Fused Gromov Wasserstein distance

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Optimal Transport for structured data

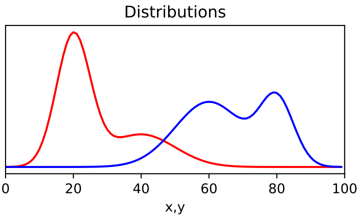
Classical Optimal Transport deals with distribution but can not leverage the specific relation amoung the component of the distribution.

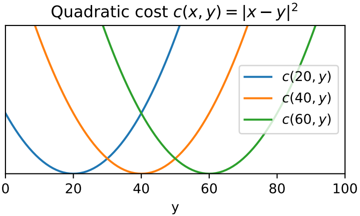
- How to include this structural information in the optimal transportation formulation ?
- How to use the new formulation in order to compare structured data (graphs, times series...)

Overview

1. Generality about Optimal Transport
   - Wasserstein distance
   - Gromov-Wasserstein distance
2. Structured data as distributions
3. A novel OT distance for structured data : Fused Gromov-Wasserstein distance

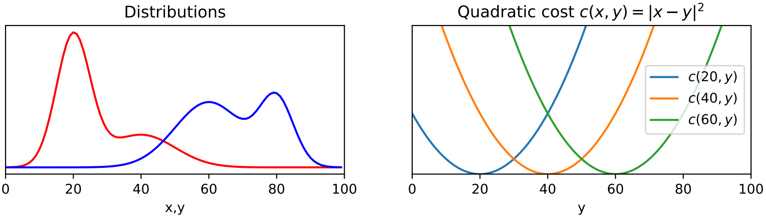
- Mathematical tools aiming at comparing distributions





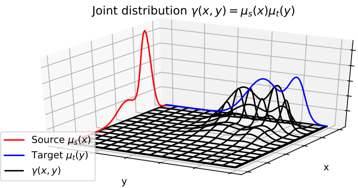
Optimal transport (Monge formulation)

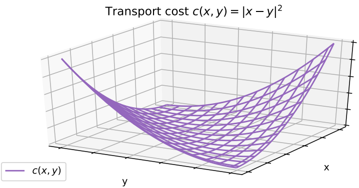
- Mathematical tools aiming at comparing distributions



- Probability measures μ_s and μ_t on Ω_s, Ω_t with a cost function $d : \Omega_s \times \Omega_t \rightarrow \mathbb{R}^+$.
- The Monge formulation aim at finding a mapping $T : \Omega_s \rightarrow \Omega_t$

$$\inf_{T\#\mu_s=\mu_t} \int_{\Omega_s} d(x, T(x))\mu_s(x)dx \tag{1}$$



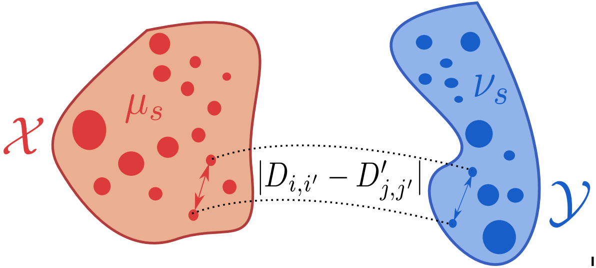


$\mu_s = \sum_{i=1}^n a_i \delta_{x_i}$ and $\mu_t = \sum_{j=1}^m b_j \delta_{y_j}$ on a commun ground space equipped with a distance

- The Kantorovich formulation seeks for a probabilistic coupling $\pi \in \Pi(\mu_s \times \mu_t)$ between μ_s and μ_t.
- π is a joint probability measure with prescribed marginals μ_s and μ_t.
- Computes the Wasserstein distance :

$$\mathcal{W}_p(\mu_s, \mu_t) = \left(\min_{\pi \in \Pi(\mu_s, \mu_t)} \sum_{i,j} d(x_i, y_j)^q \pi_{i,j} \right)^{\frac{1}{p}} \tag{2}$$

Optimal transport distance over measures with no common ground space. Compare the intrinsic distances in each space.



Inspired from Gabriel Peyré

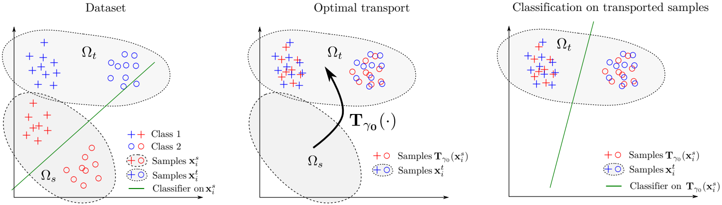
$\mu_s = \sum_i a_i \delta_{v_i}$ and $\mu_t = \sum_j b_j \delta_{w_j}$

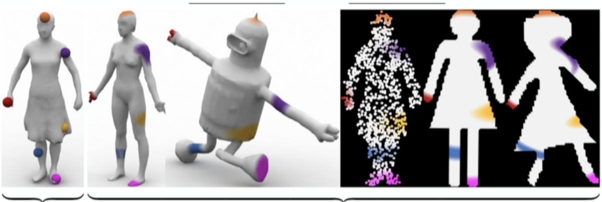
$$\mathcal{GW}_p(D, D', \mu_s, \mu_t) = \left(\min_{\pi \in \Pi(\mu_s, \mu_t)} \sum_{i,j,k,l} |D_{i,k} - D'_{j,l}|^p \pi_{i,j}\, \pi_{k,l} \right)^{\frac{1}{p}}$$

Optimal transport in Machine Learning

Numerous applications for this two distances. Some of them :

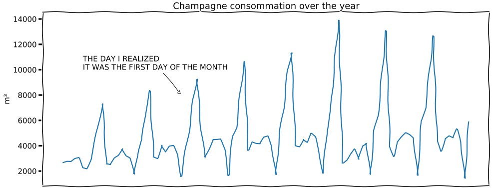
- Learning with Wasserstein Loss [FZM+15]
- Wasserstein GAN's [ACB17]
- Domain Adaptation [CFTR17]
- Image colorization [FPPA14], Dictionary Learning [RCP16] ...
- For GW : Shape comparaison [Mem11], shape barycenter [PCS16].

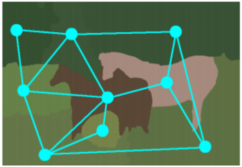




Why Structured data are interesting ?

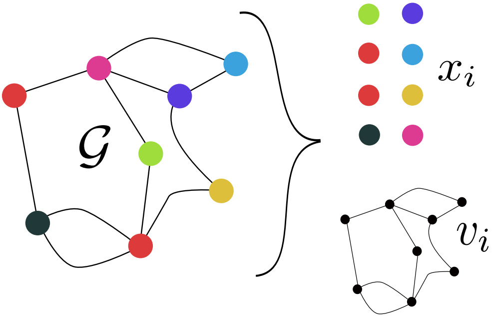
- Systems are usually complex compositions of entities and their interactions
- Crucial to include structural information in order to learn from small amounts of experience [BHB+18]
- A structure data is viewed as a combination of features informations linked within each other by some structural information.





Structured data as distributions

Graphs are natural representations of discrete structured data of the type $\mu = \sum_{i=1}^{n} a_i \delta_{(x_i, v_i)}$:



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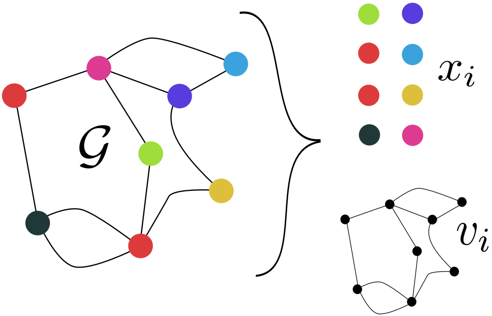


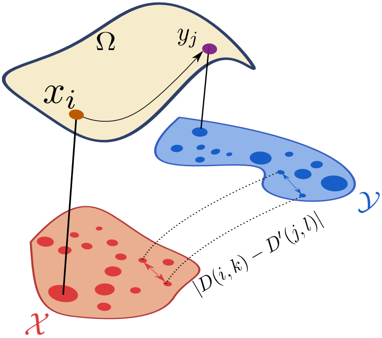
Problem when comparing two structured data on (x_i, v_i) and (y_j, w_j)

- Features value x_i and y_j can be compared through the common metric
- But no common between the structure points v_i and w_j

A novel OT distance for structured data : Fused Gromov-Wasserstein distance

→ Combining Wasserstein and Gromov-Wasserstein approach we define for measure on structured data $\mu_s = \sum_{i=1}^{n} a_i \delta_{x_i, v_i}$ and $\mu_t = \sum_{j=1}^{m} b_j \delta_{y_j, w_j}$

$$\mathcal{FGW}_{p,q,\alpha}(D, D', \mu_s, \mu_t) = \left(\min_{\pi \in \Pi(\mu_s, \mu_t)} \sum_{i,j,k,l} \left((1-\alpha) d(x_i, y_j)^q + \alpha |D_{i,k} - D'_{j,l}|^q \right)^p \pi_{i,j} \, \pi_{k,l} \right)^{\frac{1}{p}}$$



for $\alpha \in [0, 1]$ a trade off parameter between structure and features

Algorithmic solution

- Optimization problem is a non-convex Quadratic program : can be solved with Conditional gradient [FPPA14] with OT solver.
- Convergence in local minima insured by Frank-Wolfe algorithm proprieties [LJ16].

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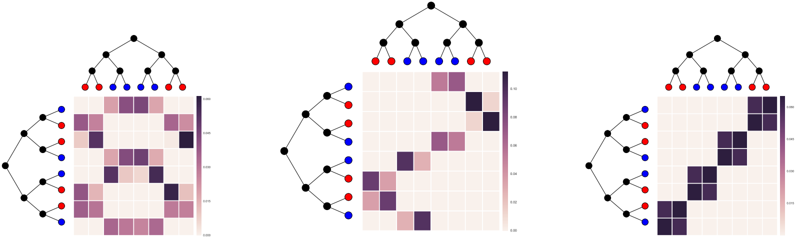
- Optimization problem is a non-convex Quadratic program : can be solved with Conditional gradient [FPPA14] with OT solver.
- Convergence in local minima insured by Frank-Wolfe algorithm proprieties [LJ16].
- Entropic regularization can be defined and allows Projected gradients with Sinkhorn [PCS16] using Bregman projections.

Optimal maps on toy trees as α increases



(c) $W = 0$ (d) $FGW \neq 0$ (e) $GW = 0$

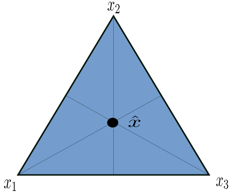
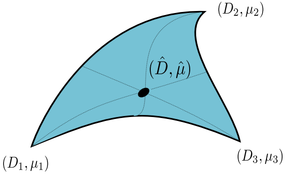
Application of FGW distance

We use our distance for graph classification and compare accuracies on classical graph datasets with state-of-the-art graph kernel approaches and CNN approach.

	Labeled Graphs			Social Graphs		Vector attributes Graph	
Dataset	MUTAG	PTC	NCI1	IMDB-B	IMDB-M	PROTEIN	ENZYMES
WL	80.72±3.0	56.97±2.0	80.22±0.5	-	-	72.9±0.5	53.7±1.4
GK	81.58±2.1	57.32±1.1	43.89±0.4	65.87±0.98	43.89±0.38	62.28±0.29	-
RW	83.68±1.66	57.26±1.30	-	-	-	74.22± 0.42	-
SP	85.79±2.51	58.53±2.55	73.00±0.51	-	-	75.07 ±0.54	-
WL-OA	84.5±1.7	**63.6±1.5**	**86.1±0.2**	-	-	76.4 ±0.4	59.9 ±1.1
PSCN $k = 10$	**88.95±4.37**	62.29±5.62	76.34±1.68	**71.00±2.29**	45.23±2.84	75.00±2.51	-
FGW CG	86.8±5.4	58.3±8.4	78.7±1.9	66.4±3.6	**48.5±3.0**	76.0±1.9	**66.3±6.5**
FGW SINK	81.6±5.9	56.9±6.6	75.3±2.3	70.6±2.8	45.5±2.8	**77.0±4.0**	55.5±5.1

FGW barycenter

We define barycenter of structured data using Fréchet mean :

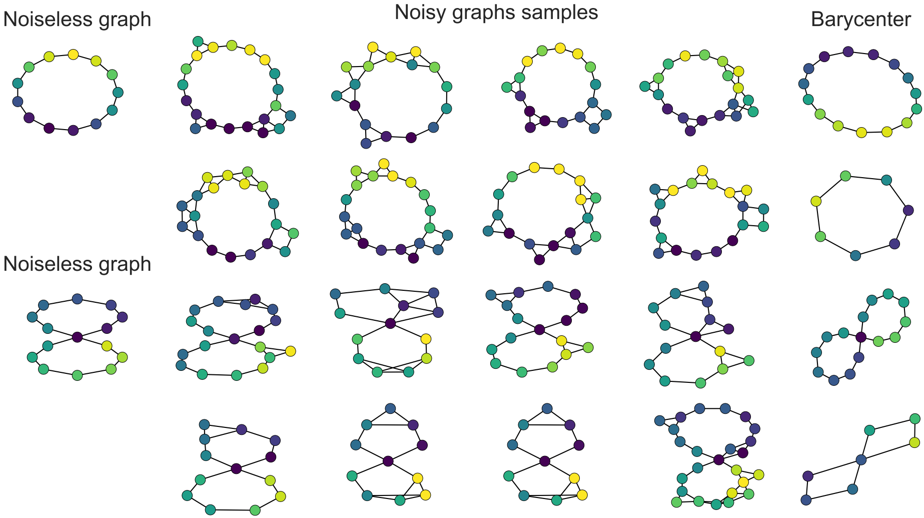
Euclidean barycenter	FGW barycenter
	
$\underset{x}{min} \sum_k \lambda_k \|x - x_k\|^2$	$\min_{D \in \mathbb{R}^{N \times N}, \mu} \sum_k \lambda_k \mathcal{FGW}_{1,q,\alpha}(D, D_k, \mu, \mu_k)$

Barycenters solved via block coordinate relaxation. Several variants of this problem :

- Computing the structure with fixed features
- Computing the features with fixed structure.
- Both features and structured unknown

FGW barycenter

We applied on toy noisy graphs :



Conclusion

- New versatile method for comparing structured data based on Optimal Transport
- Many desirable distance properties
- New notion of barycenter of structured data such as graphs or time series
- Promising applications for signal over graphs and deep learning for structured data

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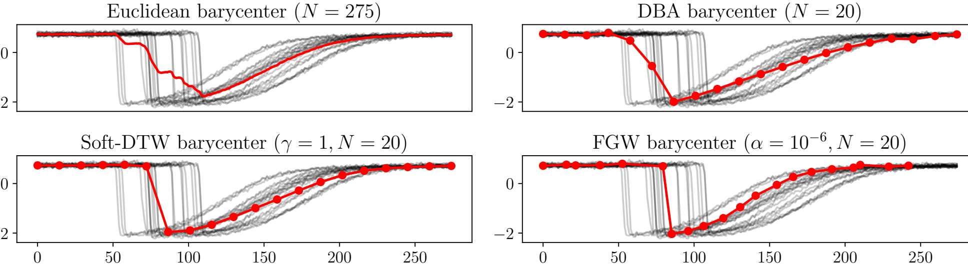
FGW barycenter

We also applied our barycenter on real time serie dataset and compare with state-of-the-art methods [CB17] [PKG11]



FGW barycenter

Application in mesh interpolation :