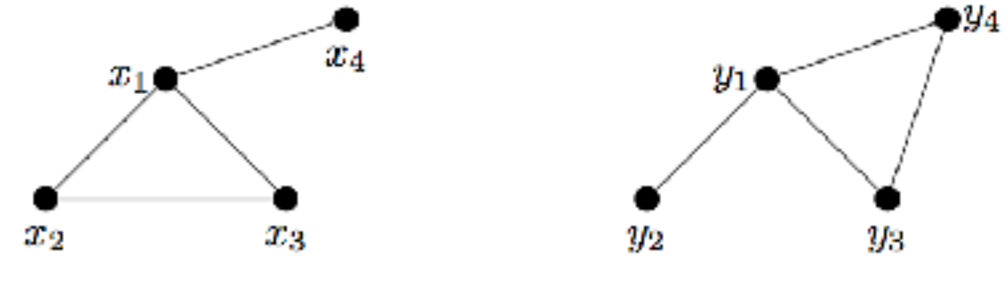
GW is a distance on the "space of all spaces":

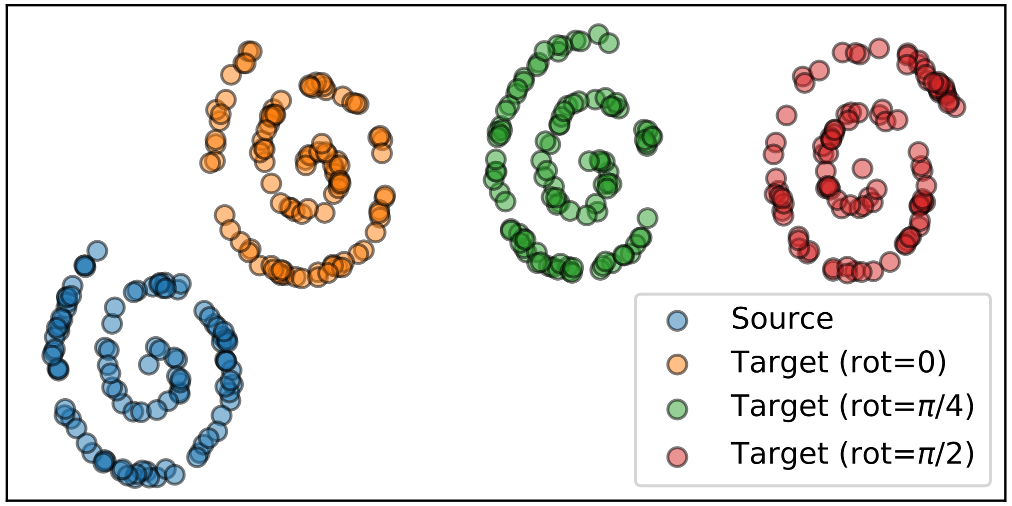
$$\mathbb{X} = \{(\mathcal{X}, d_{\mathcal{X}}, \mu \in \mathcal{P}(\mathcal{X})); d_{\mathcal{X}} \text{ metric } \} \text{ (mm-spaces)}$$

- $GW_p(d_{\mathcal{X}}, d_{\mathcal{Y}}, \mu, \nu) = 0$ iff $\exists \phi : \mathcal{X} \to \mathcal{Y}$

  ϕ is a isometry $d_{\mathcal{X}}(x,x') = d_{\mathcal{Y}}(\phi(x), \phi(x'))$

Isometry: permutations, rotations, translations,...





...to Gromov-Wasserstein

Gromov-Wasserstein distance

Gromov-Wasserstein distance

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  ϕ is measure-preserving: $\phi\#\mu = \nu$

Push-forward $\phi\#\mu$

$$\mu = \sum_{i=1}^n a_i \delta_{x_i} \underset{\phi\#\mu}{\rightarrow} \sum_{i=1}^n a_i \delta_{\phi(x_i)}$$

…to Gromov-Wasserstein

Gromov-Wasserstein distance

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(Weights are compatible)

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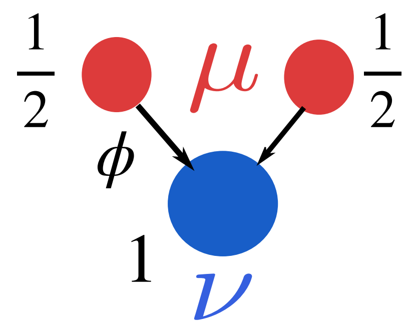
Compatible



$$\frac{1}{2} + \frac{1}{2} \rightarrow 1$$

...to Gromov-Wasserstein

Gromov-Wasserstein distance

Gromov-Wasserstein distance

$$GW_p^p(c_\mathcal{X}, c_\mathcal{Y}, \mu, \nu) = \inf_{\pi \in \Pi(\mu,\nu)} \int_{\mathcal{X}\times\mathcal{Y}} \int_{\mathcal{X}\times\mathcal{Y}} \left|c_\mathcal{X}(x,x') - c_\mathcal{Y}(y,y')\right|^p \mathrm{d}\pi(x,y)\mathrm{d}\pi(x',y'))$$

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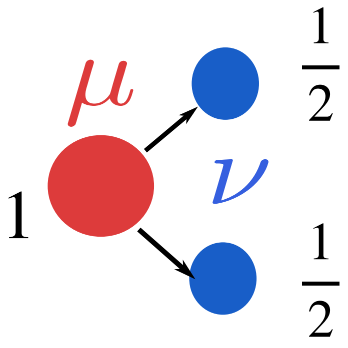
Not compatible



$$1 \nrightarrow (\frac{1}{2}, \frac{1}{2})$$

…to Gromov-Wasserstein

Gromov-Wasserstein distance

Gromov-Wasserstein = a bending invariant distance

- $GW_p(d_{\mathcal{X}}, d_{\mathcal{Y}}, \mu, \nu) = 0$ iff $\exists \phi : \mathcal{X} \to \mathcal{Y}$

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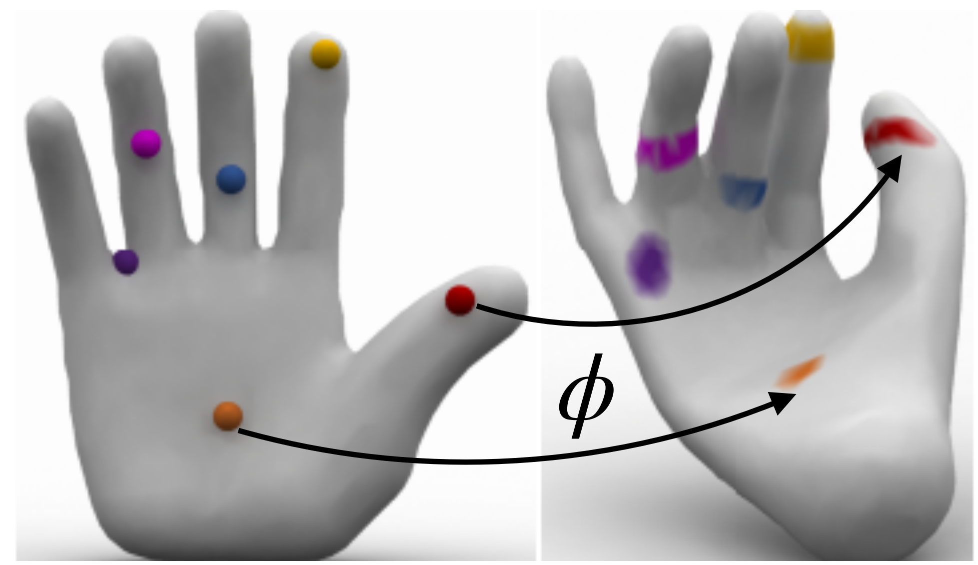


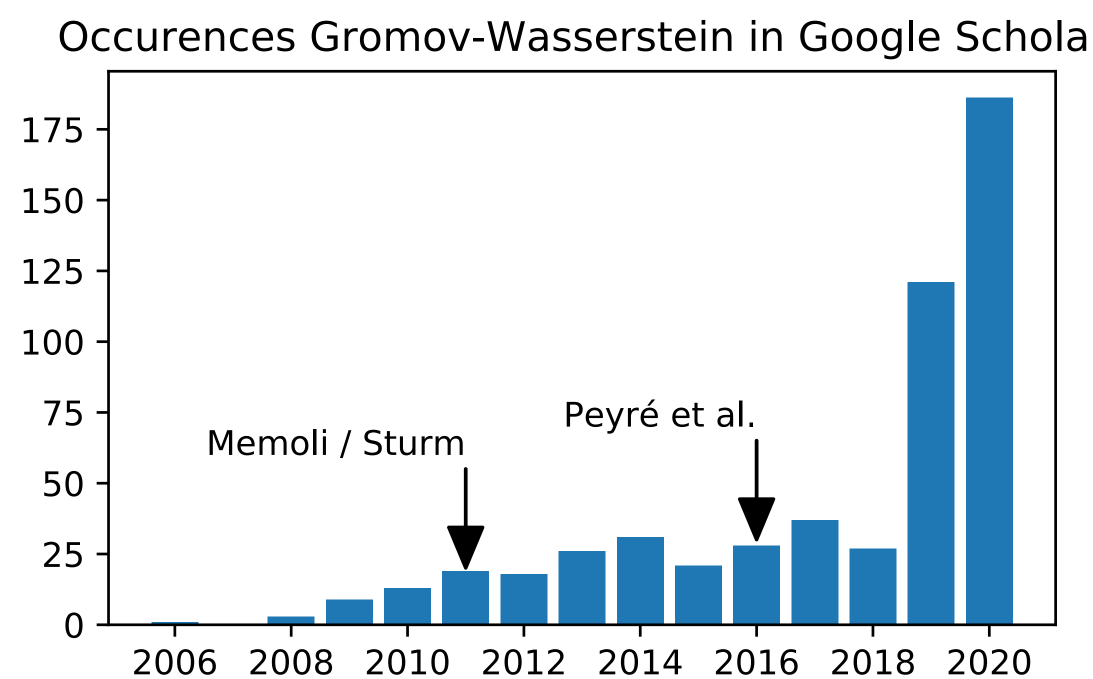
[Solomon 2016]

Applications for geometric data

Barycenter of relational data [Peyré 2016], Point clouds/meshes [Ezuz 2017]

Shape comparison [Mémoli 2011, Solomon 2016]

Graphs [Xu 2019, Fey 2020], biology [Demetci 2020], generative modeling [Bunne 2019]



Solving OT

Solving OT

A linear problem

Discrete probability measures

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

Linear Program:

$$\min_{\boldsymbol{\pi} \in \Pi(\mathbf{a},\mathbf{b})} \sum_{ij} c_{i,j} \pi_{i,j} = \min_{\boldsymbol{\pi} \in \Pi(\mathbf{a},\mathbf{b})} \langle \mathbf{C}, \boldsymbol{\pi} \rangle$$

Simplex, Network flow, Hungarian algorithms $\sim O(n^3 \log(n))$

Solving OT

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Simplex, Network flow, Hungarian algorithms $\sim O(n^3 \log(n))$

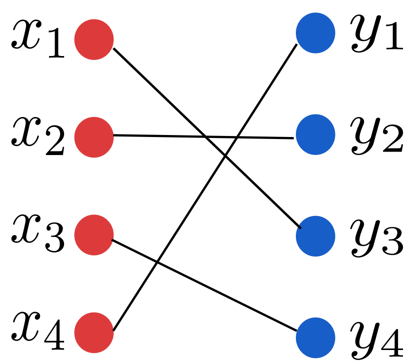
Uniform weights

$$\mathbf{a} = \mathbf{b} = \frac{\mathbf{1}_n}{n}$$

Monge Problem

$$\min_{\sigma \in S_n} \sum_{i=1}^{n} c_{i,\sigma(i)}$$

One-to-one



Solving OT

A linear problem

Discrete probability measures

$\color{red}{\mu} = \sum_{i=1}^{n} a_i \delta_{x_i}$ $\color{blue}{\nu} = \sum_{j=1}^{m} b_j \delta_{y_j}$

Linear Program:

$$\min_{\boldsymbol{\pi} \in \Pi(\color{red}{\mathbf{a}}, \color{blue}{\mathbf{b}})} \sum_{ij} c_{i,j} \pi_{i,j} = \min_{\boldsymbol{\pi} \in \Pi(\color{red}{\mathbf{a}}, \color{blue}{\mathbf{b}})} \langle \mathbf{C}, \boldsymbol{\pi} \rangle$$

Simplex, Network flow, Hungarian algorithms $\sim O(n^3 \log(n))$

Uniform weights

$$\color{red}{\mathbf{a}} = \color{blue}{\mathbf{b}} = \frac{\mathbf{1}_n}{n}$$

Monge Problem

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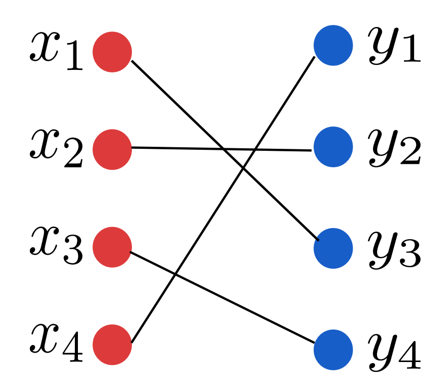


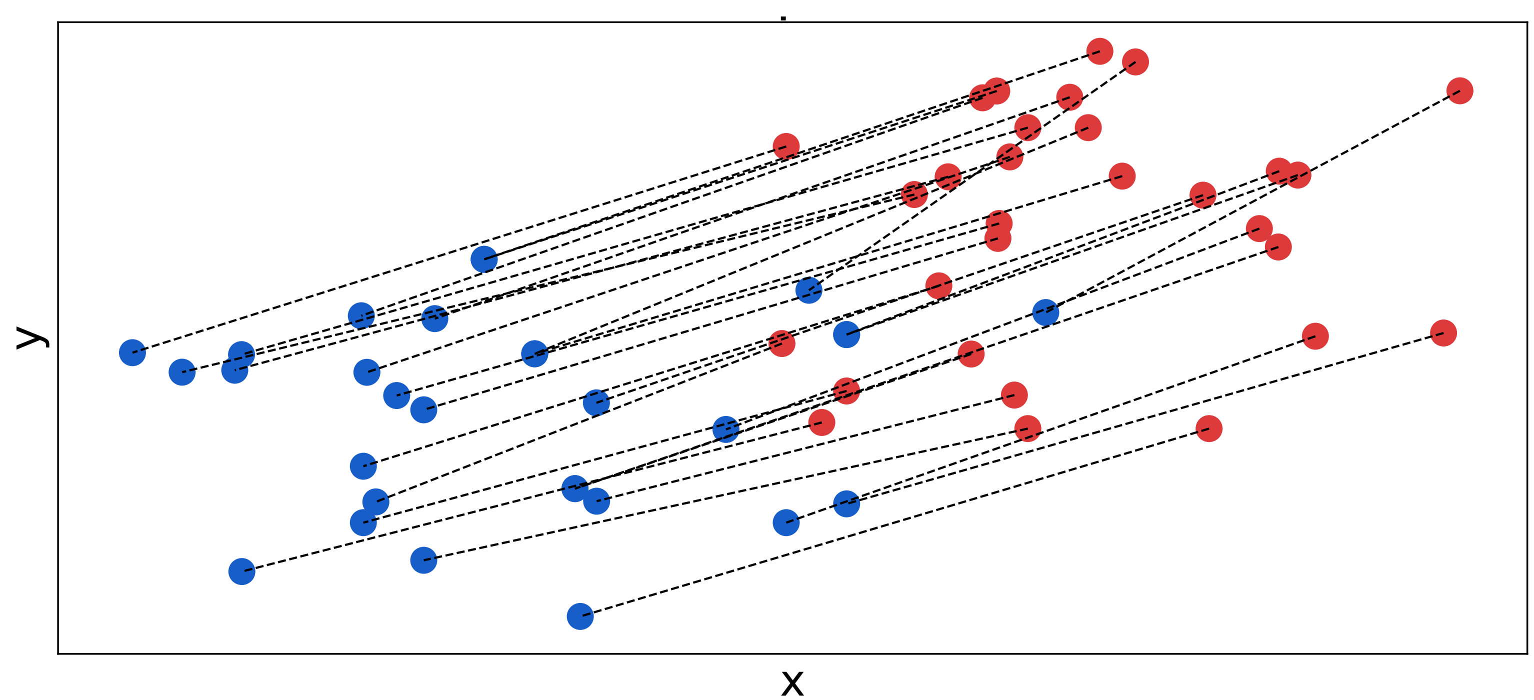
One-to-one

Fundamental theorem LP:

$$\boldsymbol{\pi}^* \leftrightarrow \sigma^* \in S_n$$

Optimal coupling is a permutation

Solves the Monge Problem

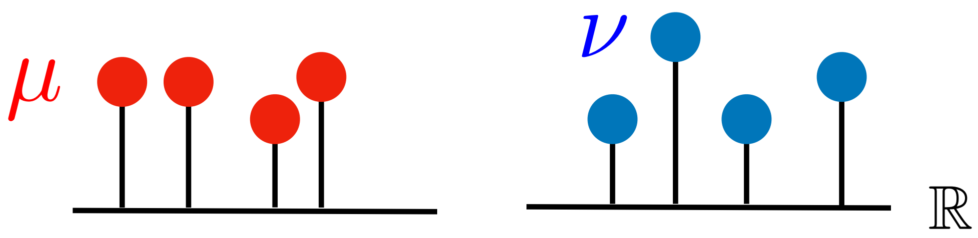


Solving OT

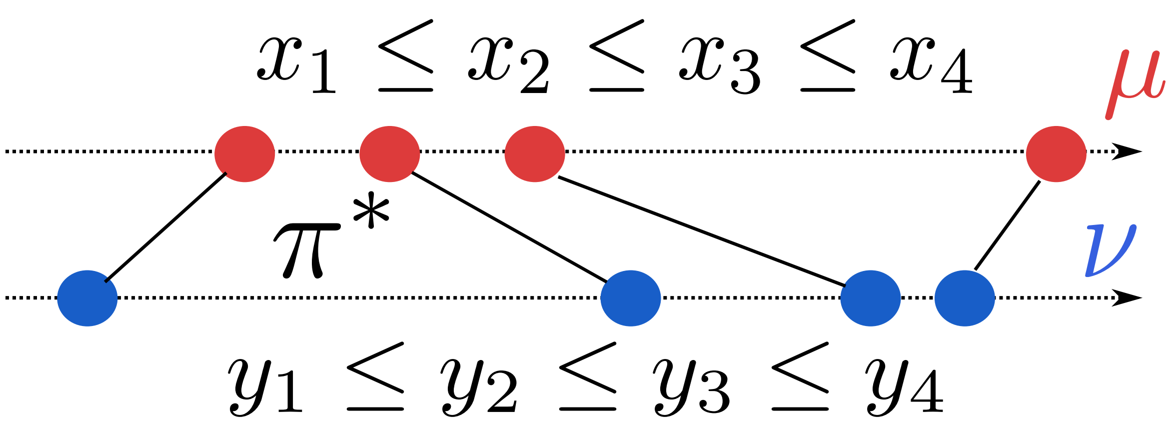
A real line problem

Two discrete probability distributions

$$\mu = \frac{1}{n}\sum_{i=1}^{n} \delta_{x_i}, \nu = \frac{1}{n}\sum_{j=1}^{n} \delta_{y_j}$$
$$x_i, y_j \in \mathbb{R}$$



In the case of Wasserstein can be solved by simple sorts $\sim O(n\log(n))$



$$\min_{\boldsymbol{\pi} \in \Pi(\frac{\mathbf{1}_n}{n}, \frac{\mathbf{1}_n}{n})} \sum_{ij} (x_i - y_j)^2 \pi_{i,j} = \min_{\sigma \in S_n} \sum_{ij} (x_i - y_{\sigma(i)})^2 \to Id$$

Solving OT

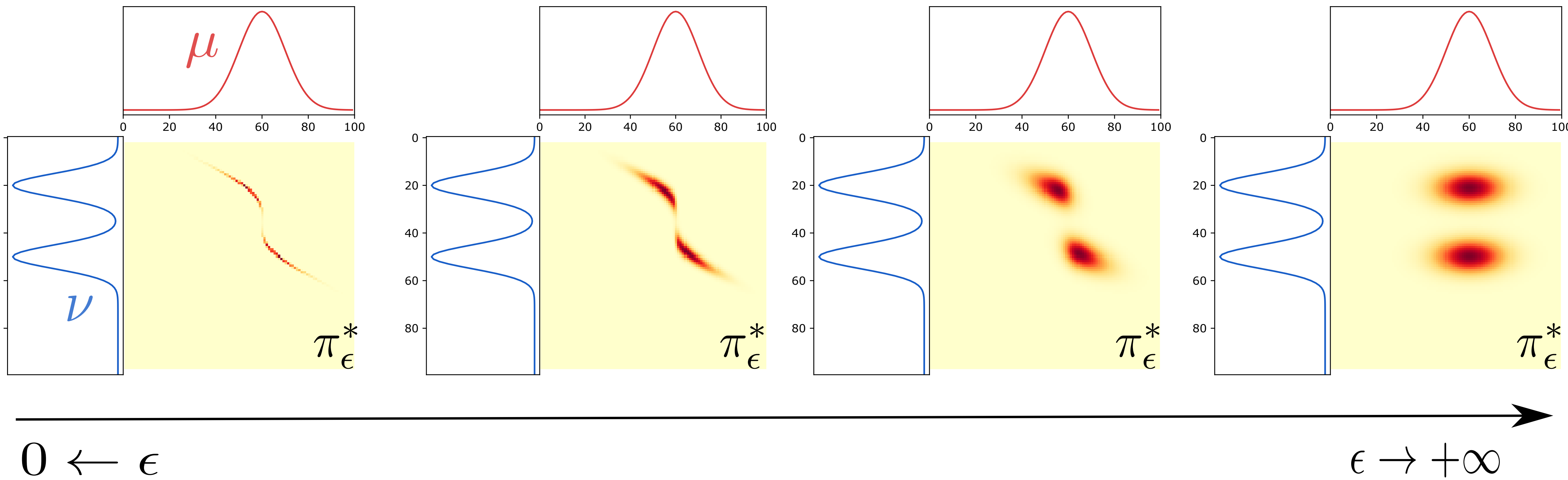
Entropic regularization

Discrete probability measures

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

Strongly convex problem: $$\min_{\boldsymbol{\pi} \in \Pi(\mathbf{a}, \mathbf{b})} \langle \mathbf{C}, \boldsymbol{\pi} \rangle - \varepsilon H(\boldsymbol{\pi})$$

- Entropy term $H(\boldsymbol{\pi}) = -\sum_{ij} (\log(\pi_{ij}) - 1)\pi_{ij}$
- Sinkhorn-Knopp algorithm: 1) fast 2) based on matrix multiplication
- τ approximate solution $\sim O(n^2 \log(n) \tau^{-3})$



Solving OT

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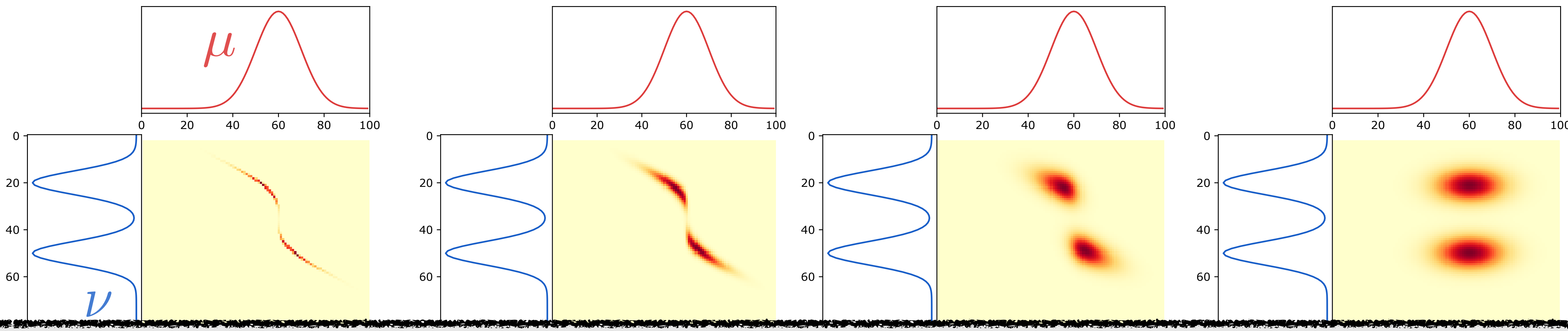


Linear OT: costly but solvable in practice

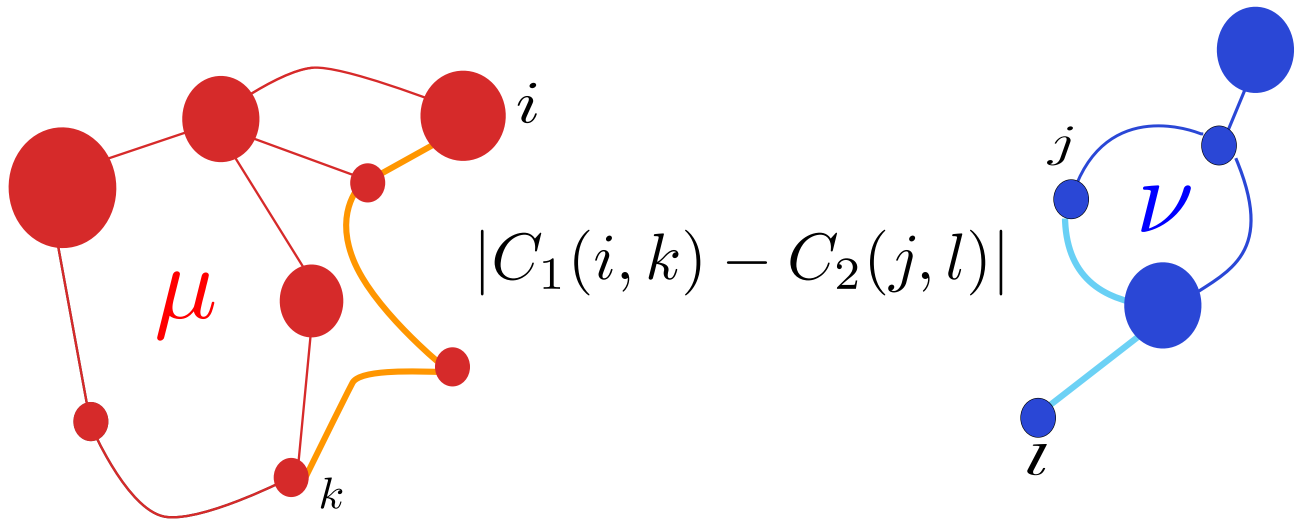
Solving OT

A quadratic problem (QP)

Discrete probability measures

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

$\mathcal{X}, \mathcal{Y} \not\subset \Omega$



$$\min_{\boldsymbol{\pi} \in \Pi(\mathbf{a},\mathbf{b})} \sum_{ijkl} |C_1(i,k) - C_2(j,l)|^p \pi_{ij} \pi_{kl}$$

Solving OT

A quadratic problem (QP)

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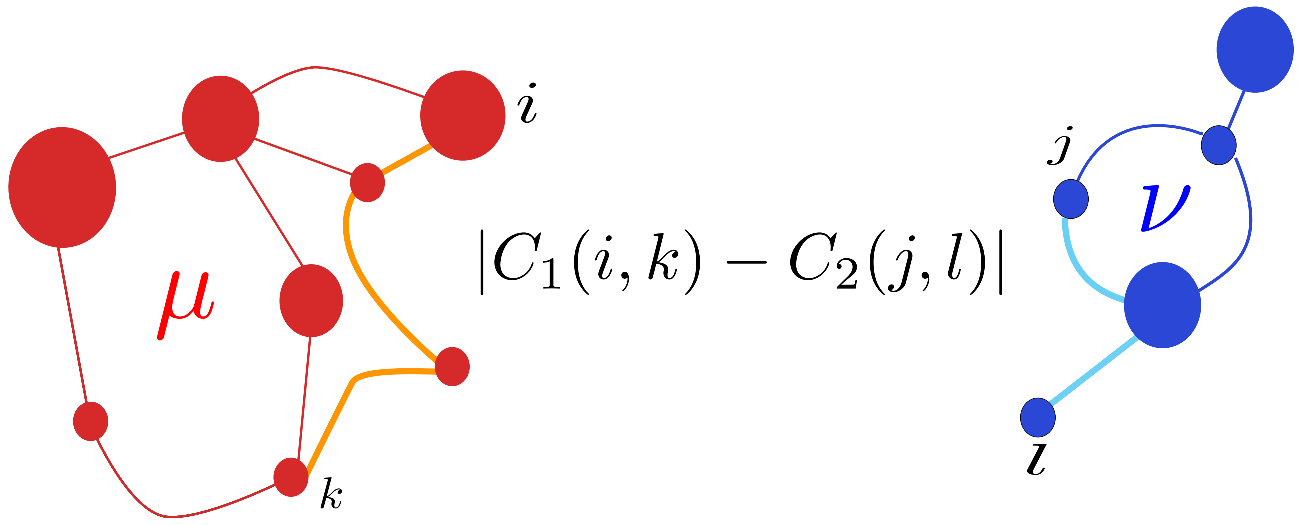

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Non convex QP: NP-hard in general (graph matching problem)

Solving OT

A quadratic problem (QP)

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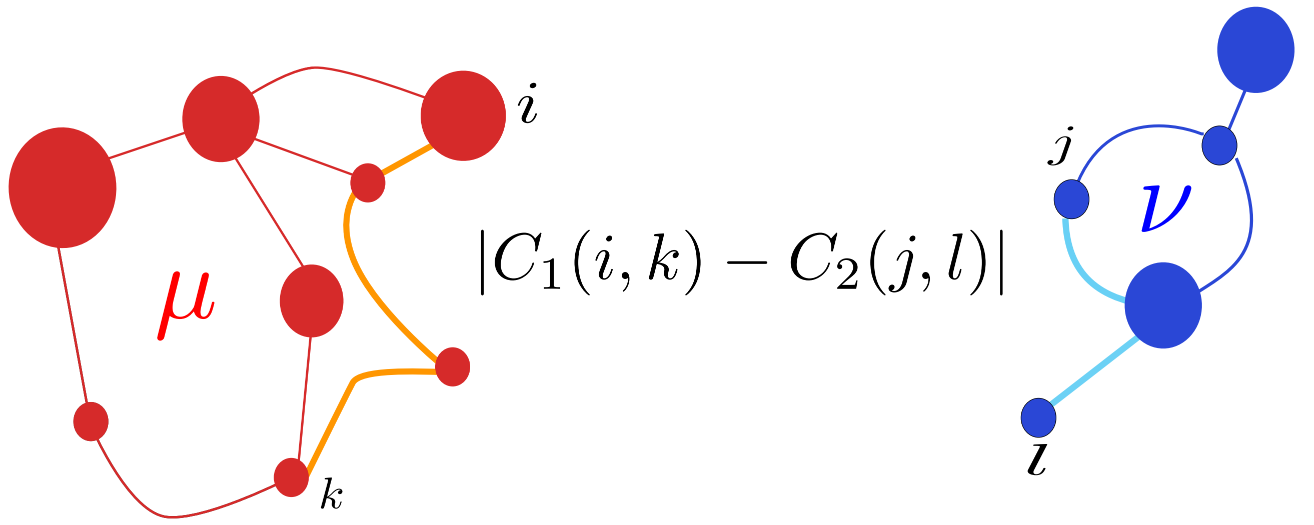

$$\min_{\boldsymbol{\pi} \in \Pi(\mathbf{a},\mathbf{b})} \sum_{ijkl} |C_1(i,k) - C_2(j,l)|^p \pi_{ij}\pi_{kl} - \varepsilon H(\boldsymbol{\pi})$$

- Non convex QP: NP-hard in general
- With entropic regularization [Peyré 2016, Solomon 2016]
- Can be solved using projected gradient descent under KL geometry
- Each gradient step: Sinkhorn algorithm

Solving OT

A quadratic problem (QP)

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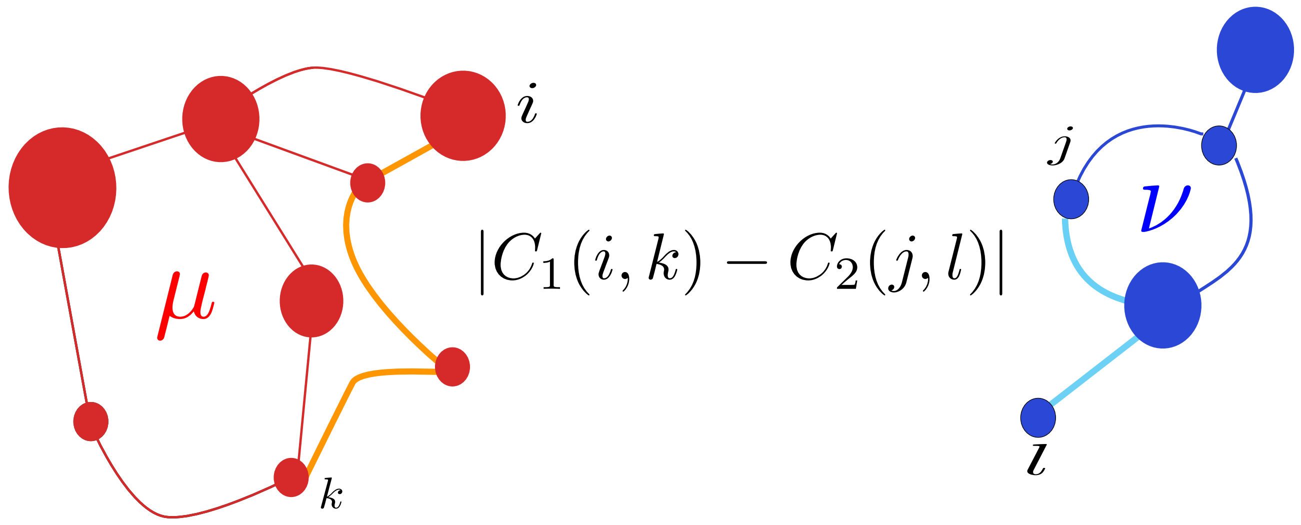

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Solving OT

A quadratic problem (QP)

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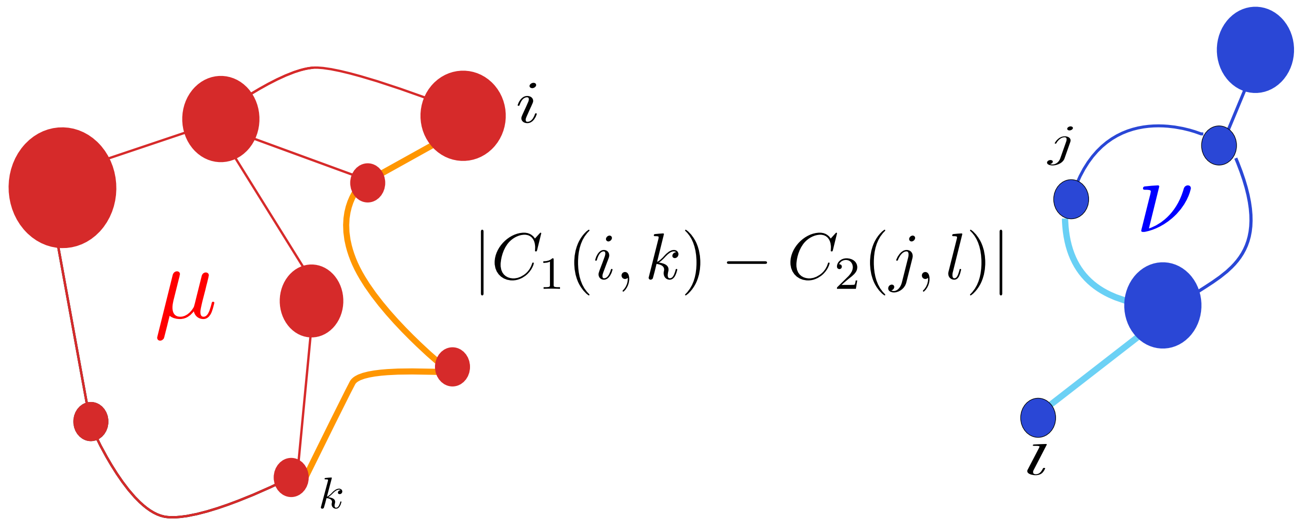

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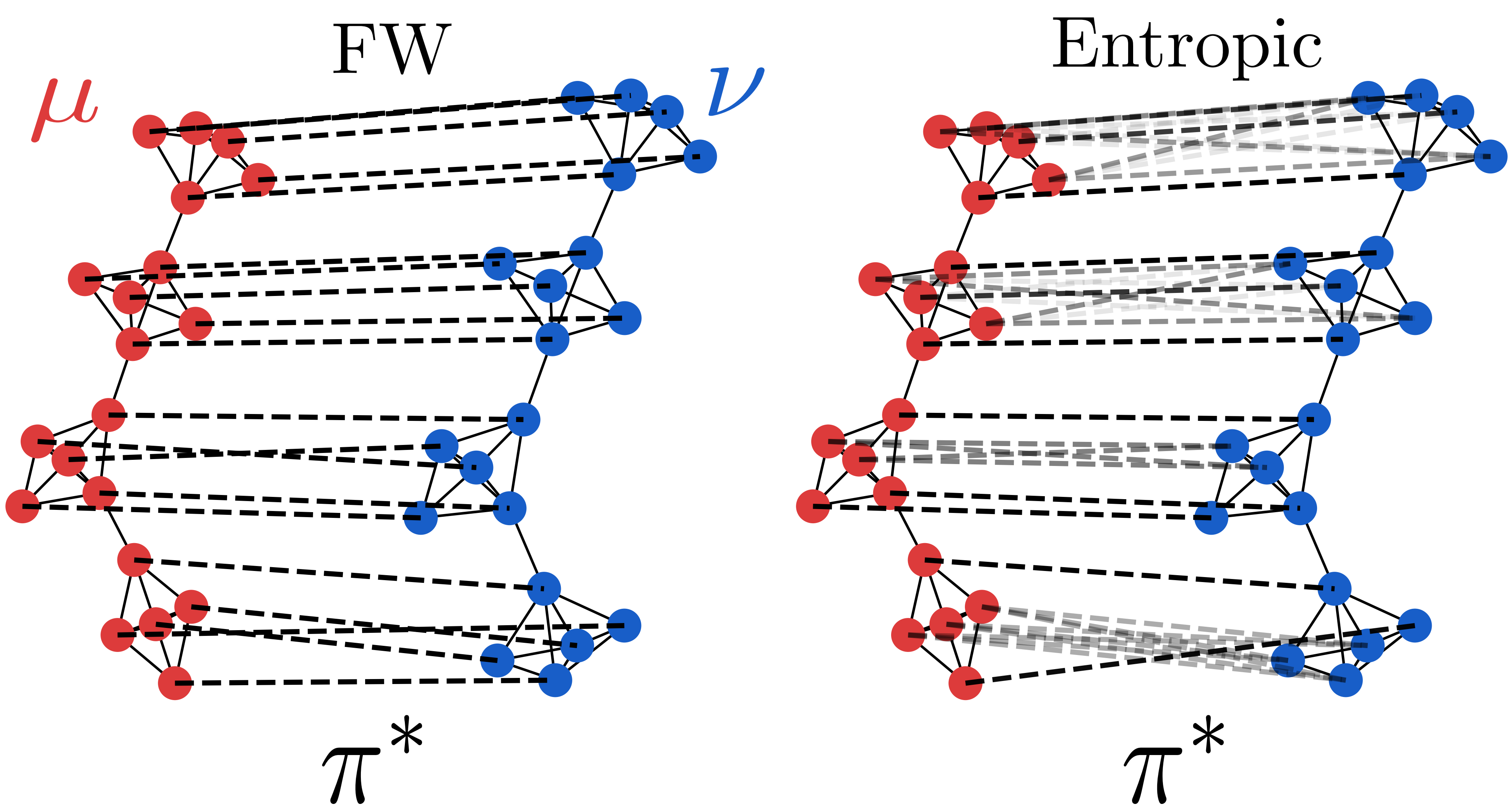
Hard to solve and even to approximate…

…to Gromov-Wasserstein

An example on graphs

> $\mathbf{C}_1, \mathbf{C}_2$ are the shortest path distance in each graph



From linear Optimal Transport…

What is it?

Input:

$$\mu \in \mathcal{P}(\mathcal{X}), \nu \in \mathcal{P}(\mathcal{Y})$$

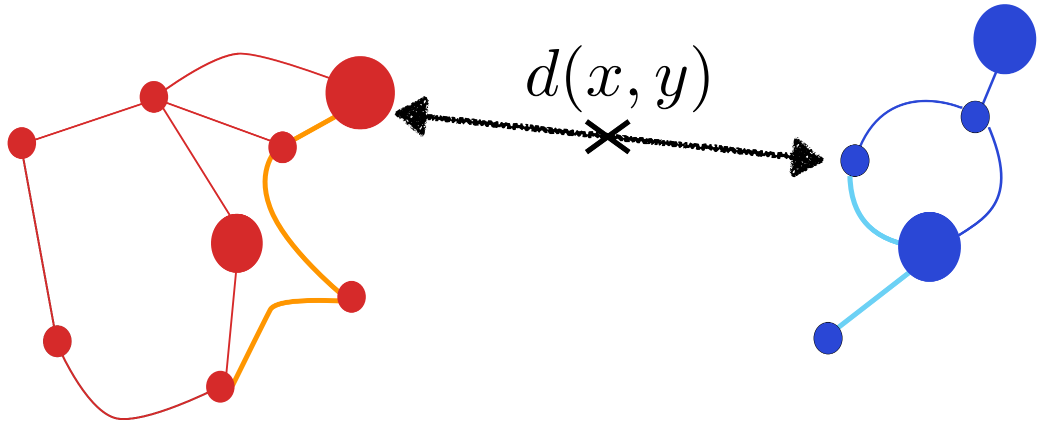
Two probability distributions

Output:

Geometric notion of distance between these distributions

Find correspondences/relations between the samples

Optimal transport for structured data



Optimal Transport for structured data

Motivations

Motivation: Is the Optimal transport framework suited for structured data ?

Problem 1: How do we model structured data ?

As probability distributions!

Problem 2: How do we compare structured data ?

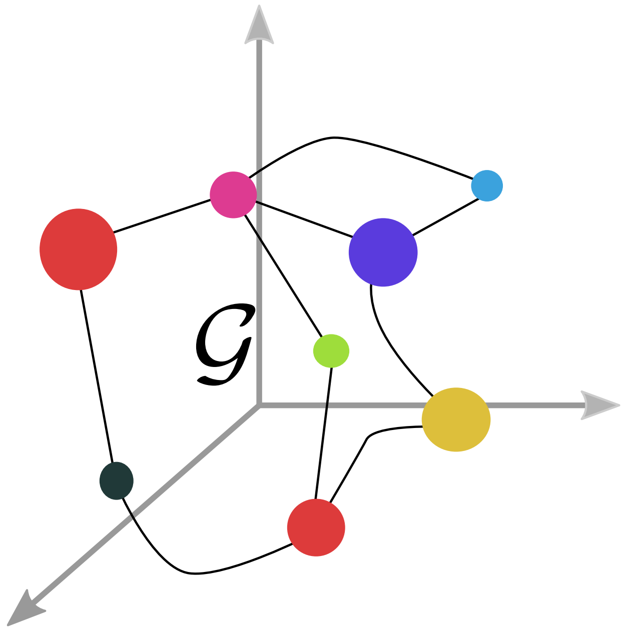
Based on the theories of Wasserstein and Gromov-Wasserstein

Optimal Transport for structured data

Structured data as probability distribution

Discrete case

- Structured data can be seen as a labeled graph
- Combines a feature **and** a structure information



Optimal Transport for structured data

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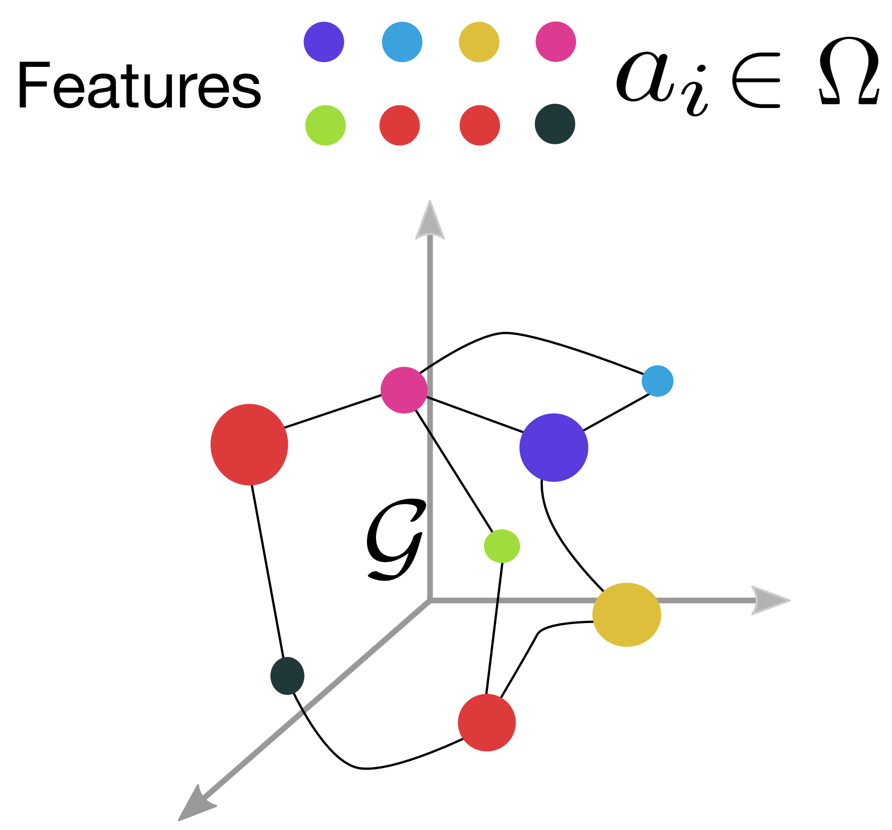

Optimal Transport for structured data

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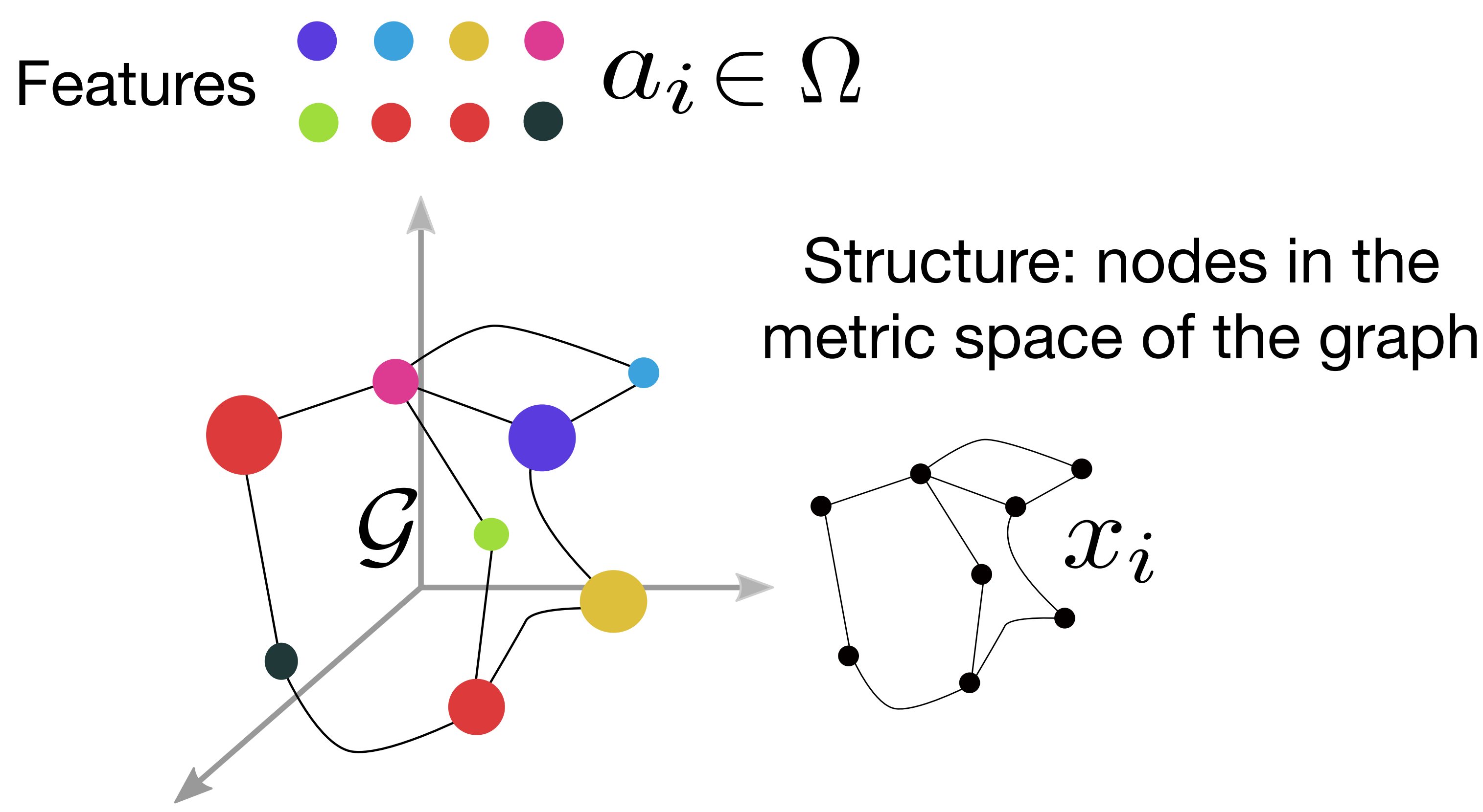
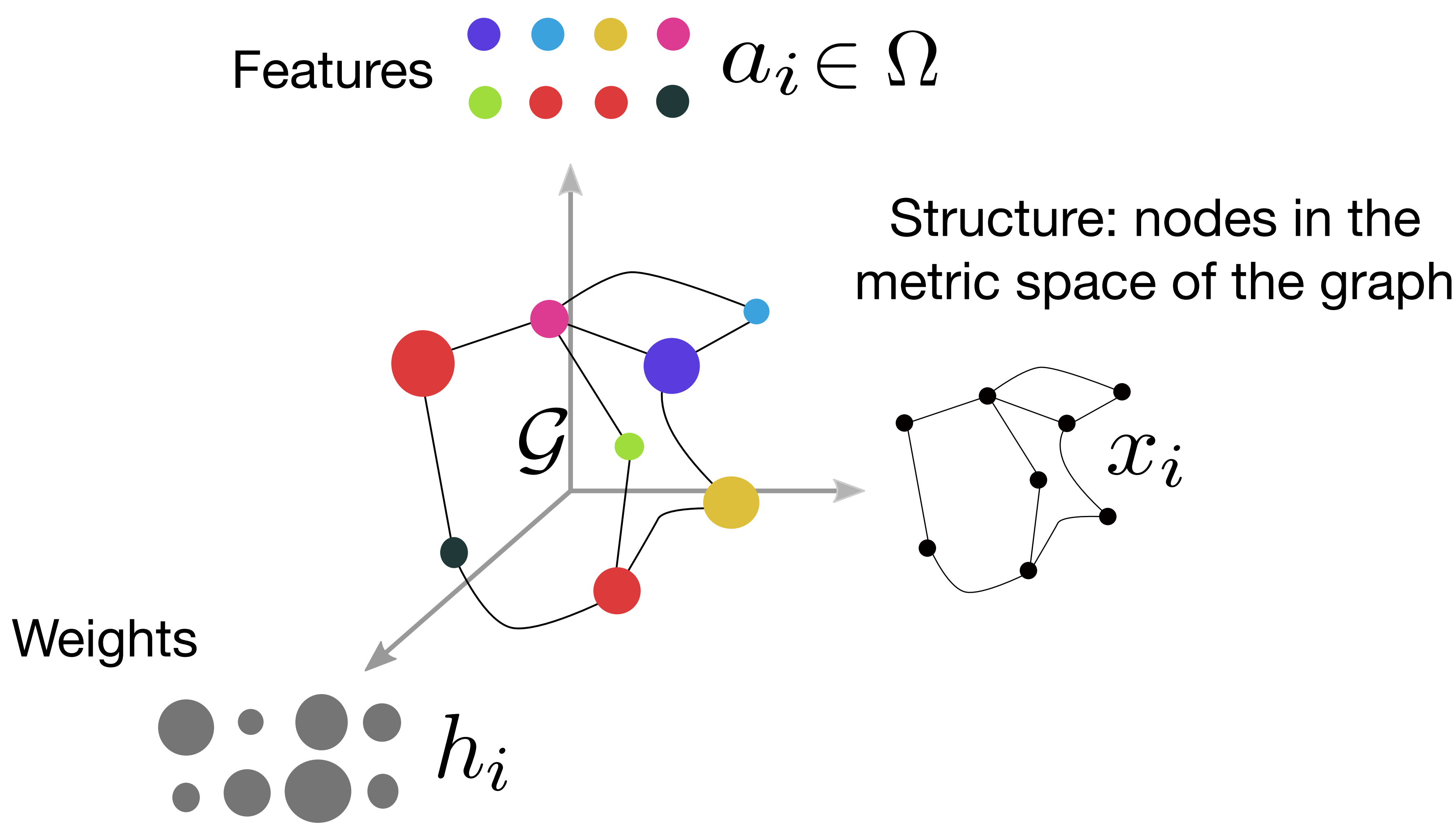


Optimal Transport for structured data

Structured data as probability distribution

Discrete case

- Structured data can be seen as a labeled graph
- Combines a feature **and** a structure information
- Add weights that encodes the relative importance of the nodes



Optimal Transport for structured data

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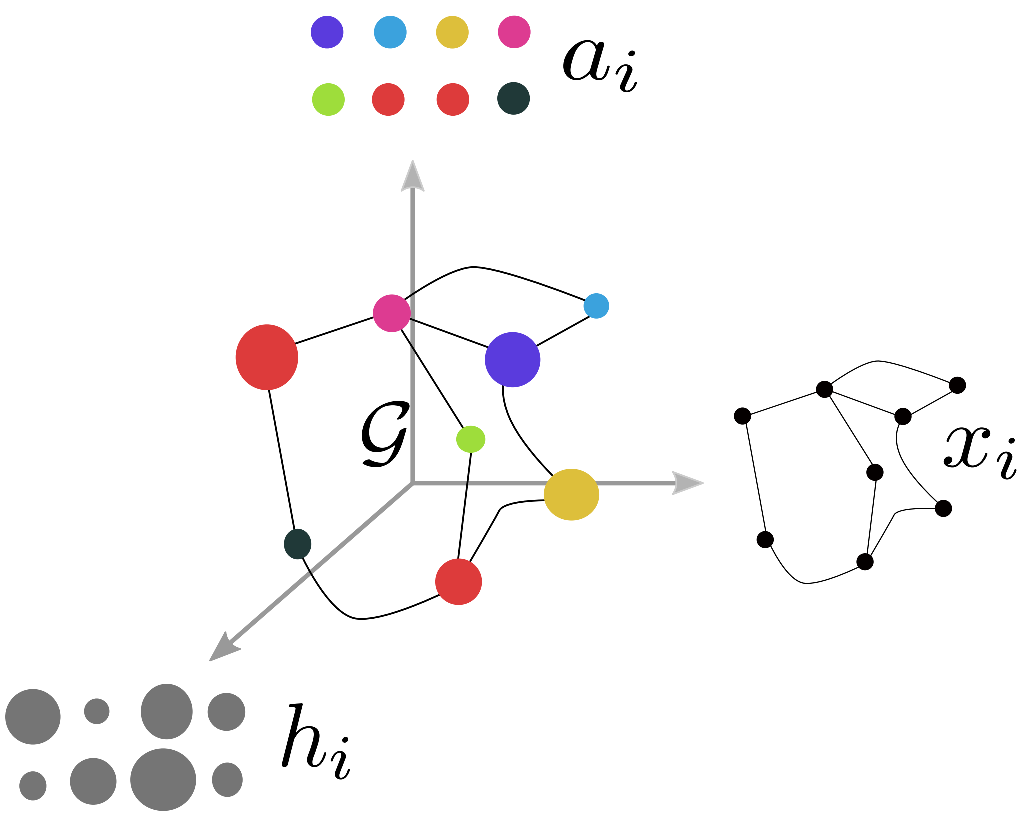
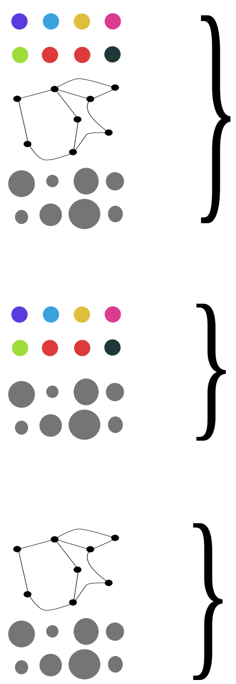


Form a probability measure



$$\mu = \sum_i h_i \delta_{(x_i, a_i)}$$

$$\mu_A = \sum_i h_i \delta_{a_i}$$

$$\mu_X = \sum_i h_i \delta_{x_i}$$

Optimal Transport for structured data

Fused Gromov-Wasserstein distance

Two structured data

$\mu = \sum_i h_i \delta_{(x_i,a_i)}, \nu = \sum_j g_j \delta_{(y_j,b_j)}$

Two matrices describing structures

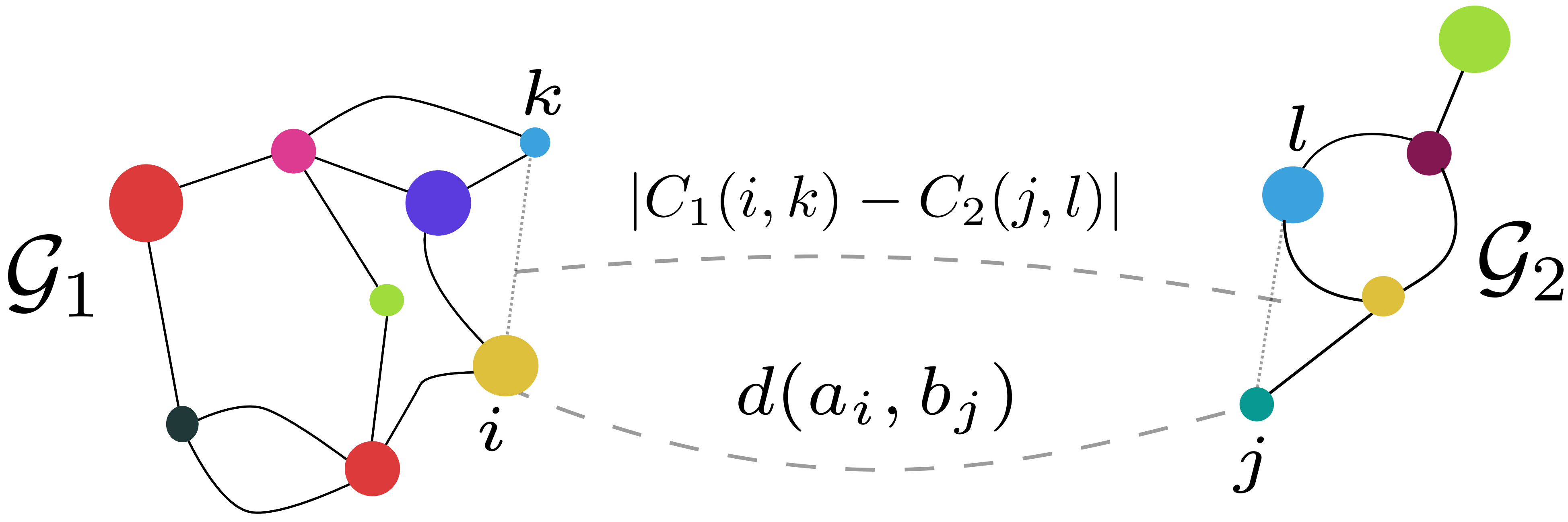
$\mathbf{C}_1, \mathbf{C}_2$

A distance between labels

$d : \Omega \times \Omega \to \mathbb{R}_+$

Fused Gromov-Wasserstein distance

$$FGW(\mathbf{M_{AB}}, \mathbf{C}_1, \mathbf{C}_2, \mathbf{h}, \mathbf{g}) = \min_{\boldsymbol{\pi} \in \Pi(\mathbf{h},\mathbf{g})} \sum_{i,j,k,l} (1-\alpha) d(a_i, b_j)^q + \alpha |C_1(i,k) - C_2(j,l)|^q \pi_{i,j} \pi_{k,l}$$



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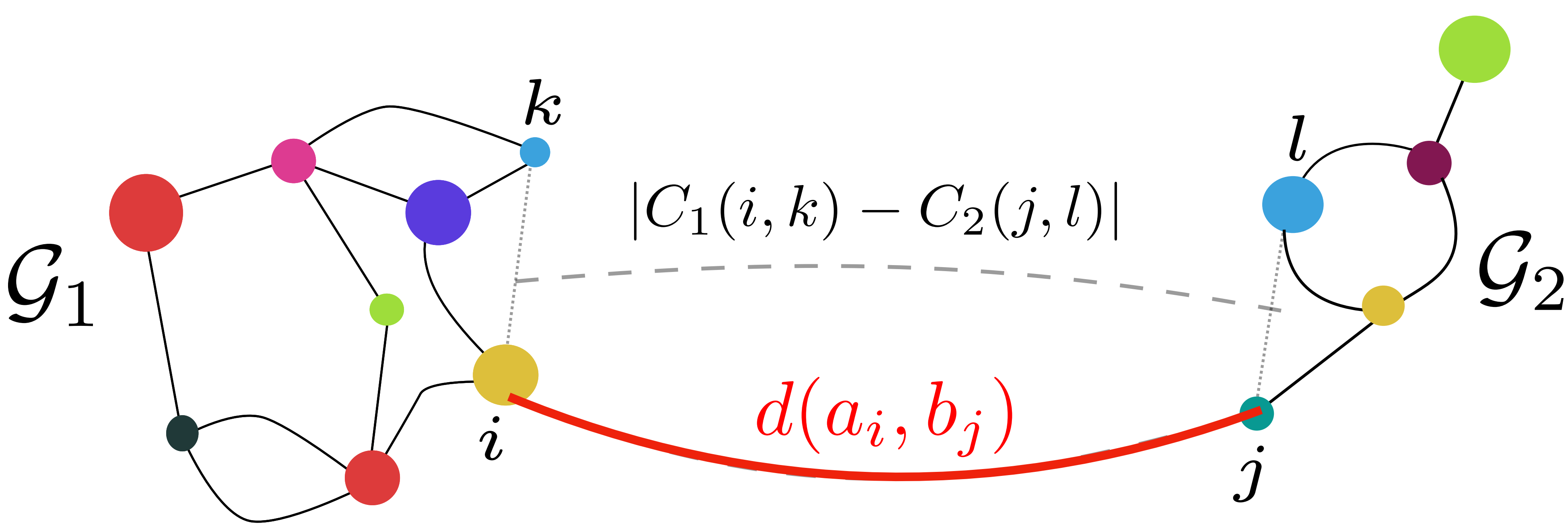

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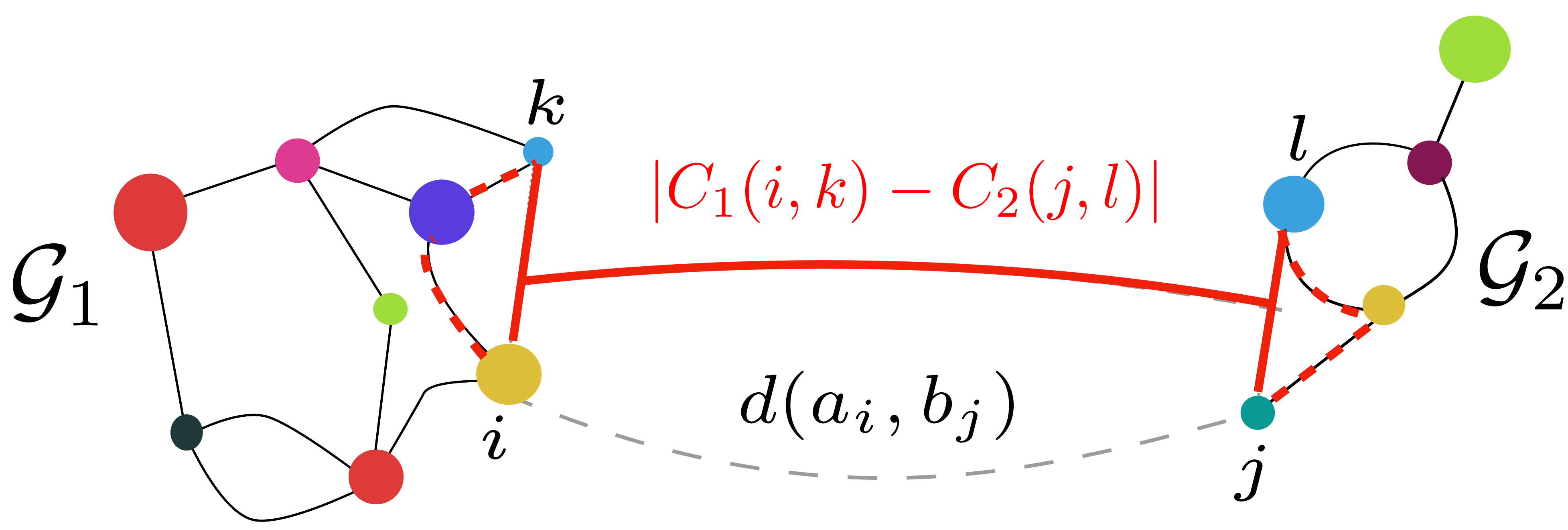

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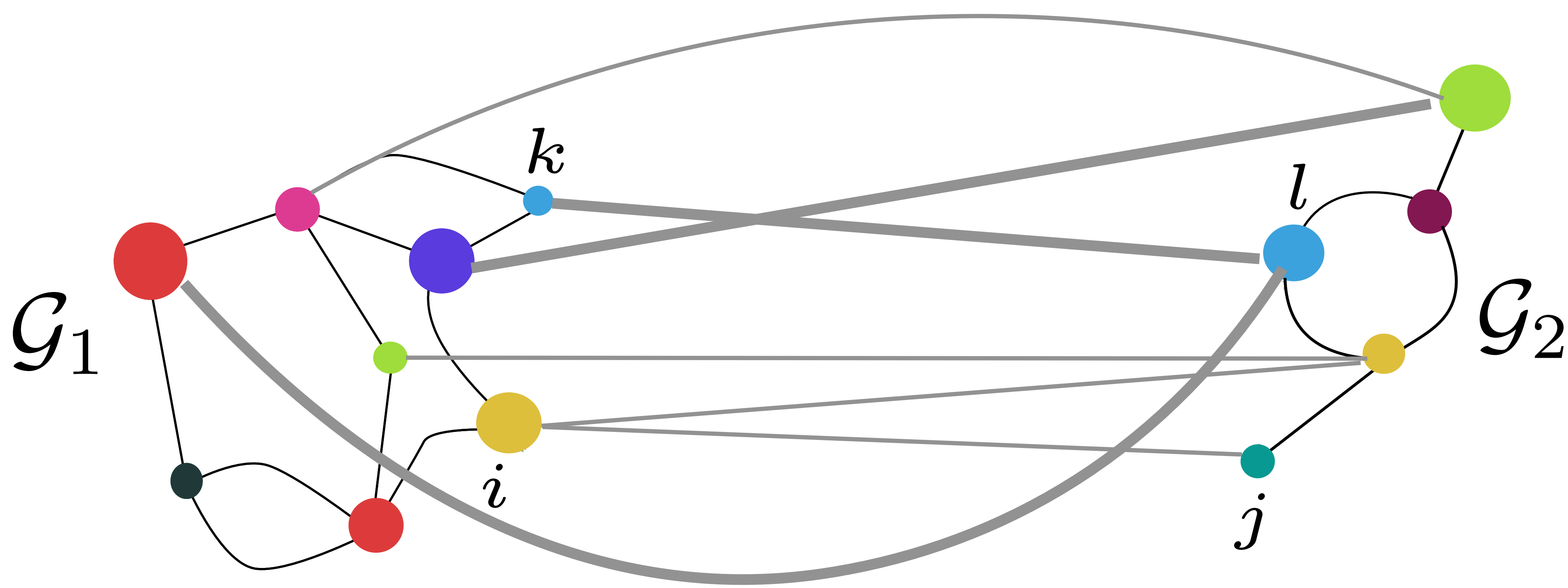
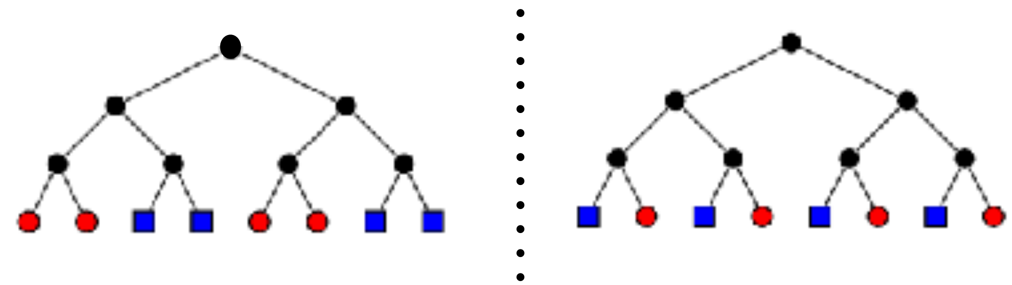


$\boldsymbol{\pi}$ **provides a soft assignment of the nodes**

Optimal Transport for structured data

Fused Gromov-Wasserstein distance: example

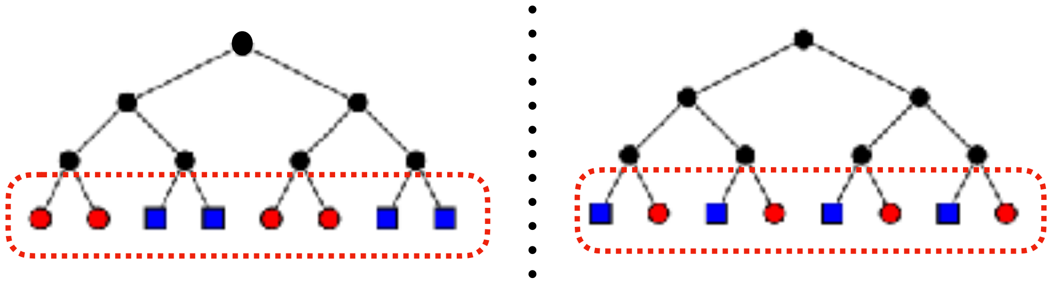
Consider two trees



Optimal Transport for structured data

Fused Gromov-Wasserstein distance: example

Consider two trees

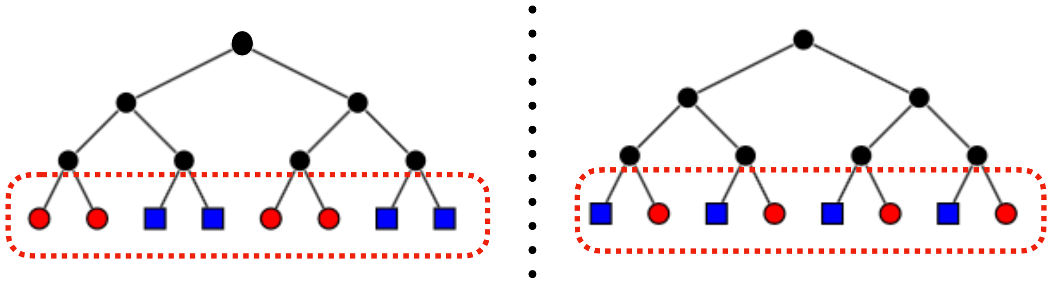


We want to compare the leaves of the trees

Optimal Transport for structured data

Fused Gromov-Wasserstein distance: example

Consider two trees



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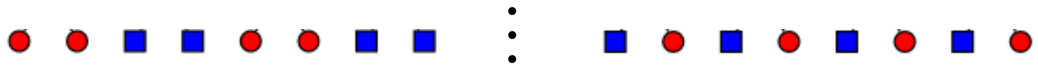
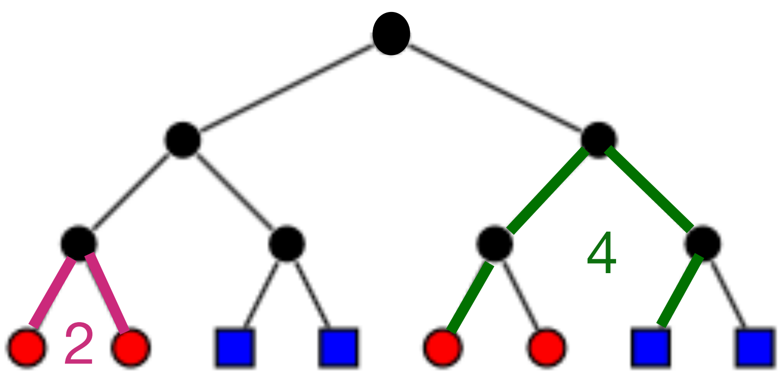


Features: blue or red

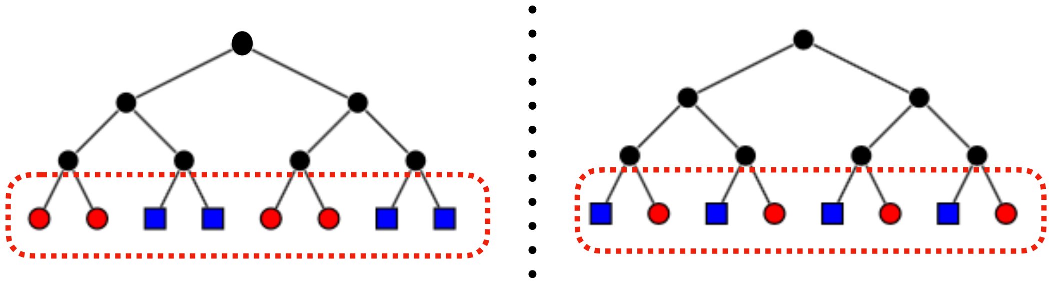
Structures : shortest path between the leaves



Optimal Transport for structured data

Fused Gromov-Wasserstein distance: example

Consider two trees



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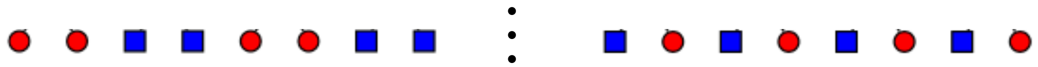

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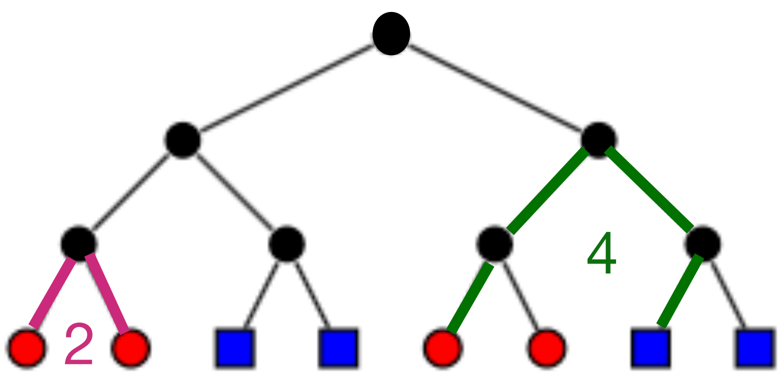
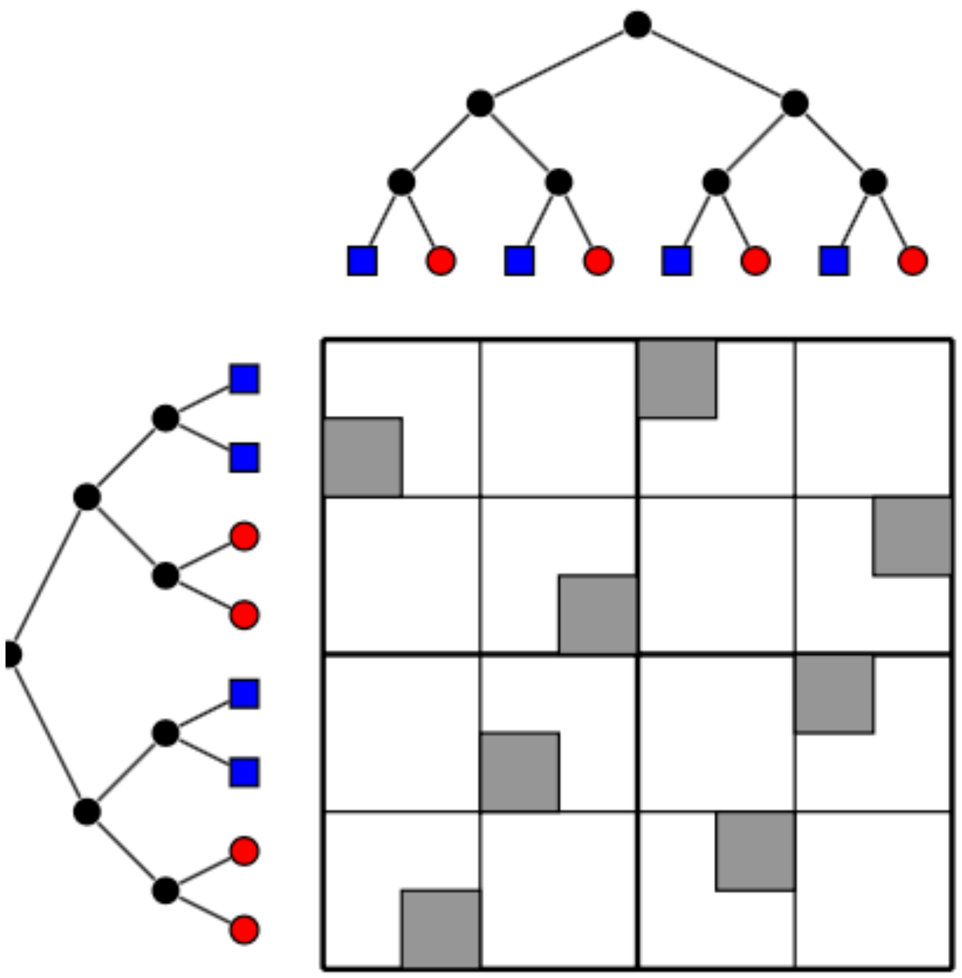


Taking both the structures and the features into account with FGW

Optimal Transport for structured data

Fused Gromov-Wasserstein distance: example

Wasserstein distance
(features only)

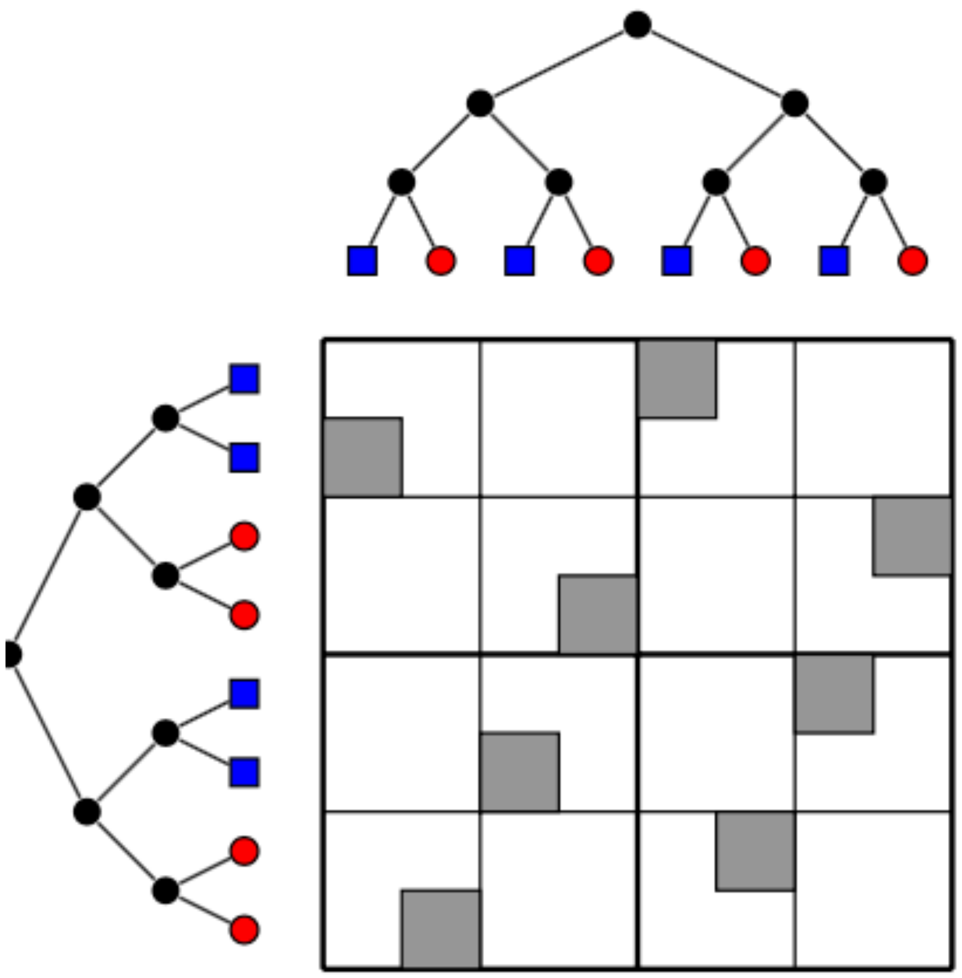


$W = 0$

Optimal Transport for structured data

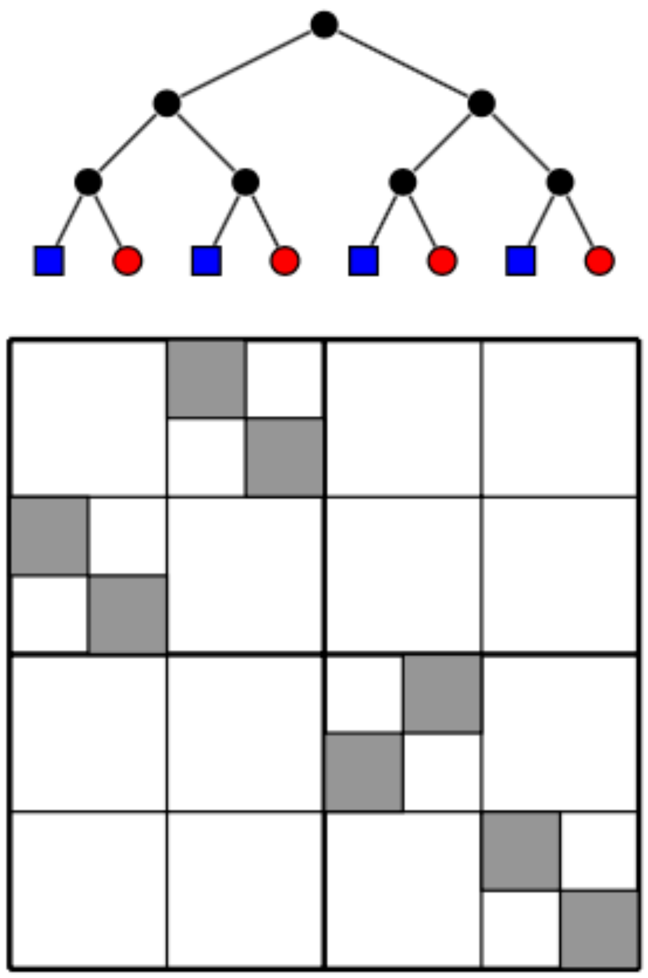
Fused Gromov-Wasserstein distance: example

Wasserstein distance (features only)



$W = 0$

Gromov-Wasserstein distance (structures only)



$GW = 0$

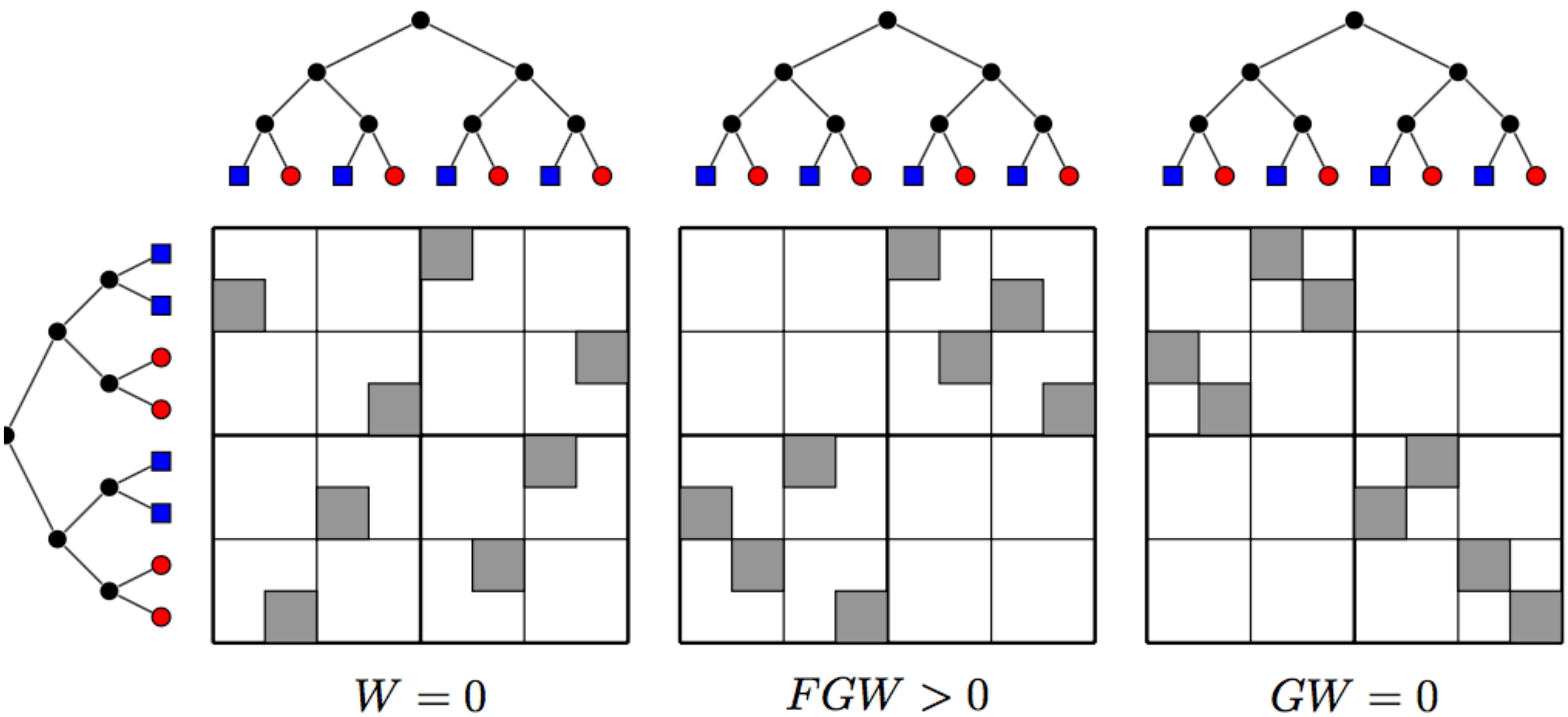
Optimal Transport for structured data

Fused Gromov-Wasserstein distance: example

Wasserstein distance (features only)

FGW

Gromov-Wasserstein distance (structures only)



Optimal Transport for structured data

Computing FGW (and GW!)

Solving FGW: a non convex QP

$$\min_{\boldsymbol{\pi} \in \Pi(\mathbf{h},\mathbf{g})} \sum_{i,j,k,l} (1-\alpha) d(a_i, b_j)^q + \alpha |C_1(i,k) - C_2(j,l)|^q \pi_{i,j} \pi_{k,l}$$

Quadratic function over polytope -> Conditional Gradient algorithm (a.k.a Frank-Wolfe)

Non convex but converges to a **local optimal solution** [Lacoste-Julien 2016]

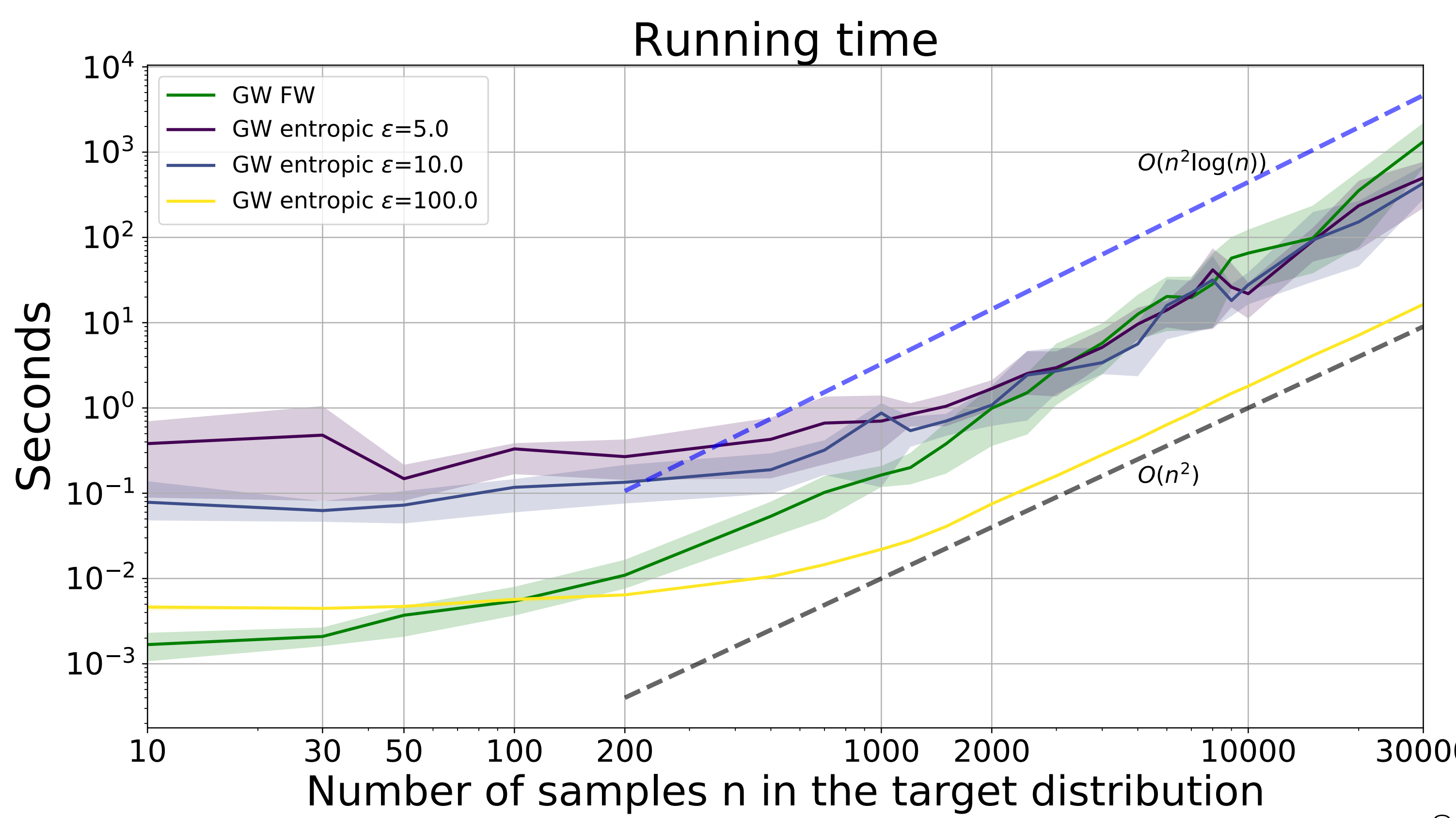
Find a **sparse** solution. FW gap = $O(\frac{1}{\sqrt{n_{iter}}})$

Algorithm 1 Conditional Gradient (CG) for *FGW*

```
π^(0) ← hg^⊤
for i = 1, ..., do
    G ← Gradient from GW loss w.r.t. π^(i-1)
    π̃^(i) ← Solve OT with ground loss G
    τ^(i) ← Line-search for GW loss with τ ∈ (0,1) (closed-form)
    π^(i) ← (1 − τ^(i)) π^(i-1) + τ^(i) π̃^(i)
end for
```

Complexity

$O(n_{iter}\ n^3)$



Optimal Transport for structured data

Fused Gromov-Wasserstein distance

A distance w.r.t strong isomorphism

- $FGW \geq 0$ and satisfies the triangle inequality
- $\mathbf{C}_1, \mathbf{C}_2$ distances. $FGW = 0$ iff $\exists \sigma$ permutations of the nodes

$$\text{(conservation of the weights) } h_i = g_{\sigma(i)}$$

$$\text{(conservation of the features) } a_i = b_{\sigma(i)}$$

$$\text{(conservation of the structures) } C_1(i,k) = C_2(\sigma(i), \sigma(k))$$

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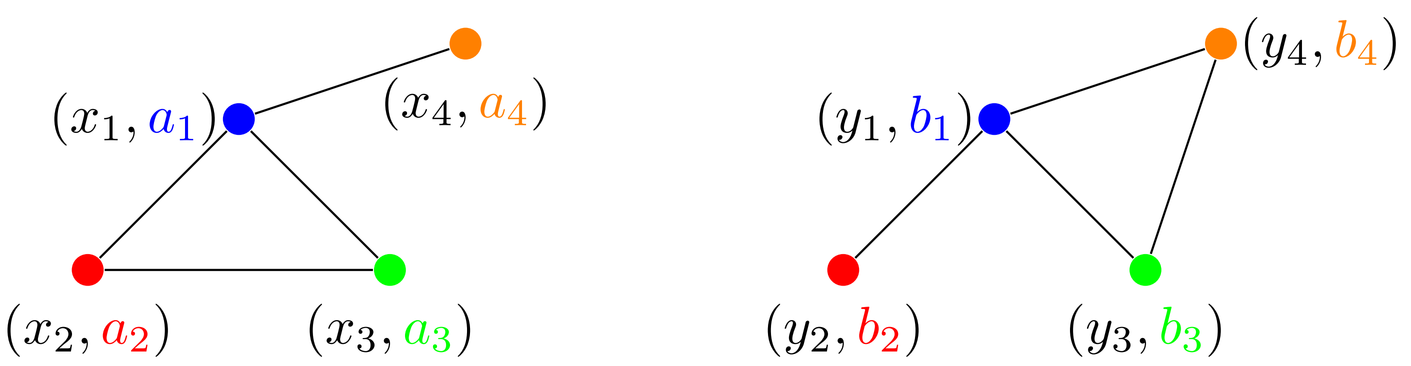
Same weights, same labels at the same place up to a permutation



Isometric + same features but not strongly isomorphic

Optimal Transport for structured data

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Other properties

Interpolates GW between the structures and W between the features

Extends to the continuous setting: geodesic properties + sample complexity

FGW in action

Optimal Transport for structured data

FGW in action

Graph classification

A set of labeled graphs $(\mathcal{G}_i, y_i)$. Structure matrices shortest path

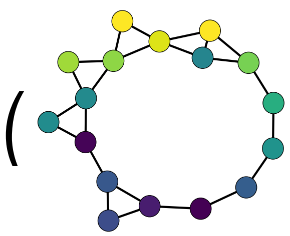
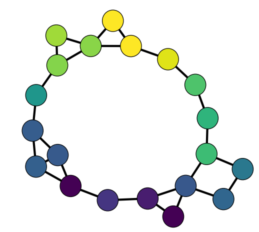
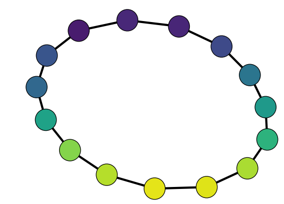
Linear classifier: SVM on the indefinite kernel $e^{-\frac{1}{\beta}FGW(\mathcal{G}_i,\mathcal{G}_j)}$

Compare with graph kernel approaches + GCN on benchmark datasets

Dataset	Labeled Graphs MUTAG	Labeled Graphs PTC	Labeled Graphs NCI1	Social Graphs IMDB-B	Vector attributes Graph SYNTHETIC	Vector attributes Graph PROTEIN	Vector attributes Graph CUNEIFORM
WL	86.21±8.15	62.17±7.80	85.13±1.61	Unapplicable(U)	U	U	U
GK	82.42±8.40	56.46±8.03	60.78±2.48	56.00±3.61	41.13±4.68	U	U
RW	79.47±8.17	55.09±7.34	58.63±2.44	U	U	U	U
SP	85.79±2.51	58.53±2.55	73.00±0.51	55.80±2.93	38.93±5.12	U	U
HOPPER	U	U	U	U	90.67±4.67	71.96±3.22	32.59±8.73
PROPA	U	U	U	U	64.67±6.70	61.34±4.38	12.59± 6.67
PSCN $k = 10$	83.47±10.26	58.34±7.71	70.65±2.58	U	**100.00±0.00**	67.95±11.28	25.19±7.73
FGW	**88.42±5.67**	**65.31±7.90**	**86.42±1.63**	**63.80±3.49**	**100.00±0.00**	**74.55±2.74**	**76.67±7.04**

Optimal Transport for structured data

FGW barycenter

Making sense of: $\frac{1}{2}($  $+$  $) =$ 

Optimal Transport for structured data

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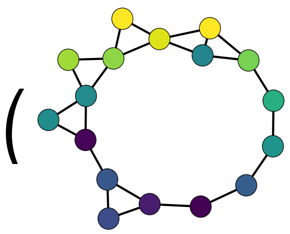
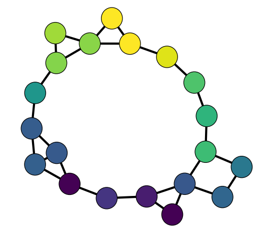
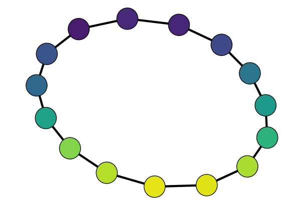
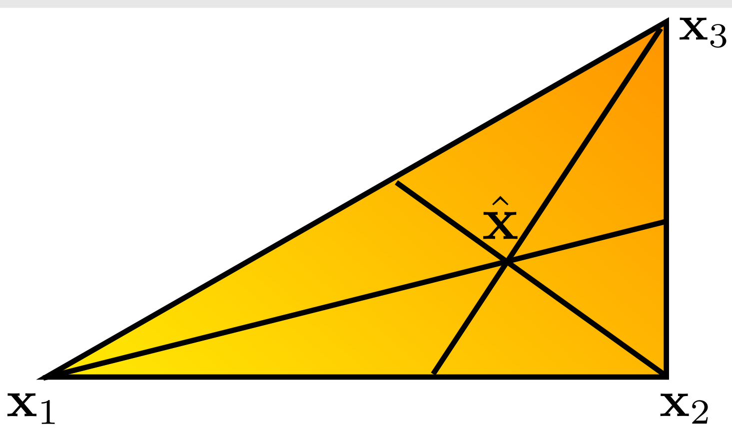
Making sense of: $\frac{1}{2}($  $+$  $) =$ 

Euclidean Barycenter: $(\mathbb{R}^d, \|.\|_2)$

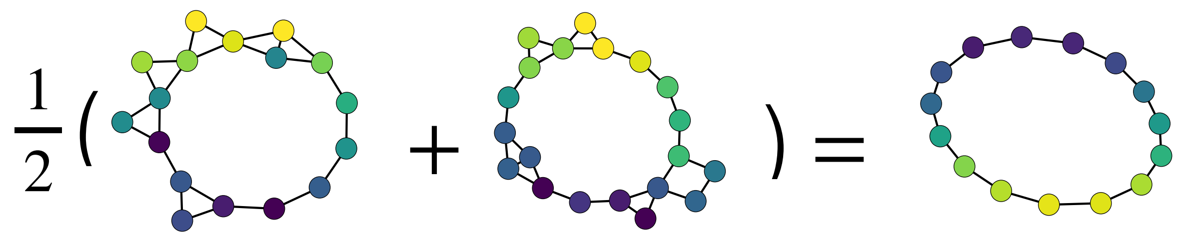
$$\inf_{\mathbf{x} \in \mathbb{R}^d} \sum_{i=1}^{n} \lambda_i \|\mathbf{x} - \mathbf{x}_i\|_2^2$$



Optimal Transport for structured data

FGW barycenter

Making sense of:



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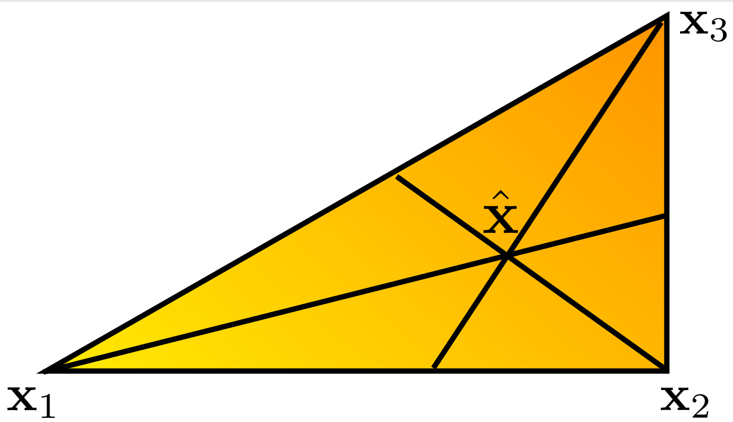
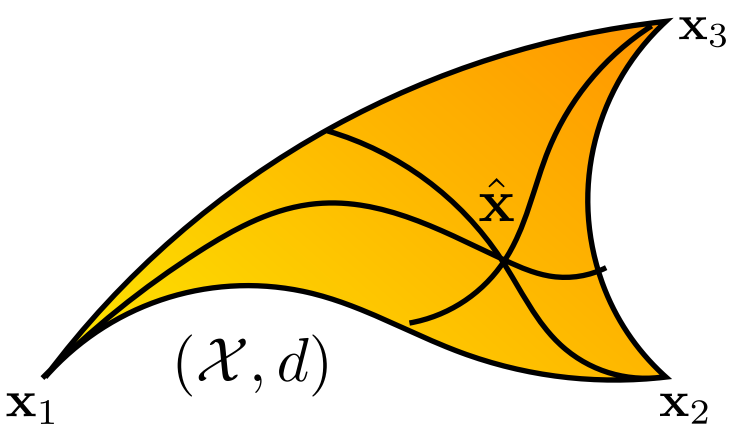
$$\inf_{\mathbf{x}\in\mathbb{R}^d} \sum_{i=1}^{n} \lambda_i \|\mathbf{x} - \mathbf{x}_i\|_2^2$$

Fréchet Barycenter: $(\mathcal{X}, d)$ metric space

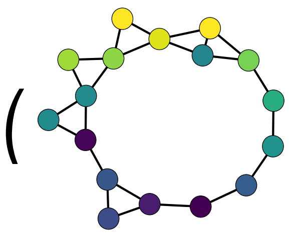
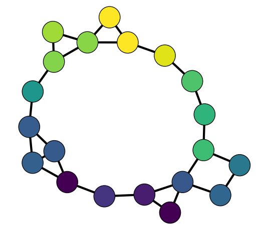
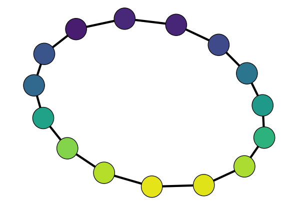
$$\inf_{x\in\mathcal{X}} \sum_{i=1}^{n} \lambda_i d(x, x_i)^p$$





Optimal Transport for structured data

FGW barycenter

Making sense of: $\frac{1}{2}($  $+$  $) =$ 

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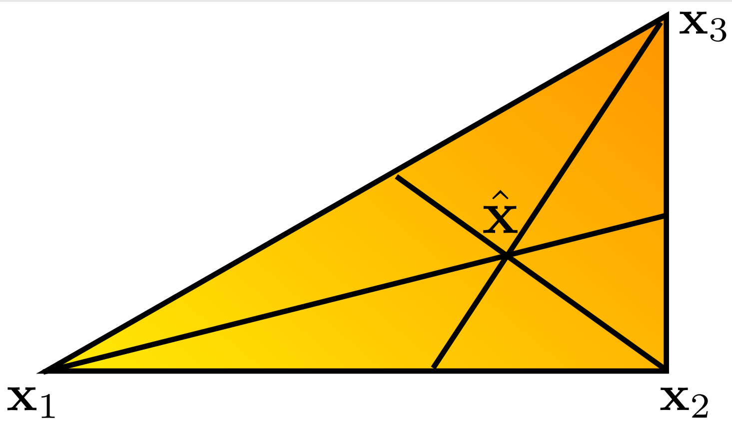

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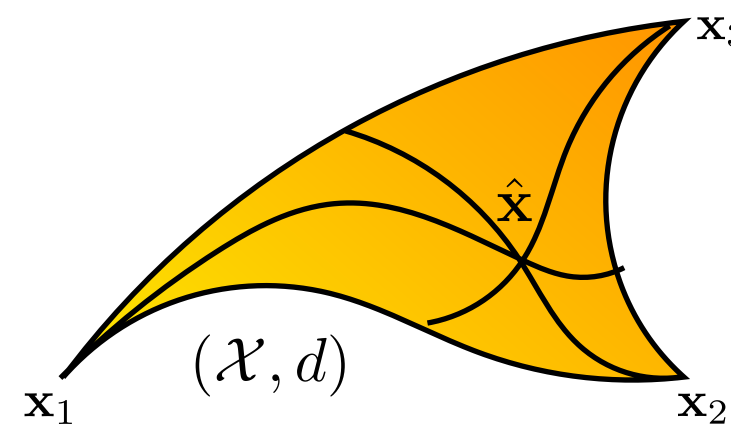


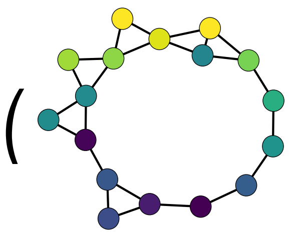
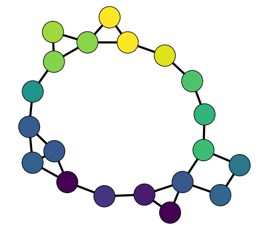
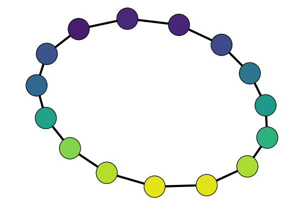
FGW barycenter

$$\min_{\mu} \sum_{k=1}^{K} \lambda_k FGW_{q,\alpha}(\mu, \mu_k)$$

- Barycenter of labeled graphs, relational data with attributes
- Consider feature space $\Omega = (\mathbb{R}^d, \|.\|_2^2)$ structured data $(\mathbf{C}_k, \mathbf{B}_k, \mathbf{h}_k)_{k=1}^K$

Optimal Transport for structured data

FGW barycenter

Making sense of: $\frac{1}{2}($  $+$  $) =$ 

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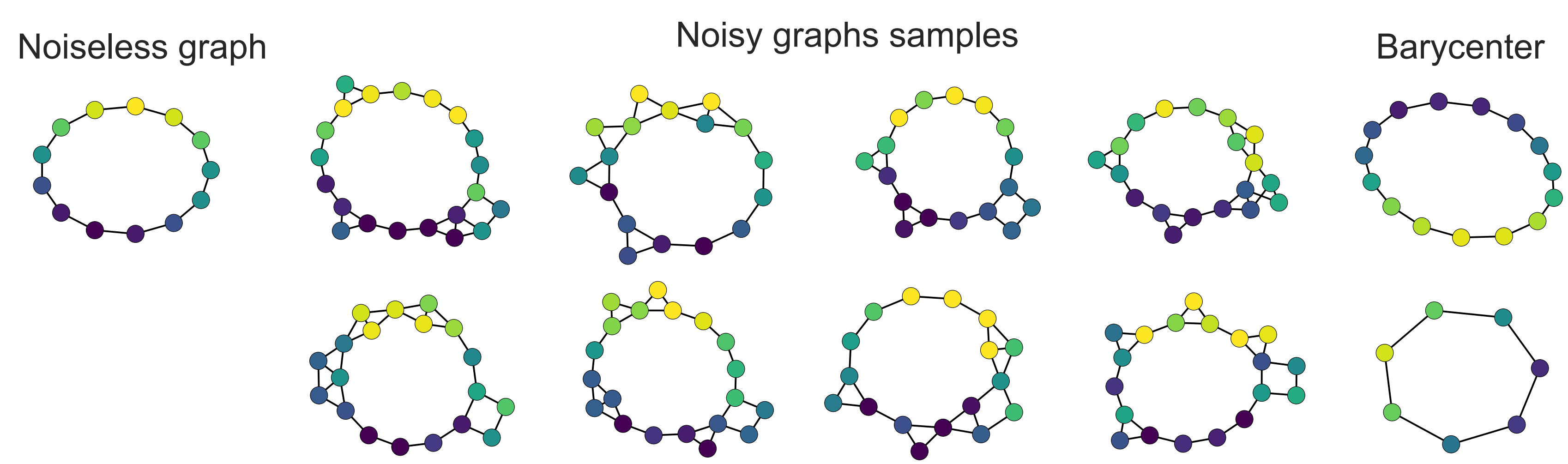
Barycenter of labeled graphs, relational data with attributes

Consider feature space $\Omega = (\mathbb{R}^d, \|.\|_2^2)$ structured data $(\mathbf{C}_k, \mathbf{B}_k, \mathbf{h}_k)_{k=1}^{K}$

Algorithm 1 FGW barycenter

Initialize $\mathbf{C} \leftarrow \mathbf{C}_0, \mathbf{A} \leftarrow \mathbf{A}_0$.
while not converged **do**
  for $k = 1 \dots K$ **do**
    $\boldsymbol{\pi}_k \leftarrow FGW(\mathbf{M}_{\mathbf{AB}_k}, \mathbf{C}, \mathbf{C}_k, \mathbf{h}, \mathbf{h}_k)$
  end for
  $\mathbf{C} \leftarrow \frac{1}{\mathbf{h}\mathbf{h}^T} \sum_{k=1}^{K} \lambda_k \boldsymbol{\pi}_k^T \mathbf{C}_k \boldsymbol{\pi}_k$
  $\mathbf{A} \leftarrow \sum_{k=1}^{K} \lambda_k \mathbf{B}_k \boldsymbol{\pi}_k^T \mathrm{diag}(\frac{1}{\mathbf{h}})$
end while



Optimal Transport for structured data

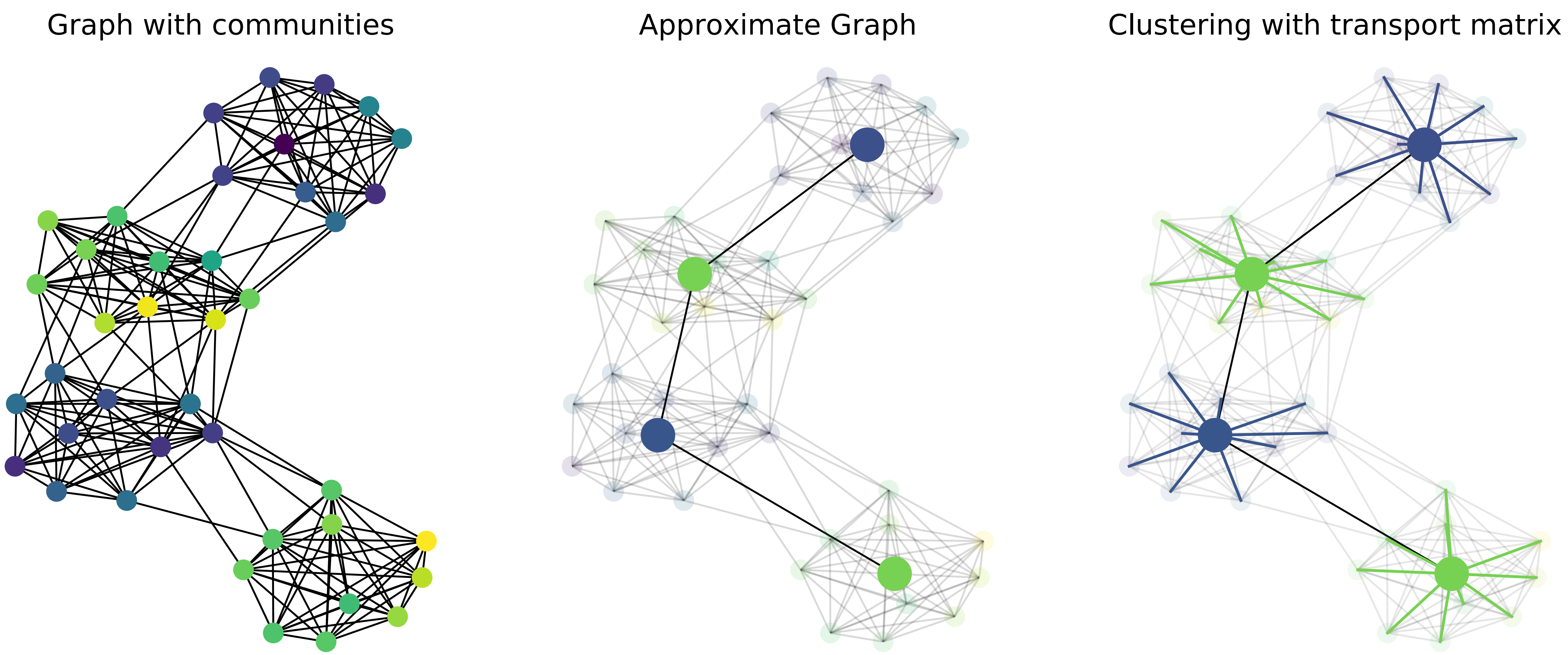
Summarization of graph

FGW coarsening

$$\min_{\mu} FGW(\mu, \nu) = \min_{\mathbf{A},\mathbf{C}_1} FGW(\mathbf{M}_{\mathbf{AB}}, \mathbf{C}_1, \mathbf{C}_2, \mathbf{h}, \mathbf{g})$$

Given a labeled graph we look for the closest graph w.r.t FGW with fewer nodes

Projection w.r.t FGW -> barycenter problem with $K = 1$



Optimal Transport for structured data

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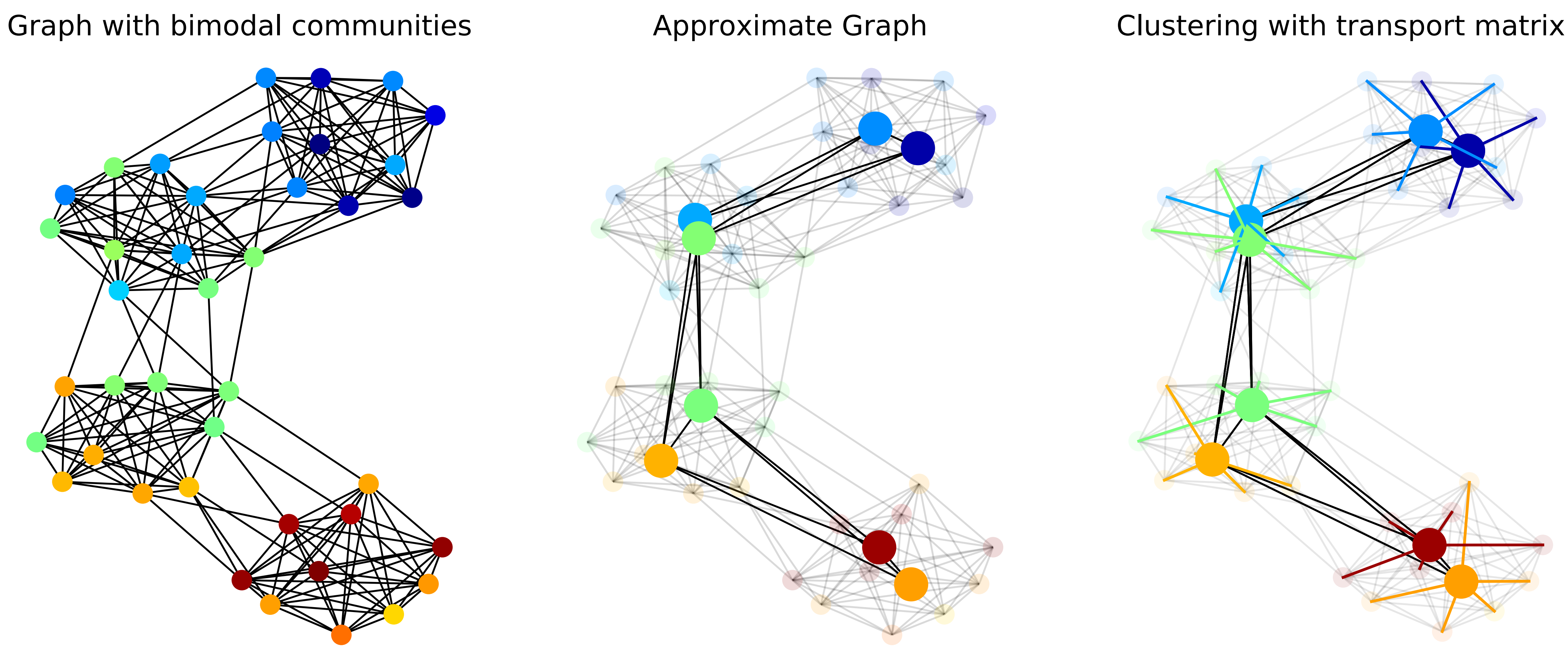


Optimal Transport for structured data

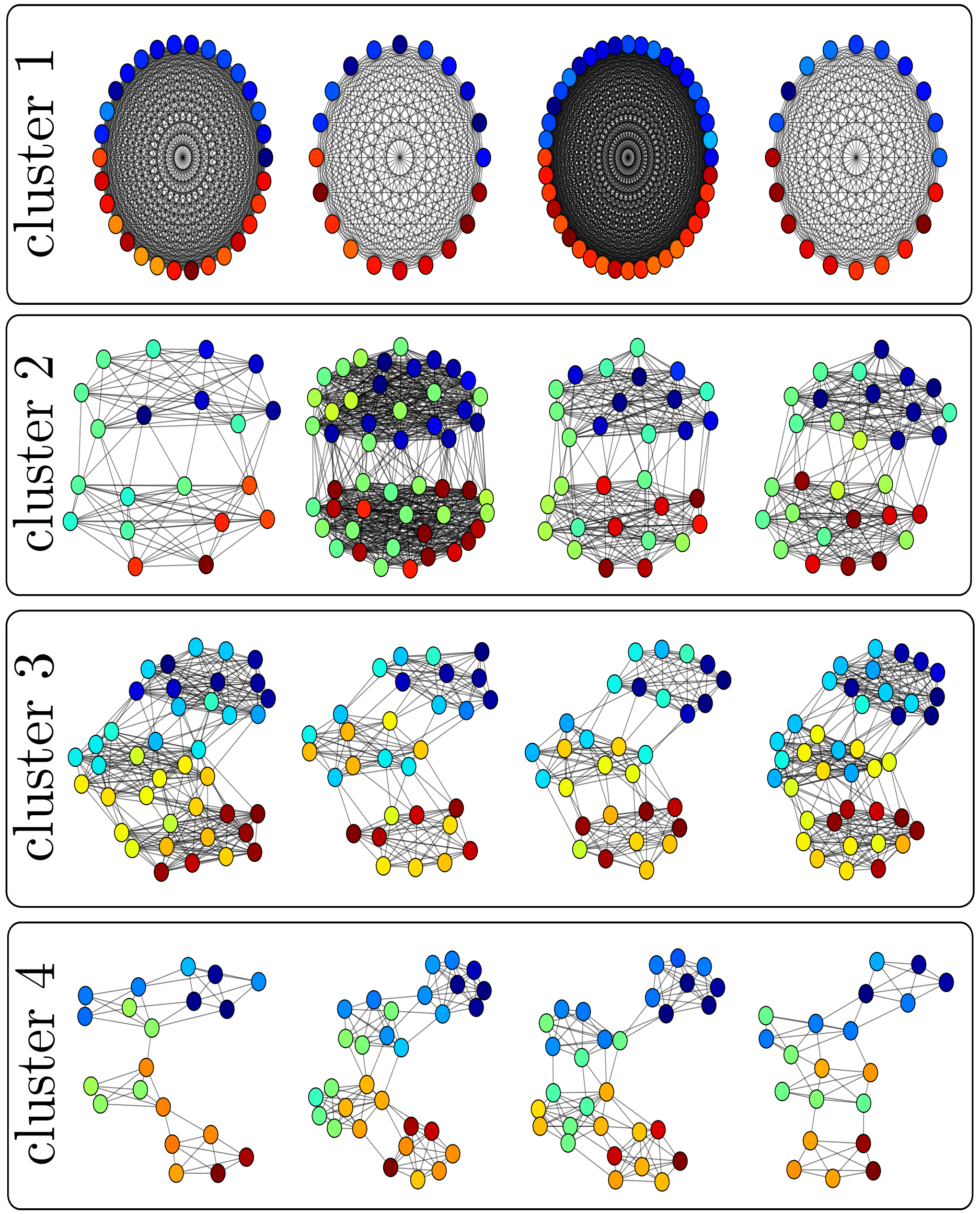
FGW clustering

Given a set of labeled graphs -> k-means using FGW barycenter

Algorithm 1 FGW clustering

Number of clusters K. Labeled graphs $(\mathbf{C}_i, \mathbf{B}_i, \mathbf{h}_i)_{i \in [\![N]\!]}$
Initialize centroids $\forall k \in [\![K]\!], \mathbf{C}_k \leftarrow \mathbf{C}_0, \mathbf{A}_k \leftarrow \mathbf{A}_0$.
while not converged **do**
    Calculate $N \times K$ FGW distances.
    for $i = 1 \dots N$ **do**
        Assign $(\mathbf{C}_i, \mathbf{B}_i, \mathbf{h}_i)$ to a cluster $k \in [\![K]\!]$
    end for
    for $k = 1 \dots K$ **do**
        $\mathbf{C}_k, \mathbf{A}_k \leftarrow$ `FGW barycenter`$((\mathbf{C}_i, \mathbf{B}_i, \mathbf{h}_i)_{i \in \text{cluster } k})$
    end for
end while

Training dataset examples



Optimal Transport for structured data

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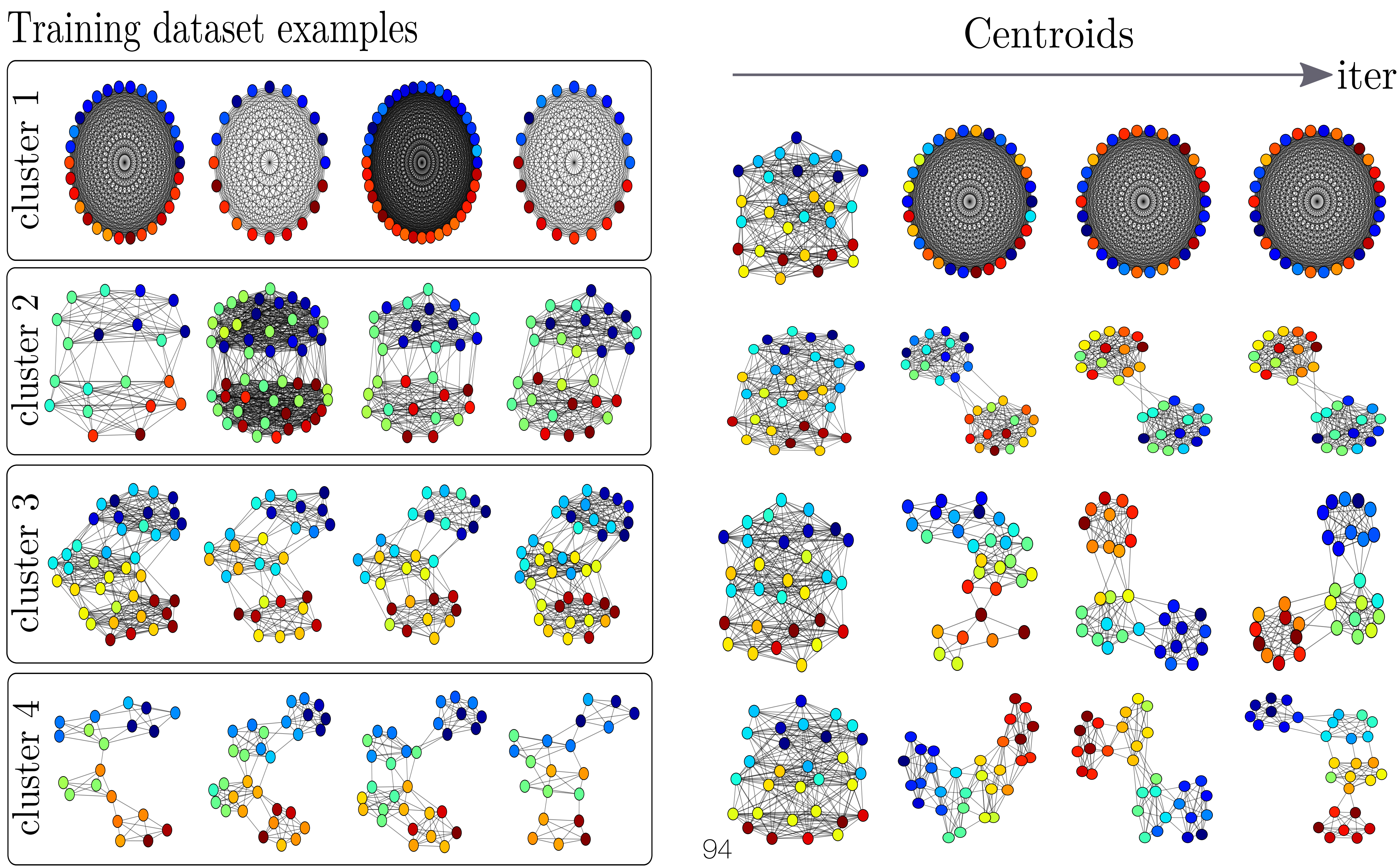
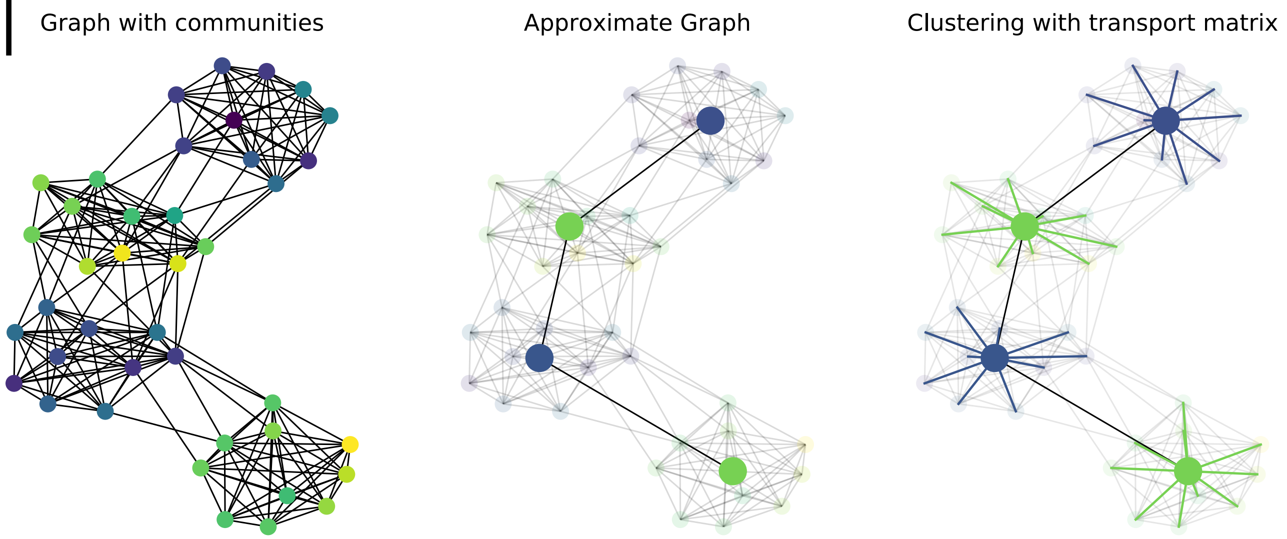
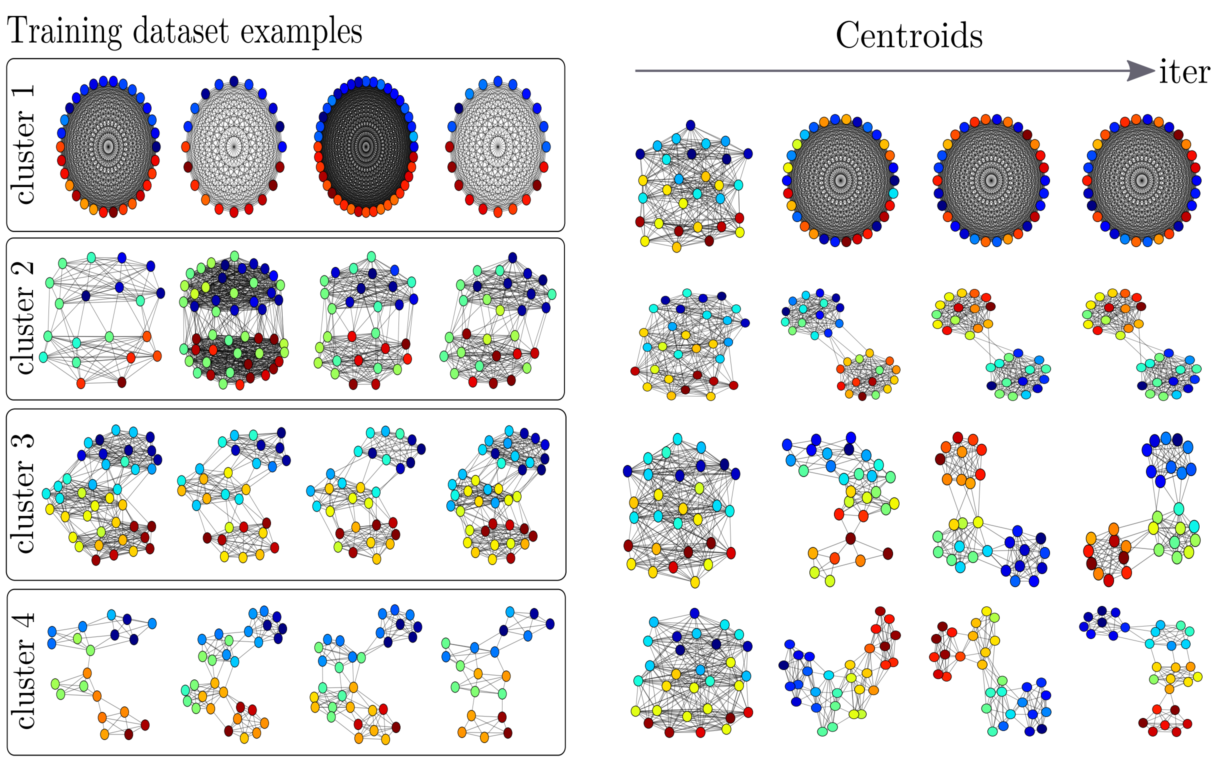


Optimal Transport for structured data

Conclusion





FGW

- OT method for structured data (**whatever sizes of graphs**)
- Provides a soft assignments of nodes + **distance between labeled graphs**
- Can be used for classification + summarization + clustering

Perspectives

- Learn structure matrices
- Use it for dynamic graph: add a temporal part
- Other formulation: match only a small portion of the nodes

CO-Optimal Transport

CO-Optimal Transport

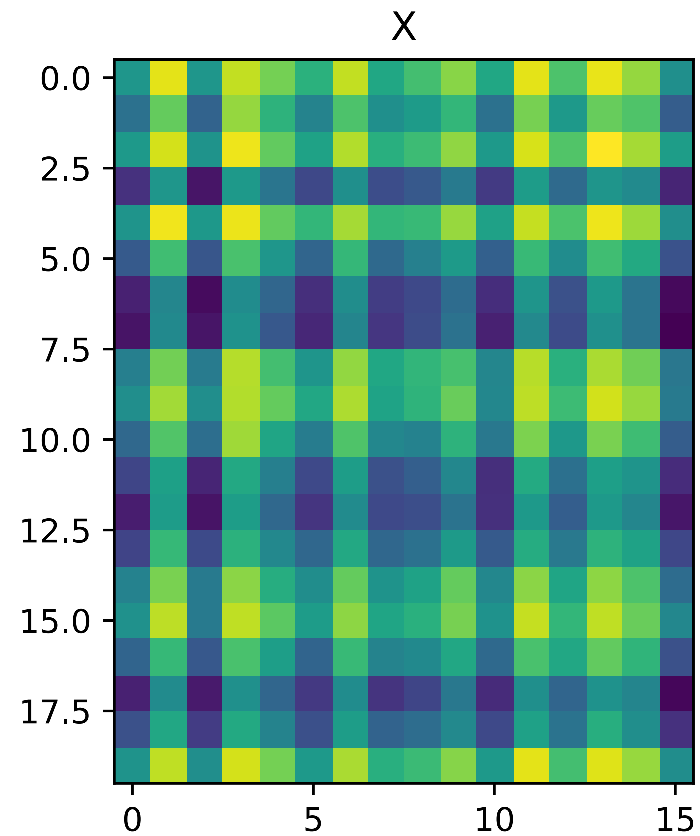
Motivations

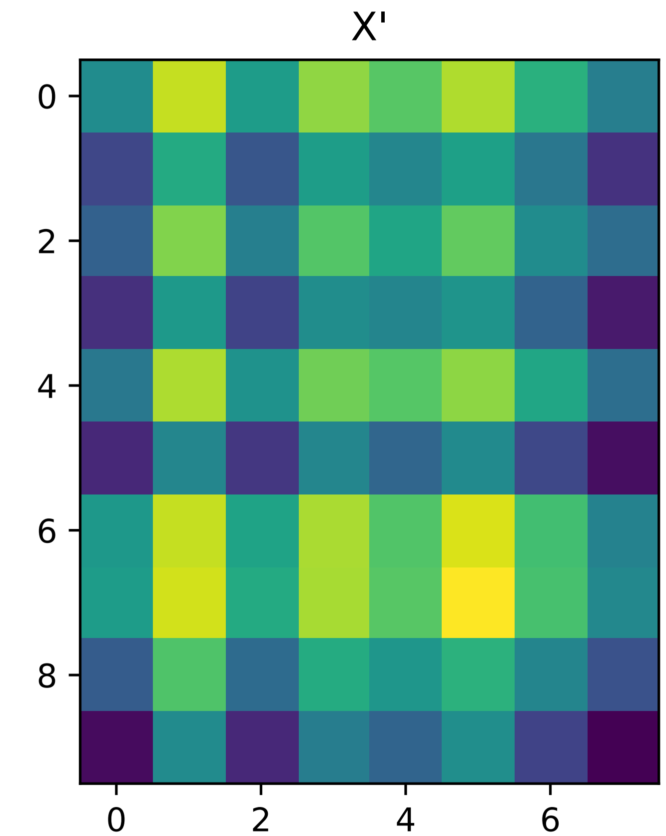
Two heterogeneous datasets

$$\mathbf{X} = [\mathbf{x}_1, \dots, \mathbf{x}_n]^T \in \mathbb{R}^{n \times d}$$

$$\mathbf{X}' = [\mathbf{x}'_1, \dots, \mathbf{x}'_{n'}]^T \in \mathbb{R}^{n' \times d'}$$

Row= samples, columns= features





We want to measure the similarity of these two datasets (interpretable way)

Image registration [Haker 2001], HDA [Yang 2018], Word embeddings [Alvarez 2018]

CO-Optimal Transport

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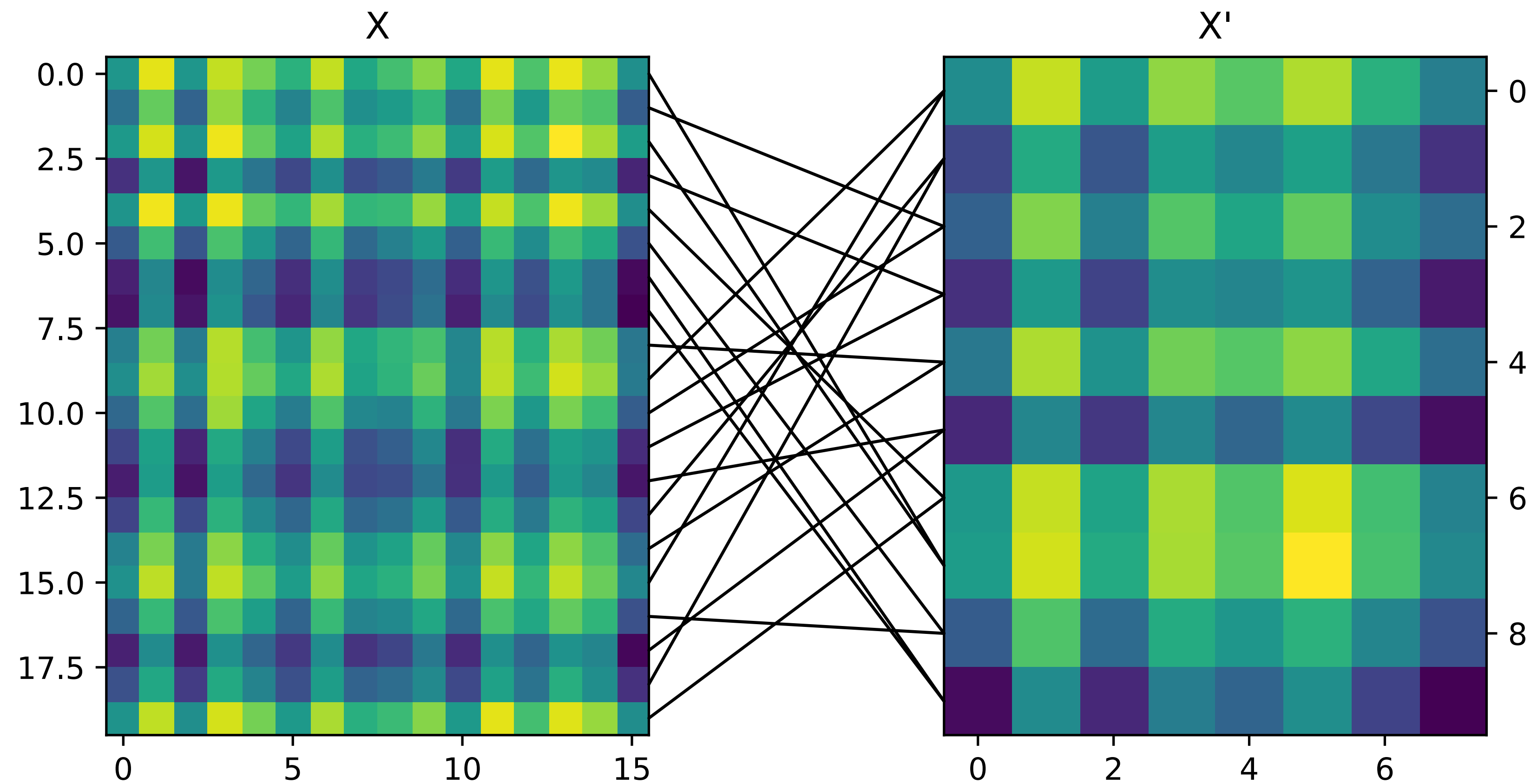
Row= samples, columns= features/variable



We can apply Gromov-Wasserstein based on the pairwise distances

$$c_X(\mathbf{x}_i, \mathbf{x}_j)$$
$$c_{X'}(\mathbf{x}'_i, \mathbf{x}'_j)$$

The OT matrix gives a reordering of the samples

CO-Optimal Transport

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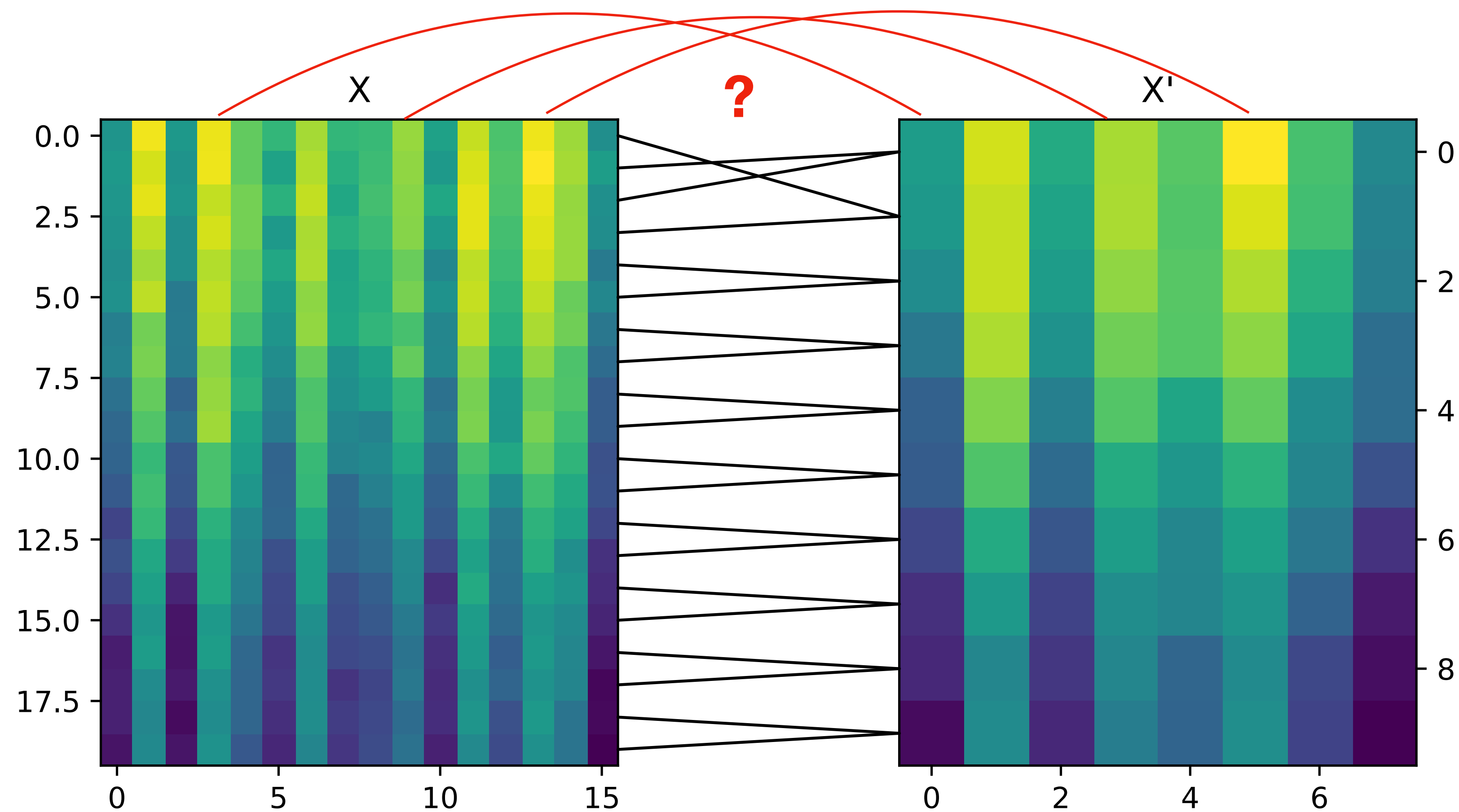

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$$c_X(\mathbf{x}_i, \mathbf{x}_j)$$
$$c_{X'}(\mathbf{x}'_i, \mathbf{x}'_j)$$

The OT matrix gives a reordering of the samples

But discards the relationship between the features…

CO-Optimal Transport

Motivations

Two heterogeneous datasets

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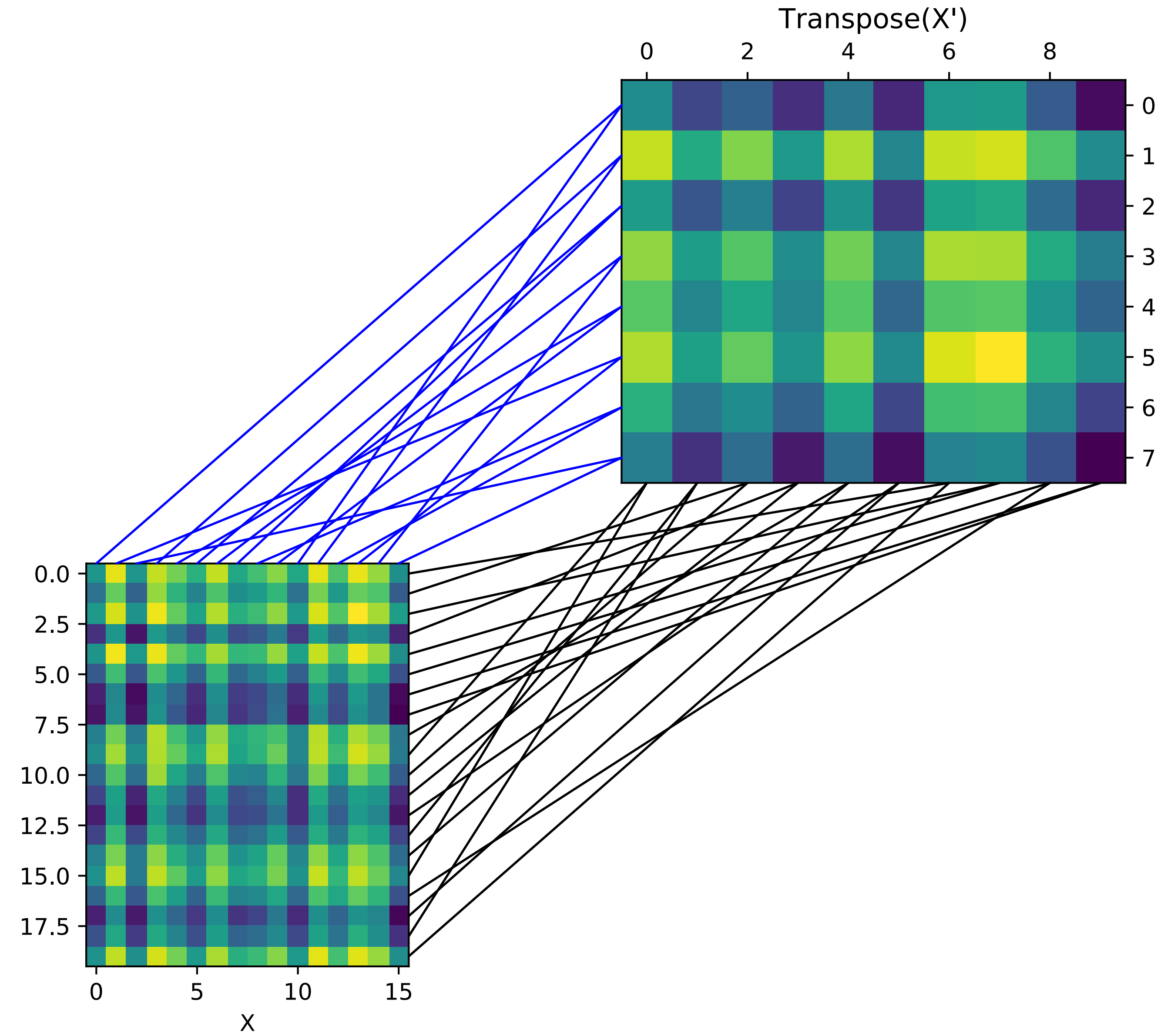

The objective of COOT is to estimate a transport matrix between the samples **and** one between the features

These matrices are estimated jointly and can be used for interpreting relationships across spaces

CO-Optimal Transport

Motivations

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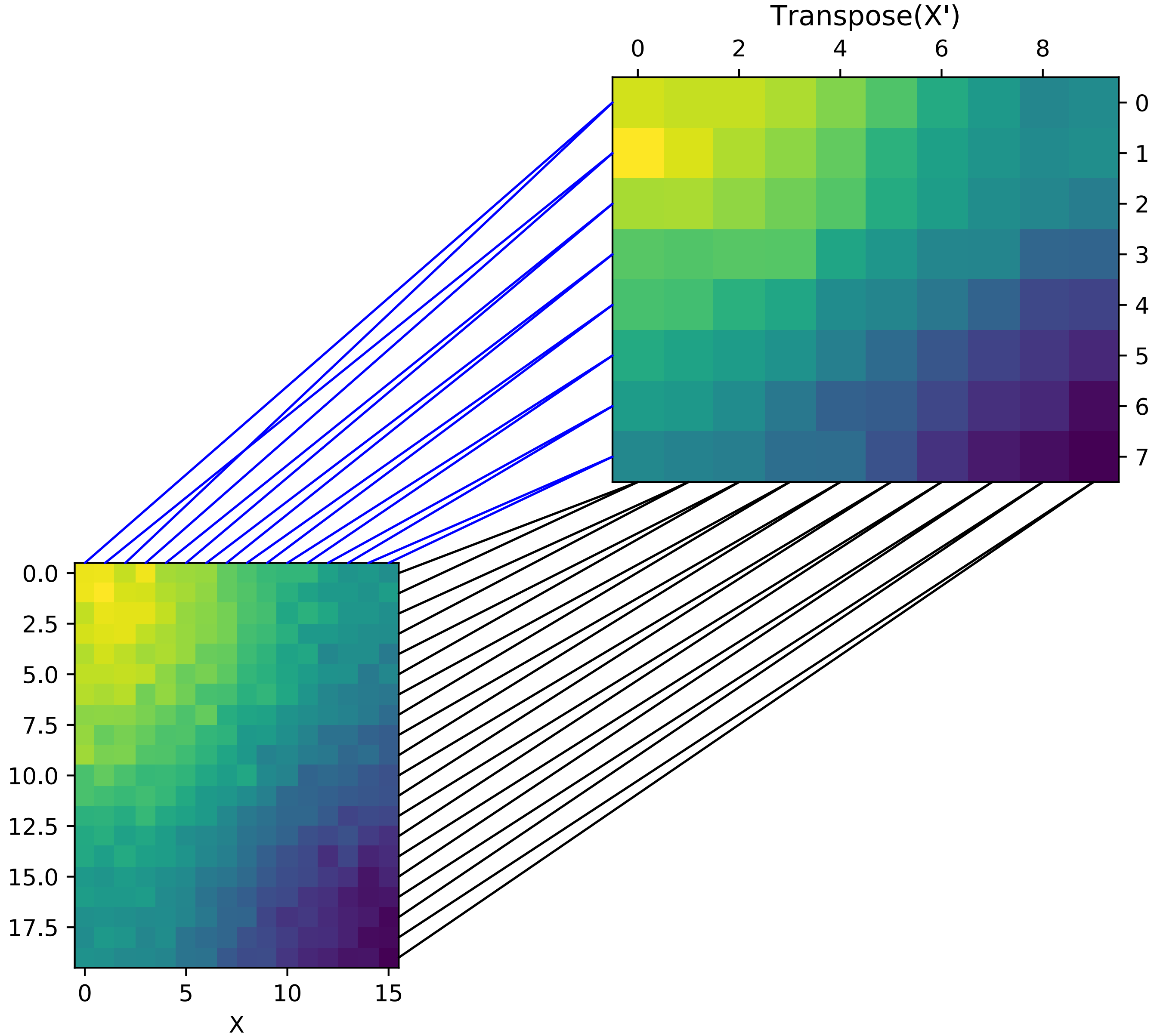

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CO-Optimal Transport

Motivations

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$\mathbf{X}' = [\mathbf{x}'_1, \ldots, \mathbf{x}'_{n'}]^T \in \mathbb{R}^{n' \times d'}$

Weights (histograms)

Samples: $\mathbf{w} \in \Sigma_n, \mathbf{w}' \in \Sigma_{n'}$

Features: $\mathbf{v} \in \Sigma_d, \mathbf{v}' \in \Sigma_{d'}$

CO-Optimal Transport

$$\min_{\substack{\boldsymbol{\pi}^s \in \Pi(\mathbf{w}, \mathbf{w}') \\ \boldsymbol{\pi}^v \in \Pi(\mathbf{v}, \mathbf{v}')}} \sum_{i,j,k,l} |X_{i,k} - X'_{j,l}|^p \boldsymbol{\pi}^s_{i,j} \boldsymbol{\pi}^v_{k,l}$$

$\boldsymbol{\pi}^s$: transport matrix between the samples

$\boldsymbol{\pi}^v$: transport matrix between the features/variables

CO-Optimal Transport

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$\boldsymbol{\pi}^s$: transport matrix between the samples

$\boldsymbol{\pi}^v$: transport matrix between the features/variables

Regularized version: add an entropy term for each transport matrix

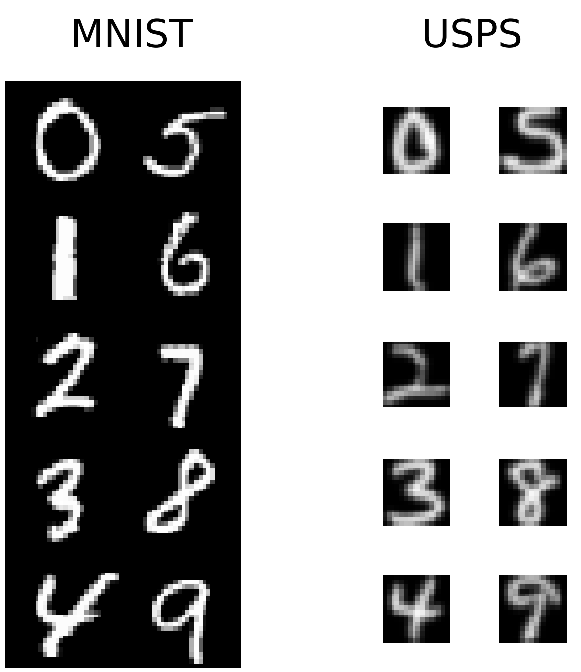
CO-Optimal Transport

Formulation & example

CO-Optimal Transport

$$\min_{\substack{\boldsymbol{\pi}^s \in \Pi(\mathbf{w},\mathbf{w}') \\ \boldsymbol{\pi}^v \in \Pi(\mathbf{v},\mathbf{v}')}} \quad \sum_{i,j,k,l} |X_{i,k} - X'_{j,l}|^p \boldsymbol{\pi}^s_{i,j} \boldsymbol{\pi}^v_{k,l}$$

MNIST/USPS example:



Samples: images, Features: pixels

$n = n' = 300$

$d = 256, d' = 784$

CO-Optimal Transport

Formulation & example

CO-Optimal Transport

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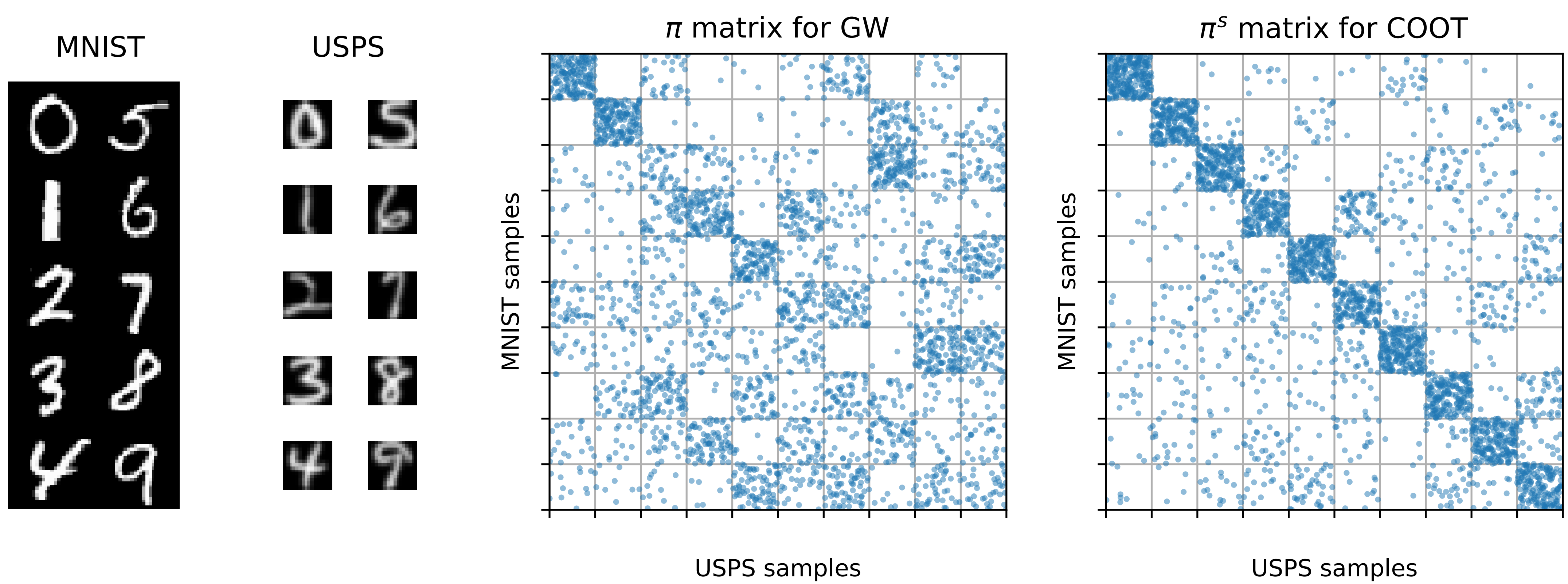
MNIST/USPS example:

Visualization of $\boldsymbol{\pi}^s$



Better class correspondence

CO-Optimal Transport

Formulation & example

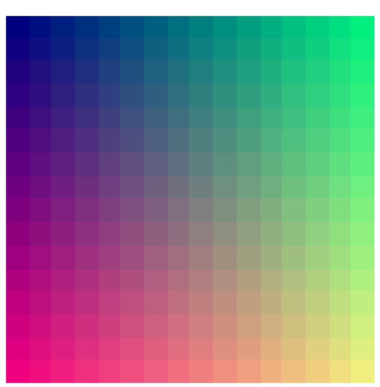
CO-Optimal Transport

$$\min_{\substack{\boldsymbol{\pi}^s \in \Pi(\mathbf{w},\mathbf{w}') \\ \boldsymbol{\pi}^v \in \Pi(\mathbf{v},\mathbf{v}')}} \quad \sum_{i,j,k,l} |X_{i,k} - X'_{j,l}|^p \boldsymbol{\pi}^s_{i,j} \boldsymbol{\pi}^v_{k,l}$$

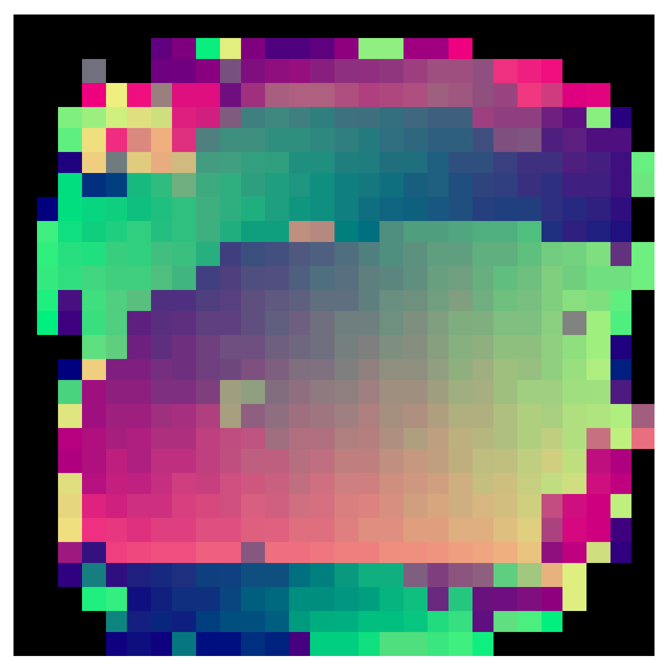
MNIST/USPS example:

Visualization of $\boldsymbol{\pi}^v$

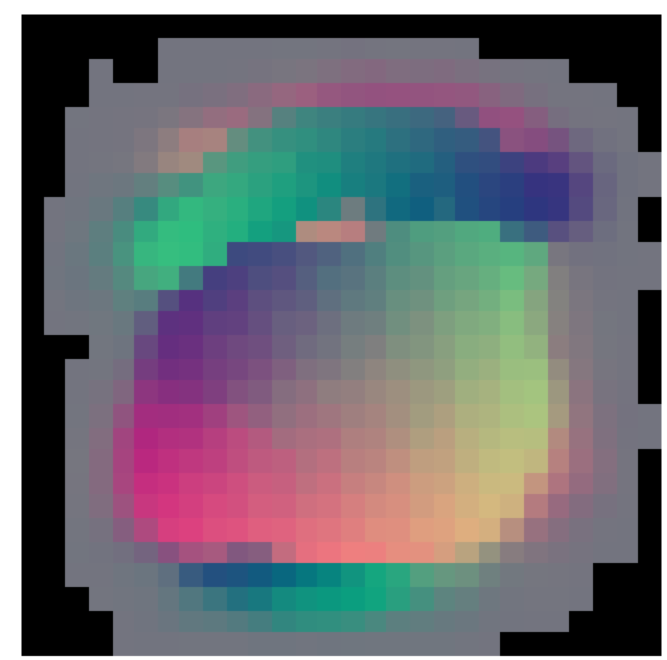
USPS colored pixels



MNIST pixels through π^v



MNIST pixels through entropic π^v



Spatial structure preserved (without supervision!)

CO-Optimal Transport

Properties

A distance w.r.t permutations of the datasets

Theorem. *COOT is a distance*

- *COOT symmetric and satisfies the triangular inequality,*

$$COOT(\mathbf{X}, \mathbf{X}'') \leq COOT(\mathbf{X}, \mathbf{X}') + COOT(\mathbf{X}', \mathbf{X}'')$$

- *Uniform weights.* $COOT(\mathbf{X}, \mathbf{X}') = 0$ *iff* $n = n', d = d'$, $\exists \sigma_1 \in S_n$ *(samples) and* $\exists \sigma_2 \in S_d$ *(features):*

$$\forall i, k \ \mathbf{X}_{i,k} = \mathbf{X}'_{\sigma_1(i), \sigma_2(k)}$$

CO-Optimal Transport

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Relation with Gromov-Wasserstein

Theorem.

- *Let* $\mathbf{C} \in \mathbb{R}^{n \times n}, \mathbf{C}' \in \mathbb{R}^{n' \times n'}$ *be any symmetric matrices, then:*

$$COOT(\mathbf{C}, \mathbf{C}', \mathbf{w}, \mathbf{w}', \mathbf{w}, \mathbf{w}') \leq GW(\mathbf{C}, \mathbf{C}', \mathbf{w}, \mathbf{w}').$$

- *When* $\mathbf{C}$ *and* $\mathbf{C}'$ *are squared Euclidean distance matrices:*

$$COOT(\mathbf{C}, \mathbf{C}', \mathbf{w}, \mathbf{w}', \mathbf{w}, \mathbf{w}') = GW(\mathbf{C}, \mathbf{C}', \mathbf{w}, \mathbf{w}')$$

and the optimal transport matrices $\boldsymbol{\pi}^{GW} = \boldsymbol{\pi}^{s} = \boldsymbol{\pi}^{v}$.

CO-Optimal Transport

Solving COOT

CO-Optimal Transport

$$\min_{\substack{\boldsymbol{\pi}^s \in \Pi(\mathbf{w},\mathbf{w}') \\ \boldsymbol{\pi}^v \in \Pi(\mathbf{v},\mathbf{v}')}} \quad \sum_{i,j,k,l} |X_{i,k} - X'_{j,l}|^p \boldsymbol{\pi}^s_{i,j} \boldsymbol{\pi}^v_{k,l}$$

Non-convex bilinear program: NP-Hard

BCD procedure: alternates OT problems -> converges to a local minima [Konno 1976]

Algorithm 1 BCD for COOT

1: $\pi^s_{(0)} \leftarrow \mathbf{w}\mathbf{w}'^T, \pi^v_{(0)} \leftarrow \mathbf{v}\mathbf{v}'^T, k \leftarrow 0$
2: **while** $k <$ maxIt **and** $err > 0$ **do**
3: $\quad \boldsymbol{\pi}^v_{(k)} \leftarrow OT(\mathbf{v}, \mathbf{v}', \mathbf{L}(\mathbf{X}, \mathbf{X}') \otimes \boldsymbol{\pi}^s_{(k-1)})$
4: $\quad \boldsymbol{\pi}^s_{(k)} \leftarrow OT(\mathbf{w}, \mathbf{w}', \mathbf{L}(\mathbf{X}, \mathbf{X}') \otimes \boldsymbol{\pi}^v_{(k-1)})$
5: $\quad err \leftarrow ||\boldsymbol{\pi}^v_{(k-1)} - \boldsymbol{\pi}^v_{(k)}||_F$
6: $\quad k \leftarrow k + 1$
7: **end while**

CO-Optimal Transport

Solving COOT

CO-Optimal Transport

$$\min_{\substack{\boldsymbol{\pi}^s \in \Pi(\mathbf{w},\mathbf{w}') \\ \boldsymbol{\pi}^v \in \Pi(\mathbf{v},\mathbf{v}')}} \quad \sum_{i,j,k,l} |X_{i,k} - X'_{j,l}|^p \boldsymbol{\pi}^s_{i,j} \boldsymbol{\pi}^v_{k,l}$$

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1: $\pi^s_{(0)} \leftarrow \mathbf{w}\mathbf{w}'^T, \pi^v_{(0)} \leftarrow \mathbf{v}\mathbf{v}'^T, k \leftarrow 0$

2: **while** $k <$ maxIt **and** $err > 0$ **do**

3: $\quad \boldsymbol{\pi}^v_{(k)} \leftarrow OT(\mathbf{v}, \mathbf{v}', \mathbf{L}(\mathbf{X}, \mathbf{X}') \otimes \boldsymbol{\pi}^s_{(k-1)}) \sim O(n^3 \log(n)) \; (p = 2)$

4: $\quad \boldsymbol{\pi}^s_{(k)} \leftarrow OT(\mathbf{w}, \mathbf{w}', \mathbf{L}(\mathbf{X}, \mathbf{X}') \otimes \boldsymbol{\pi}^v_{(k-1)}) \sim O(d^3 \log(d)) \; (p = 2)$

5: $\quad err \leftarrow ||\boldsymbol{\pi}^v_{(k-1)} - \boldsymbol{\pi}^v_{(k)}||_F$

6: $\quad k \leftarrow k + 1$

7: **end while**

CO-Optimal Transport

Solving COOT

CO-Optimal Transport

$$\min_{\substack{\boldsymbol{\pi}^s \in \Pi(\mathbf{w},\mathbf{w}') \\ \boldsymbol{\pi}^v \in \Pi(\mathbf{v},\mathbf{v}')}} \sum_{i,j,k,l} |X_{i,k} - X'_{j,l}|^p \boldsymbol{\pi}^s_{i,j} \boldsymbol{\pi}^v_{k,l}$$

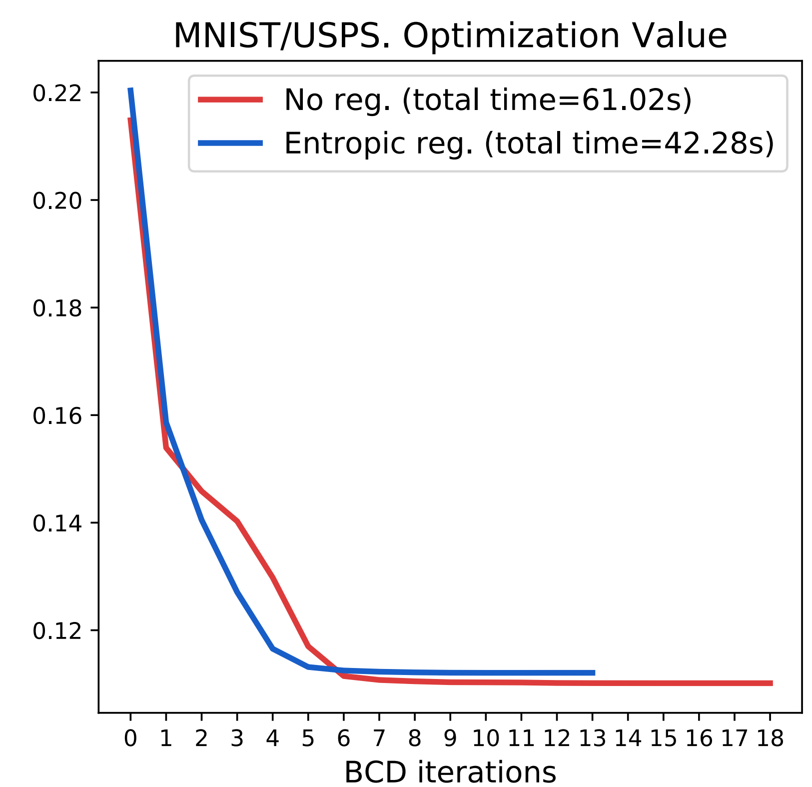
Non-convex bilinear program: NP-Hard

BCD procedure: alternates OT problems -> converges to a local minima [Konno 1976]

Algorithm 1 BCD for COOT

1: $\pi^s_{(0)} \leftarrow \mathbf{w}\mathbf{w}'^T, \pi^v_{(0)} \leftarrow \mathbf{v}\mathbf{v}'^T, k \leftarrow 0$
2: **while** $k <$ maxIt **and** $err > 0$ **do**
3: $\quad \boldsymbol{\pi}^v_{(k)} \leftarrow OT(\mathbf{v}, \mathbf{v}', \mathbf{L}(\mathbf{X}, \mathbf{X}') \otimes \boldsymbol{\pi}^s_{(k-1)})$
4: $\quad \boldsymbol{\pi}^s_{(k)} \leftarrow OT(\mathbf{w}, \mathbf{w}', \mathbf{L}(\mathbf{X}, \mathbf{X}') \otimes \boldsymbol{\pi}^v_{(k-1)})$
5: $\quad err \leftarrow ||\boldsymbol{\pi}^v_{(k-1)} - \boldsymbol{\pi}^v_{(k)}||_F$
6: $\quad k \leftarrow k + 1$
7: **end while**

In practice BCD converges in few iterations



CO-Optimal Transport

Domain adaptation in a nutshell

Given a source domain with labels

$$\mathbf{X}_s = \{\mathbf{x}_i^s\}_{i=1}^{N_s}$$
$$\mathbf{Y}_s = \{\mathbf{y}_i^s\}_{i=1}^{N_s}$$

CO-Optimal Transport

Domain adaptation in a nutshell

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A target domain

$$\mathbf{X}_t = \{\mathbf{x}_i^t\}_{i=1}^{N_t}$$

Apply/learn a classifier on

CO-Optimal Transport

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Apply/learn a classifier on

A target domain

$$\mathbf{X}_t = \{\mathbf{x}_i^t\}_{i=1}^{N_t}$$

related but
different domains..

CO-Optimal Transport

Domain adaptation in a nutshell

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$$\mathbf{X}_s = \{\mathbf{x}_i^s\}_{i=1}^{N_s}$$
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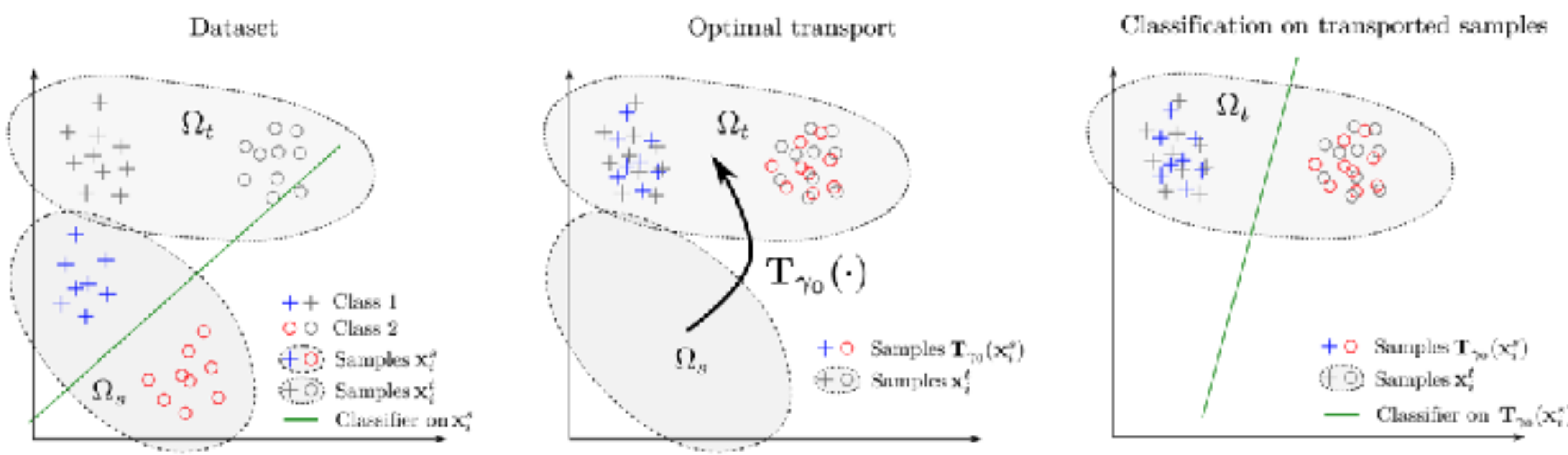

[Courty 2015]

$$\boldsymbol{\pi}^s \leftarrow OT(\mathbf{X}_s, \mathbf{X}_t)$$

Barycentric mapping:

$$\hat{\mathbf{X}}_s = T_{\boldsymbol{\pi}^s}(\mathbf{X}_s) = N_s \boldsymbol{\pi}^s \mathbf{X}_t$$

[Redko 2019]

Label propagation:

$$\hat{\mathbf{Y}}_t = \boldsymbol{\pi}^s \mathbf{Y}_s$$

CO-Optimal Transport

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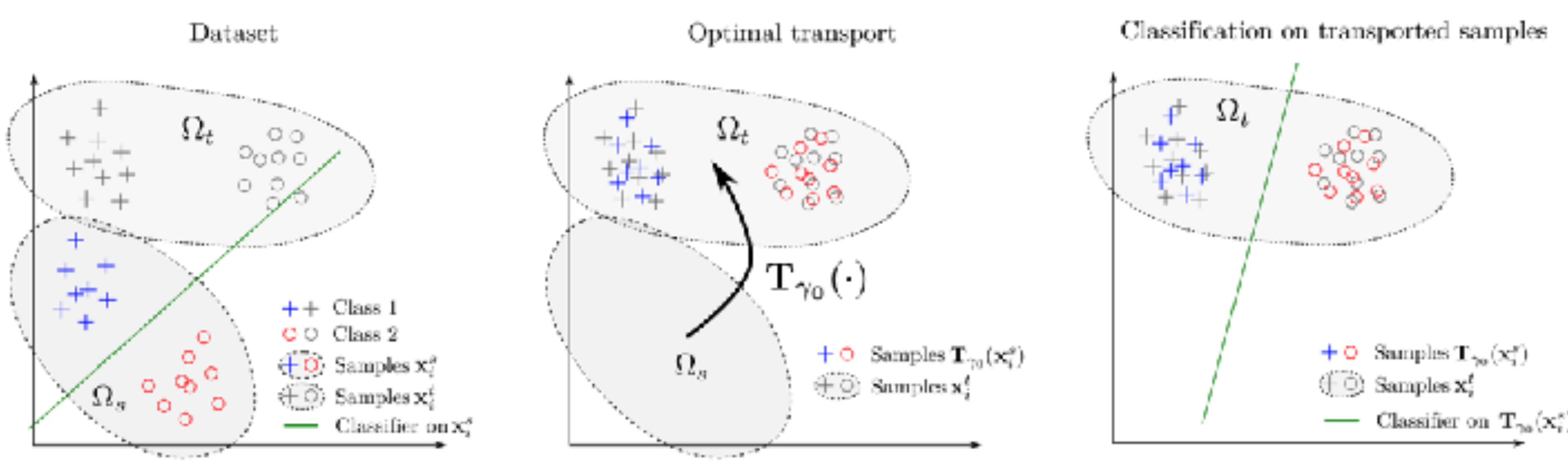

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[Redko 2019]

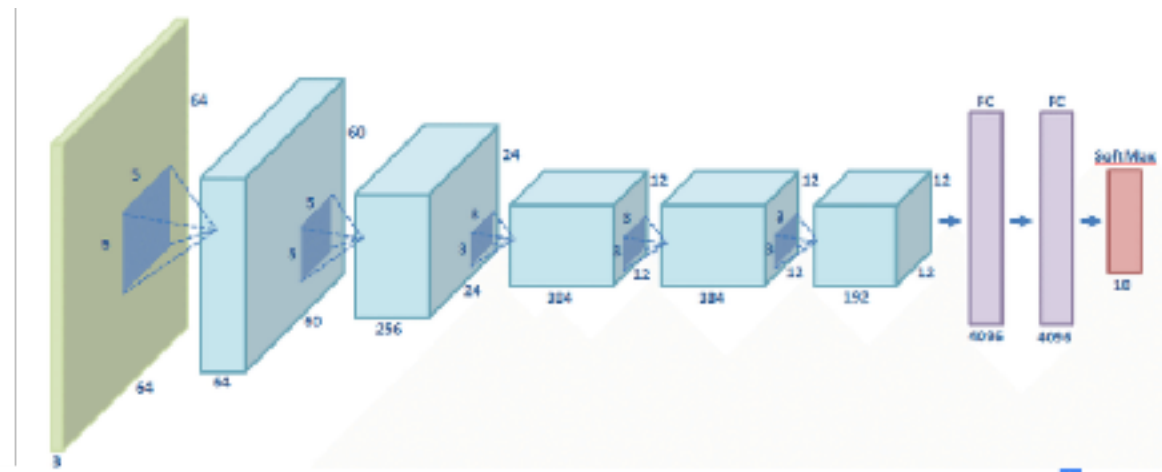
Label propagation:

$$\hat{\mathbf{Y}}_t = \boldsymbol{\pi}^s \mathbf{Y}_s$$

$$\text{(HDA) } \mathbf{X}_s \in \mathbb{R}^{N_s \times d} \text{ and } \mathbf{X}_t \in \mathbb{R}^{N_t \times d'} \text{ with } d \neq d'$$

CO-Optimal Transport

COOT in action: Heterogeneous Domain Adaptation



- Caltech/Officie dataset [Saenko 2010] $\boldsymbol{\pi}^s, \boldsymbol{\pi}^v \leftarrow \mathrm{COOT}(\mathbf{X}_s, \mathbf{X}_t)$
- Adaptation from two different embeddings from Decaf to GoogleNet $\mathbb{R}^{4096} \rightarrow \mathbb{R}^{1024}$
- Unsupervised HDA + Semi supervised HDA (3 samples per class)
- Label propagation [Redko 2019] $\hat{\mathbf{Y}}_t = \boldsymbol{\pi}^s \mathbf{Y}_s$

CO-Optimal Transport

COOT in action: Heterogeneous Domain Adaptation

Semi supervised HDA

Domains	No-adaptation baseline	CCA	KCCA	EGW	SGW	COOT
C→W	69.12±4.82	11.47±3.78	66.76±4.40	11.35±1.93	78.88±3.90	**83.47±2.60**
W→C	83.00±3.95	19.59±7.71	76.76±4.70	11.00±1.05	92.41±2.18	**93.65±1.80**
W→W	82.18±3.63	14.76±3.15	78.94±3.94	10.18±1.64	93.12±3.14	**93.94±1.84**
W→A	84.29±3.35	17.00±12.41	78.94±6.13	7.24±2.78	93.41±2.18	**94.71±1.49**
A→C	83.71±1.82	15.29±3.88	76.35±4.07	9.82±1.37	80.53±6.80	**89.53±2.34**
A→W	81.88±3.69	12.59±2.92	81.41±3.93	12.65±1.21	87.18±5.23	**92.06±1.73**
A→A	84.18±3.45	13.88±2.88	80.65±3.03	14.29±4.23	82.76±6.63	**92.12±1.79**
C→C	67.47±3.72	13.59±4.33	60.76±4.38	11.71±1.91	77.59±4.90	**83.35±2.31**
C→A	66.18±4.47	13.71±6.15	63.35±4.32	11.82±2.58	75.94±5.58	**82.41±2.79**
Mean	78.00±7.43	14.65±2.29	73.77±7.47	11.12±1.86	84.65±6.62	**89.47±4.74**
p-value	$<.001$	$<.001$	$<.001$	$<.001$	$<.001$	-

Caltech/Officie dataset [Saenko 2010]

$$\boldsymbol{\pi}^s, \boldsymbol{\pi}^v \leftarrow \mathrm{COOT}(\mathbf{X}_s, \mathbf{X}_t)$$

Adaptation from two different embeddings from Decaf to GoogleNet $\mathbb{R}^{4096} \rightarrow \mathbb{R}^{1024}$

Unsupervised HDA + Semi supervised HDA (3 samples per class)

Label propagation [Redko 2019] $\hat{\mathbf{Y}}_t = \boldsymbol{\pi}^s \mathbf{Y}_s$

CO-Optimal Transport

COOT in action: Heterogeneous Domain Adaptation

Unsupervised HDA

Domains	CCA	KCCA	EGW	COOT
C→W	14.20±8.60	21.30±15.64	10.55±1.97	**25.50±11.76**
W→C	13.35±3.70	18.60±9.44	10.60±0.94	**35.40±14.61**
W→W	10.95±2.36	13.25±6.34	10.25±2.26	**37.10±14.57**
W→A	14.25±8.14	23.00±22.95	9.50±2.47	**34.25±13.03**
A→C	11.40±3.23	11.50±9.23	11.35±1.38	**17.40±8.86**
A→W	19.65±17.85	28.35±26.13	11.60±1.30	**30.95±18.19**
A→A	11.75±1.82	14.20±4.78	13.10±2.35	**42.85±17.65**
C→C	12.00±4.69	14.95±6.79	12.90±1.46	**42.85±18.44**
C→A	15.35±6.30	23.35±17.61	12.95±2.63	**33.25±15.93**
Mean	13.66±2.55	18.72±5.33	11.42±1.24	**33.28±7.61**
p-value	<.001	<.001	<.001	-

Caltech/Officie dataset [Saenko 2010]

$\boldsymbol{\pi}^s, \boldsymbol{\pi}^v \leftarrow \mathrm{COOT}(\mathbf{X}_s, \mathbf{X}_t)$

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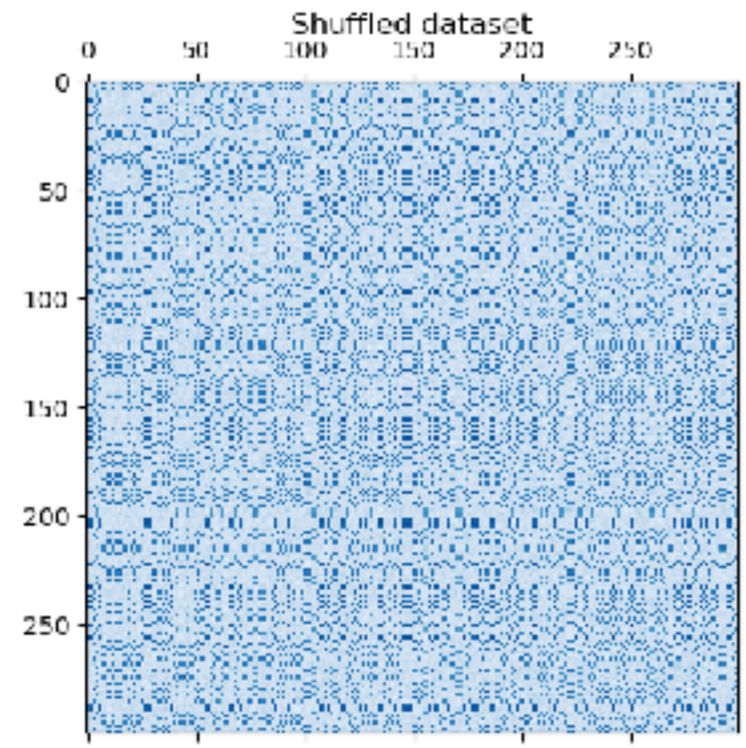
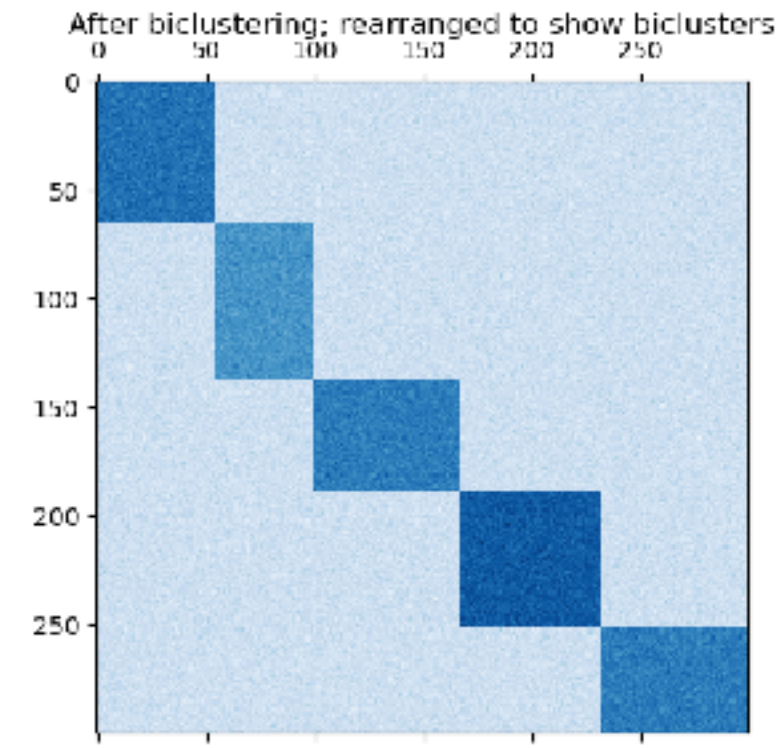
CO-Optimal Transport

COOT in action: CO-clustering

Search for a simultaneous clustering of both samples and features of a dataset

$$\mathbf{X} \in \mathbb{R}^{n \times d}$$





CO-Optimal Transport

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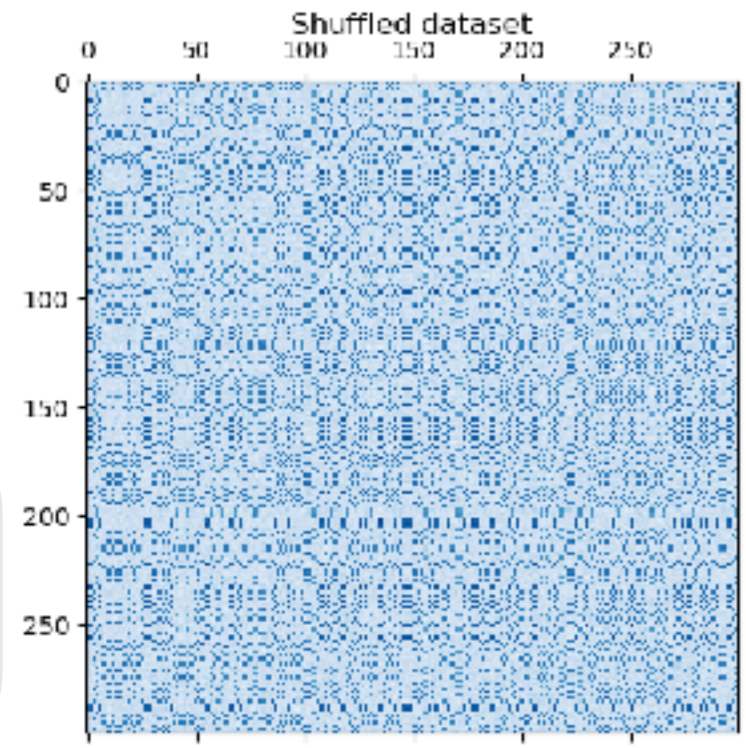
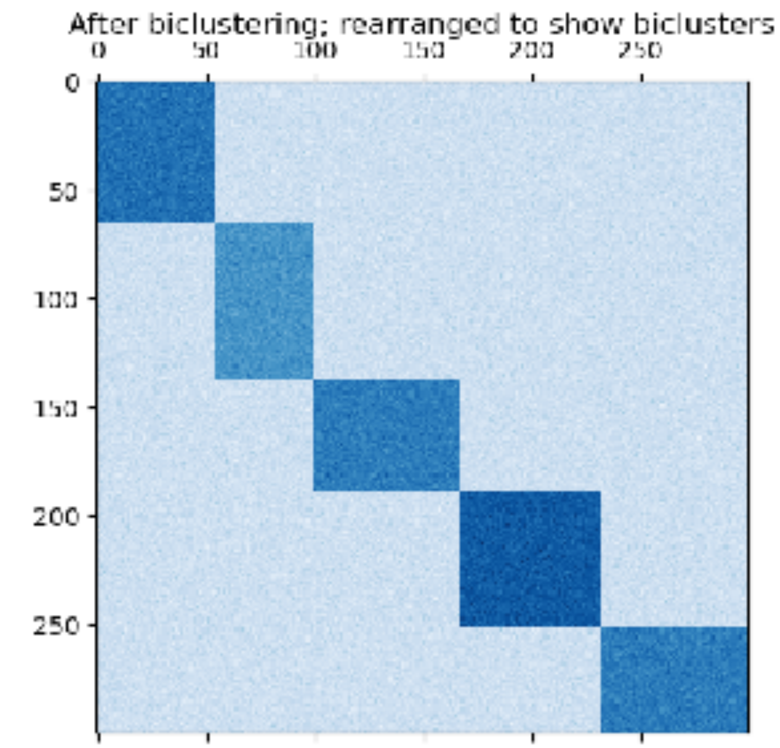




COOT CO-clustering

$$\min_{\mathbf{X}_c \in \mathbb{R}^{n' \times d'}} \text{COOT}(\mathbf{X}, \mathbf{X}_c)$$

$\mathbf{X}_c$ with $n' < n,\ d' < d$ that summarizes $\mathbf{X}$ in the best way possible.

Solved by BCD

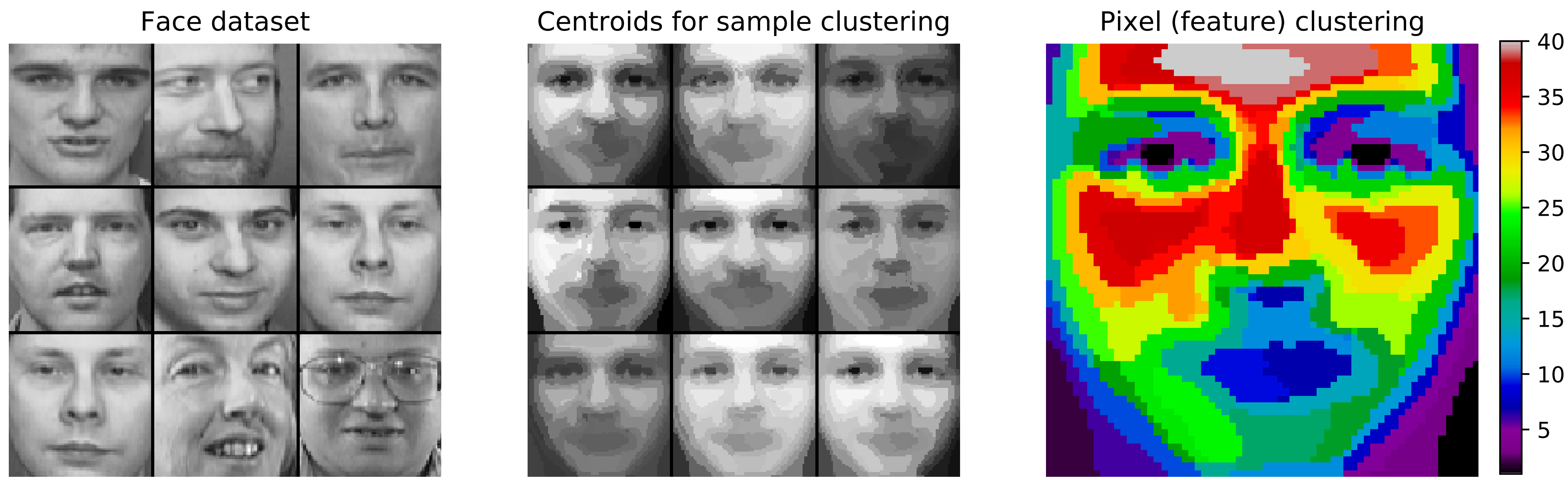
1. Obtain $\boldsymbol{\pi}^s$ and $\boldsymbol{\pi}^v$ by solving $\text{COOT}(\mathbf{X}, \mathbf{X}_c)$
2. Set $\mathbf{X}_c$ to $n'd'\boldsymbol{\pi}^{s\top}\mathbf{X}\boldsymbol{\pi}^v$.

CO-Optimal Transport

COOT in action: CO-clustering

$$\min_{\mathbf{X}_c \in \mathbb{R}^{n' \times d'}} \mathrm{COOT}(\mathbf{X}, \mathbf{X}_c)$$

Olivetti faces dataset [Samaria 1994]



CO-Optimal Transport

COOT in action: CO-clustering

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Olivetti faces dataset
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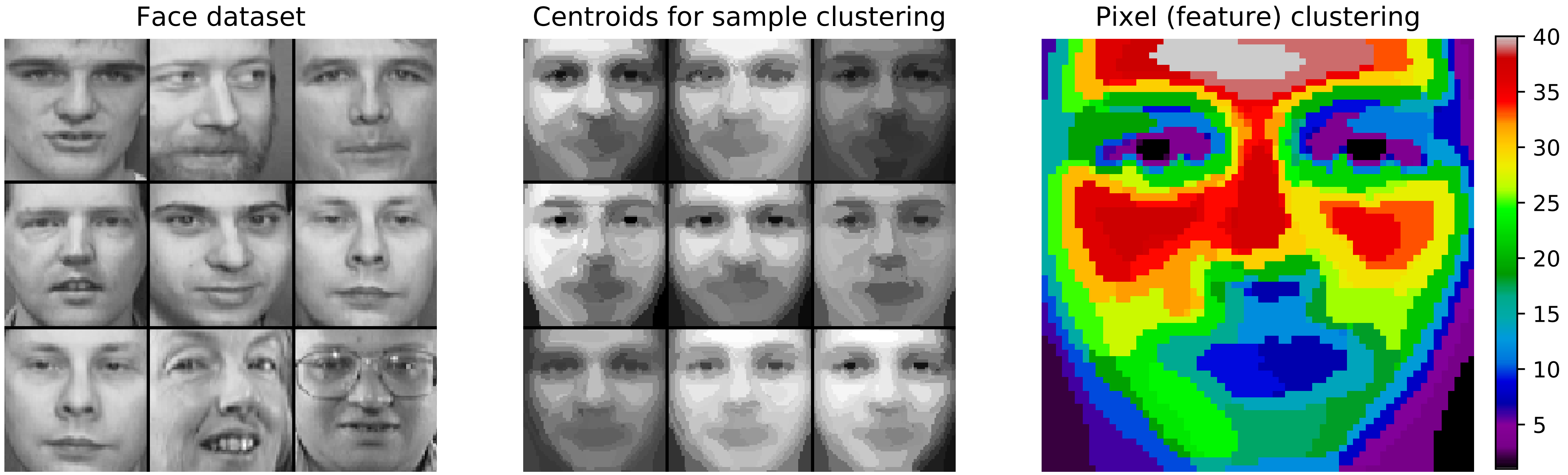

SOTA on simulated benchmark dataset from [Laclau 2017]

CO-Optimal Transport

COOT in action: CO-clustering

$$\min_{\mathbf{X}_c \in \mathbb{R}^{n' \times d'}} \mathrm{COOT}(\mathbf{X}, \mathbf{X}_c)$$

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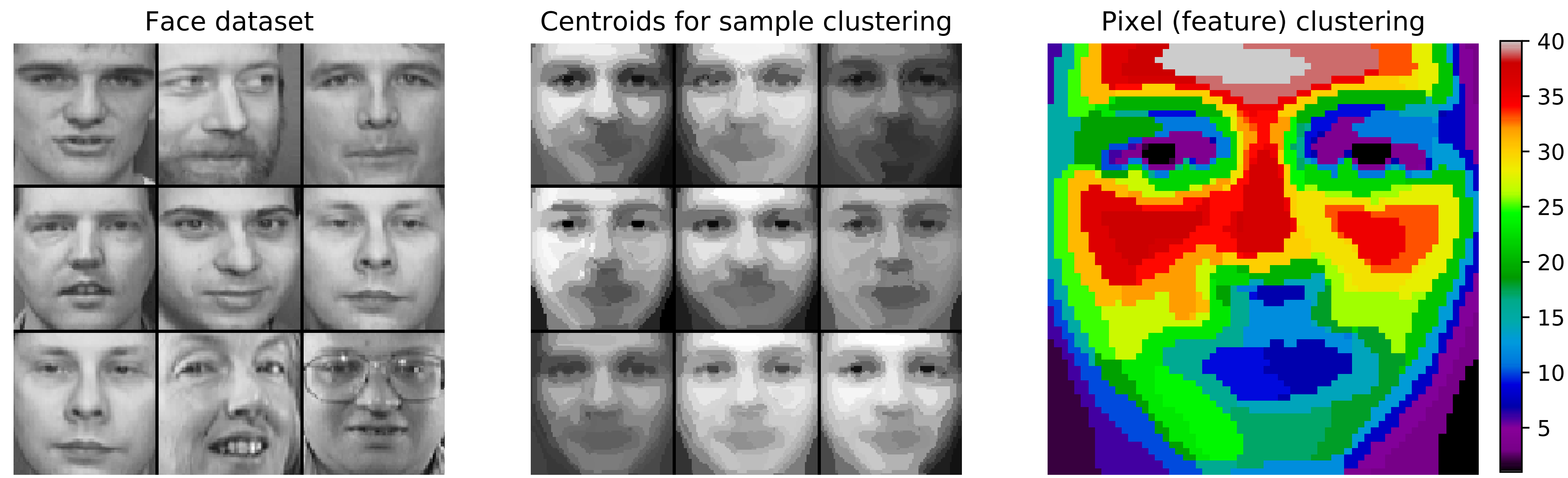


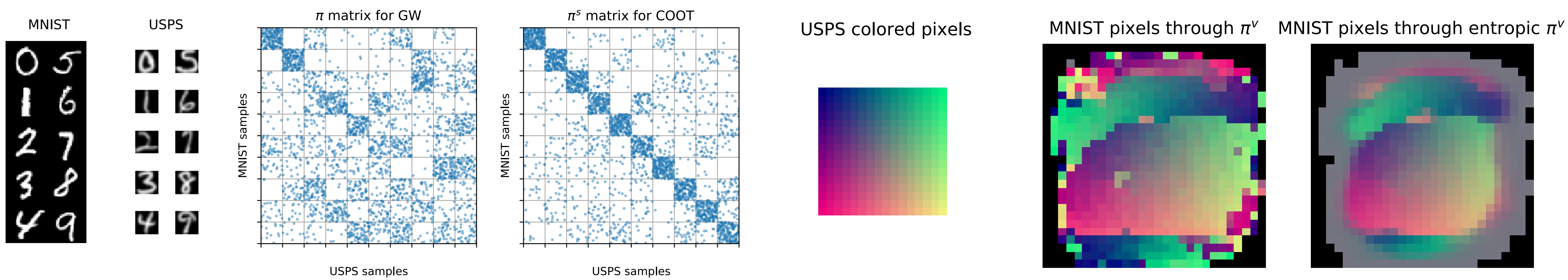
SOTA on simulated benchmark dataset from [Laclau 2017]

Movielens dataset (users and films)

M1	M20
Shawshank Redemption (1994)	Police Story 4: Project S (Chao ji ji hua) (1993)
Schindler's List (1993)	Eye of Vichy, The (Oeil de Vichy, L') (1993)
Casablanca (1942)	Promise, The (Versprechen, Das) (1994)
Rear Window (1954)	To Cross the Rubicon (1991)
Usual Suspects, The (1995)	Daens (1992)

CO-Optimal Transport

Conclusion: take away messages



COOT

OT method for heterogeneous dataset

Provides interpretable correspondences between samples and features

Works well for HDA + Can be applied for co-clustering

Perspectives

Study the statistics of COOT $(n, d \to \infty \ ?)$

Other formulations (unbalanced, extension to labeled dataset)

Effect of the entropic regularization (convergence), effect of the feature weights)

Thank you!