Learning on graphs with Gromov-Wasserstein

From unsupervised learning to GNN

R. Flamary - CMAP, École Polytechnique, Institut Polytechnique de Paris

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Optimal Transport and Machine Leranin Workshow, Neurips 2023, New Orleans.

Collaborators about OT on graphs


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T. Vayer


L. Chapel


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H. Tran


G. Gasso


M. Corneli


H. Van Assel


C. Vincent-Cuaz

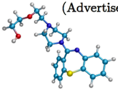

A. Thual


B. Thirion

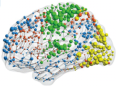

F. d'Alché-Buc


L. Brogat-Motte

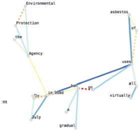
Social networks (Advertisement)



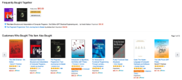
Drug/Material molecules (Chemistry)



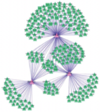
Brain connectivity (Neuroscience)



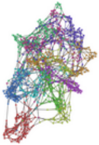
Words relationships (NLP)



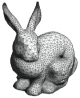
Recommender systems (Amazon, Netflix)



Gene Regulatory Network

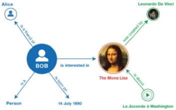
= 

Graphs/ Networks

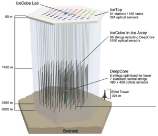


3D Meshes (Computer Graphics)

Transportation networks



Knowledge graph (Causality)



Neutrino detection (High-energy Physics)

- Classical approach: spectral and Fourier based analysis and processing (GNN)
- What I will talk about: modeling graph as probability distributions (and use OT)

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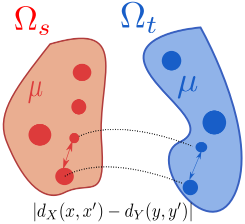
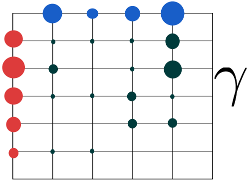
Dictionary learning with OT

Structured graph prediction with OT

Graph classification with OT

Optimal Transport and divergences between graphs





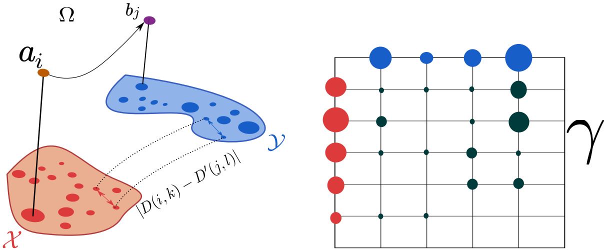
Inspired from Gabriel Peyré

GW for discrete distributions [Memoli, 2011]

$$\mathcal{GW}_p^p(\mu_s,\mu_t) = \min_{T\in\Pi(\mu_s,\mu_t)} \sum_{i,j,k,l} |D_{i,k} - D'_{j,l}|^p T_{i,j}\, T_{k,l}$$

with $\mu_s = \sum_i a_i \delta_{\mathbf{x}_i^s}$ and $\mu_t = \sum_j b_j \delta_{x_j^t}$ and $D_{i,k} = \|\mathbf{x}_i^s - \mathbf{x}_k^s\|$, $D'_{j,l} = \|\mathbf{x}_j^t - \mathbf{x}_l^t\|$

- Distance between metric measured spaces : across different spaces.
- Search for an OT plan that preserve the pairwise relationships between samples.
- Entropy regularized GW proposed in [Peyré et al., 2016].
- Fused GW interpolates between Wass. and GW [Vayer et al., 2018].



FGW for discrete distributions [Vayer et al., 2018]

$$\mathcal{FGW}_p^p(\mu_s, \mu_t) = \min_{T \in \Pi(\mu_s, \mu_t)} \sum_{i,j,k,l} \left((1-\alpha) C_{i,j}^q + \alpha |D_{i,k} - D'_{j,l}|^q\right)^p T_{i,j} T_{k,l}$$

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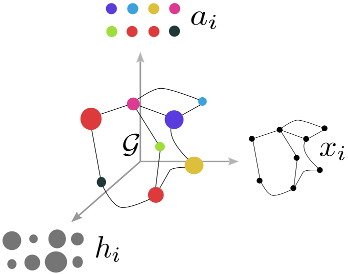


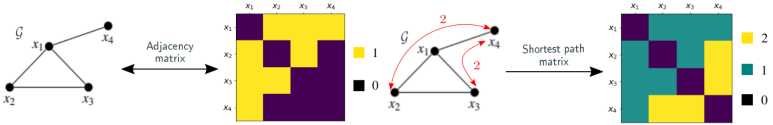
$$\mu = \sum_i h_i \delta_{(x_i, a_i)}$$

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

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

Graph as a distribution $(\boldsymbol{D}, \mathbf{F}, \boldsymbol{h})$

- The positions x_i are implicit and represented as the pairwise matrix $\boldsymbol{D}$.
- Possible choices for $\boldsymbol{D}$: Adjacency matrix, Laplacian, Shortest path, ...



- The node features can be compared between graphs and stored in $\mathbf{F}$.
- h_i are the masses on the nodes of the graphs (uniform by default).

Unbalanced Gromov-Wasserstein [Séjourné et al., 2020]

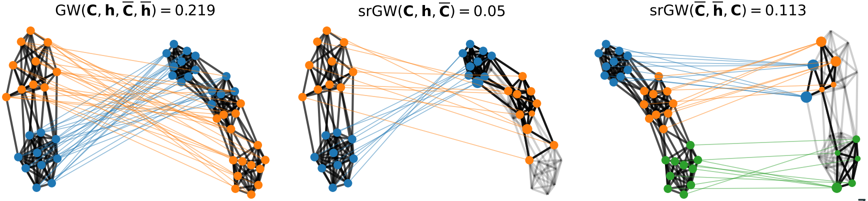
$$\min_{T\in\Pi(\mu_s,\mu_t)} \sum_{i,j,k,l} |D_{i,k} - D'_{j,l}|^p T_{i,j}\, T_{k,l} + \lambda^u D_\varphi(\mathbf{T}\mathbf{1}_m, \mathbf{a}) + \lambda^u D_\varphi(\mathbf{T}^\top \mathbf{1}_n, \mathbf{b})$$

- The marginal constraints are relaxed by penalizing with divergence D_φ.
- Partial GW proposed in [Chapel et al., 2020]
- Unbalanced FGW [Thual et al., 2022] and Low rank [Scetbon et al., 2023].

Semi-relaxed (F)GW [Vincent-Cuaz et al., 2022a]

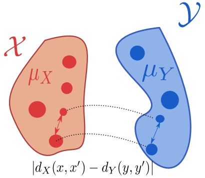
$$\min_{T\geq 0, \mathbf{T}\mathbf{1}_m=\mathbf{a}} \sum_{i,j,k,l} |D_{i,k} - D'_{j,l}|^p T_{i,j}\, T_{k,l}$$

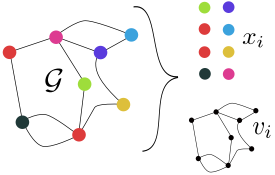
- Second marginal constraint relaxed: optimal weights $\mathbf{b}$ w.r.t. GW.
- Very fast solver (Frank-Wolfe) because constraints are separable

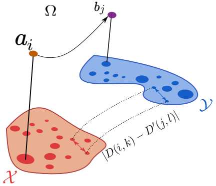


Learning on graphs with optimal transport

GW and FGW : the swiss army knife of OT on graphs







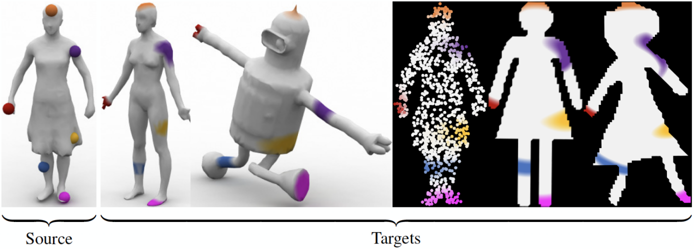
GW and extensions

- GW [Memoli, 2011] and FGW [Vayer et al., 2018] are versatile distances for graph and structured data seen as distribution.
- Unbalanced [Séjourné et al., 2020] and semi-relaxed [Vincent-Cuaz et al., 2022a].

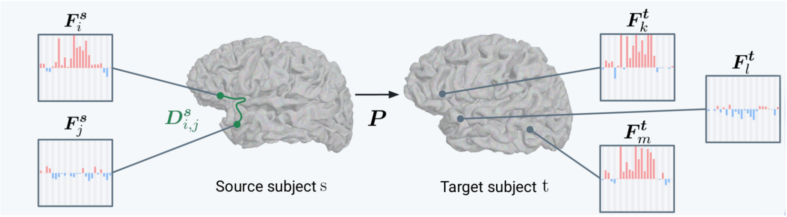
GW tools

- OT plan gives interpretable alignment between graphs.
- GW geometry allows barycenter and interpolation between graphs.
- GW provides similarity between graphs (data fitting).

Shape matching between surfaces with GW [Solomon et al., 2016]



Brain alignment between individuals with unbalanced FGW [Thual et al., 2022]



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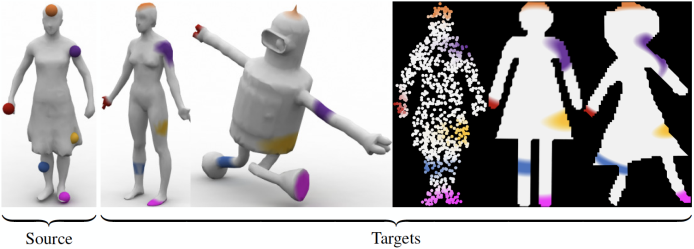

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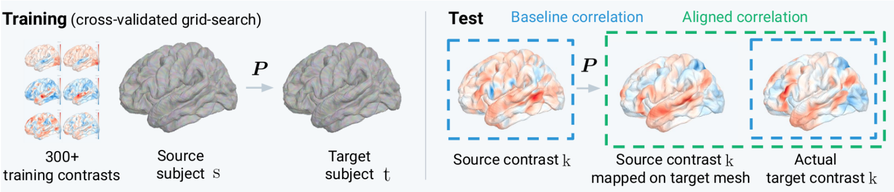

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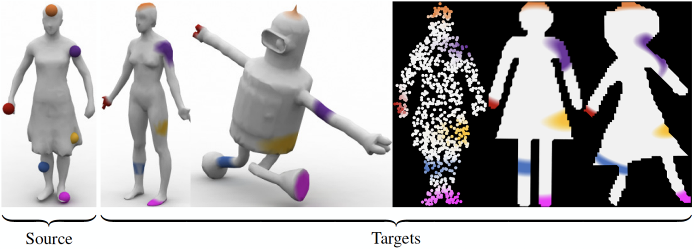

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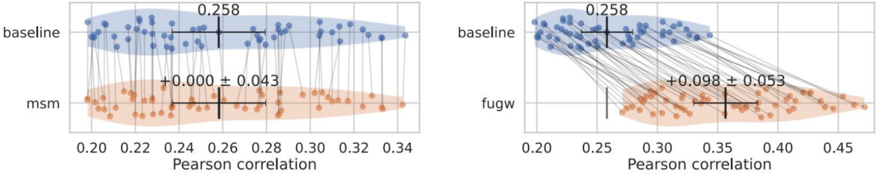
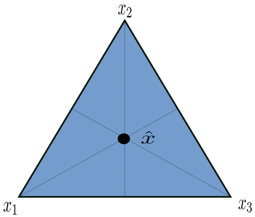
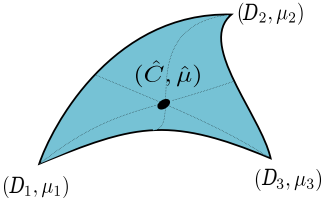


Euclidean barycenter



$$\underset{x}{min} \sum_k \lambda_k \|x - x_k\|^2$$

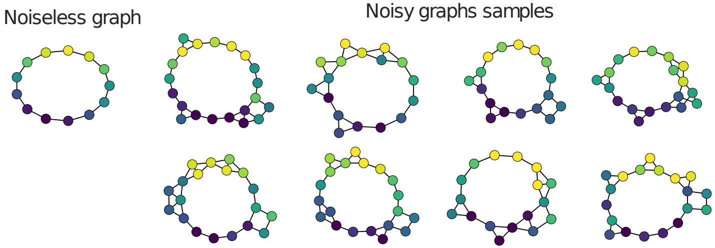
FGW barycenter



$$\min_{D \in \mathbb{R}^{n \times n}, \mu} \sum_i \lambda_i \mathcal{FGW}(D_i, D, \mu_i, \mu)$$

FGW barycenter

- Estimate FGW barycenter using Fréchet means (Proposed in [Peyré et al., 2016] for GW).
- Barycenter optimization solved via block coordinate descent (on $\mathbf{T}, D, \{a_i\}_i$).
- Use for data augmentation /mixup in [Ma et al., 2023].



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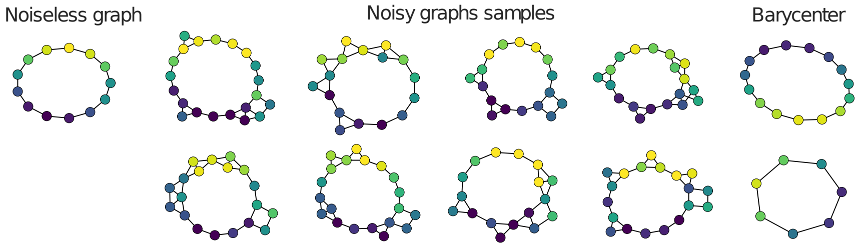

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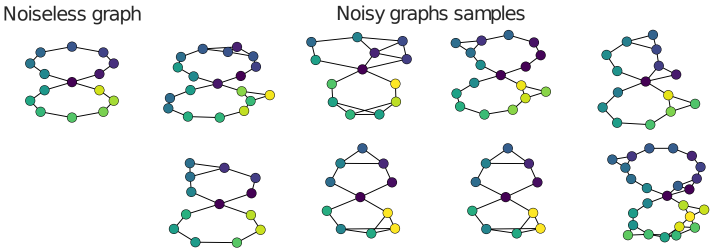

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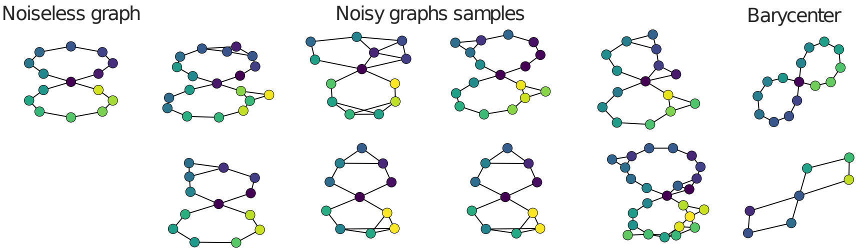
(F)GW barycenter



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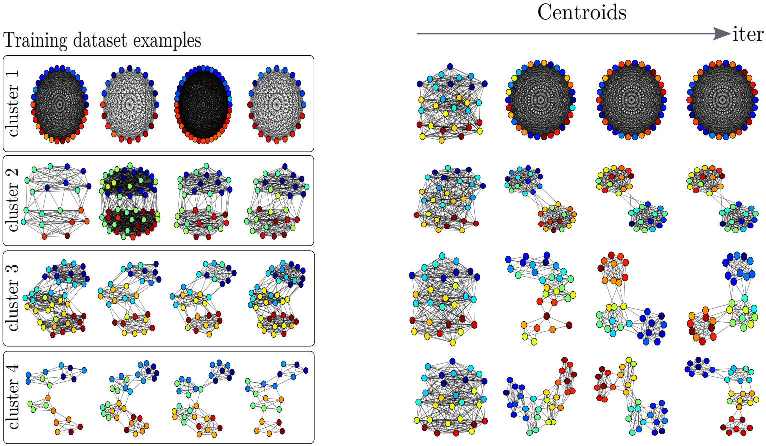
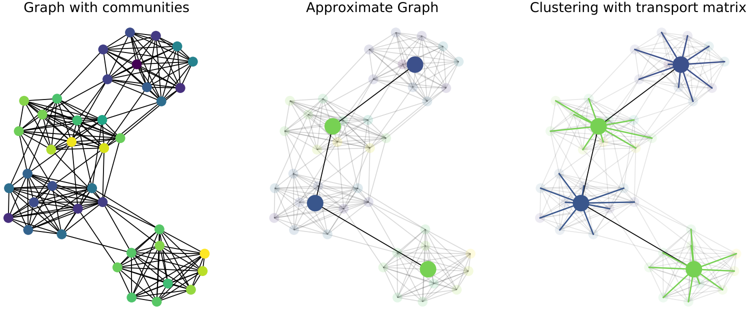
FGW for graphs based clustering



- Clustering of multiple real-valued graphs. Dataset composed of 40 graphs (10 graphs $\times$ 4 types of communities)
- k-means clustering using the FGW barycenter

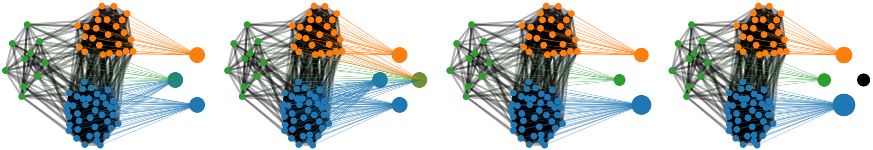


Graph approximation and community clustering [Vayer et al., 2018]

$$\min_{\mathbf{D},\mu} \quad \mathcal{FGW}(\mathbf{D}, \mathbf{D}_0, \mu, \mu_0)$$

- Approximate the graph $(\mathbf{D}_0, \mu_0)$ with a small number of nodes.
- OT matrix give the clustering affectation.
- Semi-relaxed GW estimates cluster proportions [Vincent-Cuaz et al., 2022a].
- Connections with spectral clustering [Chowdhury and Needham, 2021].
- Connection with Dimensionality reduction [Van Assel et al., 2023].

FGW baryenter for community clustering



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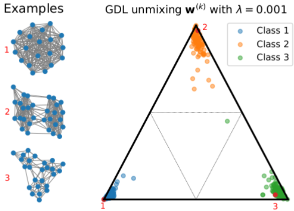
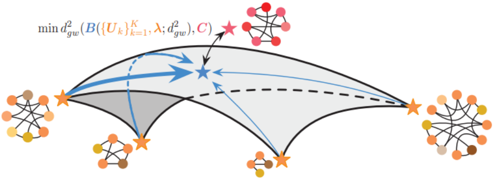




Representation learning for graphs

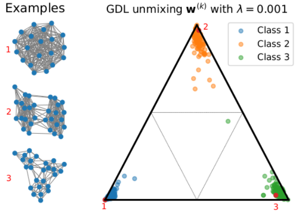
$$\min_{\{\overline{\mathbf{C}_k}\}_k, \{\mathbf{w}_i\}_i} \frac{1}{N} \sum_i GW(\mathbf{C}_i, \widehat{\mathbf{C}}(\mathbf{w}_i))$$

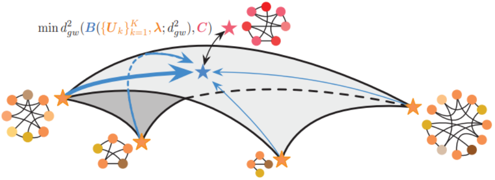
- Learn a dictionary $\{\overline{\mathbf{C}_k}\}_k$ of graph templates to describe a continuous manifold.
- The representation is learned by minimizing the (F)GW distance between the graph reconstruction from the embedding in the dictionary.
- Online Graph Dictionary learning : Linear model [Vincent-Cuaz et al., 2021].

$$\widehat{\mathbf{C}}(\mathbf{w}) = \sum_k w_k \overline{\mathbf{C}_k}$$

- GW Factorization : Nonlinear (GW barycenter) model [Xu, 2020].

Graph representation learning: Dictionary Learning





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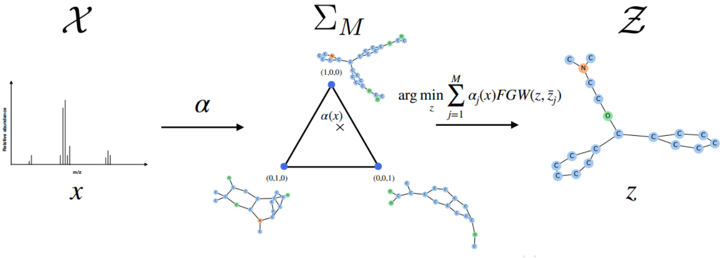


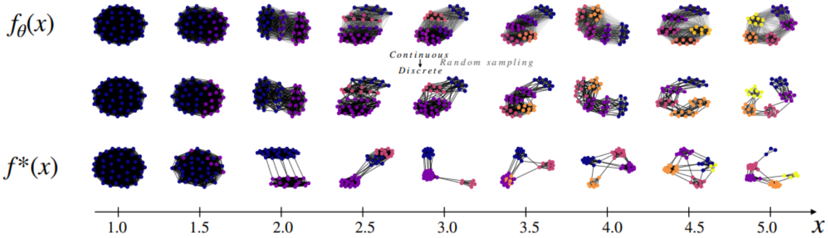
Structured prediction with GW barycenter [Brogat-Motte et al., 2022]

$$f(\mathbf{x}) = \widehat{\mathbf{C}}(\mathbf{w}(\mathbf{x})) = \text{argmin}_{\mathbf{C}} \sum_k w_k(\mathbf{x}) GW(\mathbf{C}, \overline{\mathbf{C}}_i)$$

- Prediction of the graph with a GW barycenter with weights conditioned by $\mathbf{x}$.
- Dictionary $\{\overline{\mathbf{C}}_k\}_k$ and conditional weights $\mathbf{w}(x)$ learned simultaneously with

$$\min_{\{\overline{\mathbf{C}}_k\}_k, \mathbf{w}(\cdot)} \quad \frac{1}{N} \sum_i GW(f(\mathbf{x}_i), \mathbf{C}_i)$$

- Both parametric and non parametric estimators [Brogat-Motte et al., 2022].



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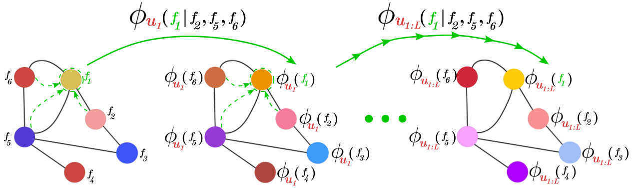
- Both parametric and non parametric estimators [Brogat-Motte et al., 2022].

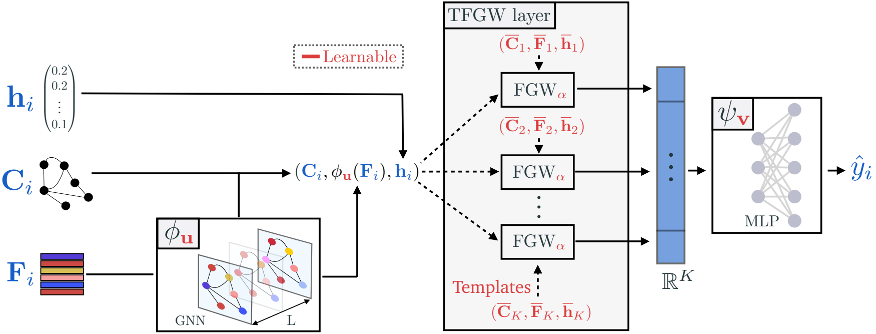
Graph kernels and FGW

- Graph kernels still SOTA on many datasets : WWL [Togninalli et al., 2019].
- FGW can be used in a non-positive "kernel" [Vayer et al., 2019a].
- Graph dictionary learning methods provide euclidean embeddings for kernels [Vincent-Cuaz et al., 2021, Vincent-Cuaz et al., 2022a].

Graph Neural Networks [Bronstein et al., 2017]



- Each layer of the GNN compute features on graph node using the values from the connected neighbors : message passing principle.
- The final pooling step must remain invariant to permutations (min, max, mean).
- Can we encode graphs as distributions in GNN?

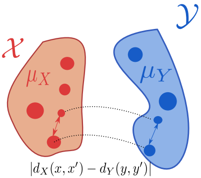


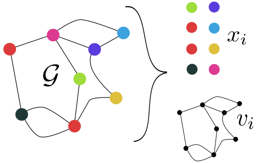
Template based FGW layer (TFGW) [Vincent-Cuaz et al., 2022b]

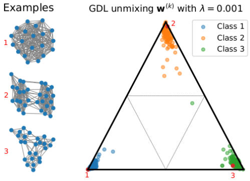
- Principle: represent a graph through its distances to learned templates.
- Novel pooling layer derived from OT distances.
- New end-to-end GNN models for graph-level tasks.
- Learnable parameters are illustrated in red above.

category	model	MUTAG	PTC	ENZYMES	PROTEIN	NCI1	IMDB-B	IMDB-M	COLLAB
Ours	TFGW ADJ (L=2)	**96.4(3.3)**	**72.4(5.7)**	73.8(4.6)	**82.9(2.7)**	**88.1(2.5)**	**78.3(3.7)**	**56.8(3.1)**	**84.3(2.6)**
($\phi_{\mathbf{u}}$ = GIN)	TFGW SP (L=2)	94.8(3.5)	70.8(6.3)	**75.1(5.0)**	82.0(3.0)	86.1(2.7)	74.1(5.4)	54.9(3.9)	80.9(3.1)
OT emb.	OT-GNN (L=2)	91.6(4.6)	68.0(7.5)	66.9(3.8)	76.6(4.0)	82.9(2.1)	67.5(3.5)	52.1(3.0)	80.7(2.9)
	OT-GNN (L=4)	92.1(3.7)	65.4(9.6)	67.3(4.3)	78.0(5.1)	83.6(2.5)	69.1(4.4)	51.9(2.8)	81.1(2.5)
	WEGL	91.0(3.4)	66.0(2.4)	60.0(2.8)	73.7(1.9)	75.5(1.4)	66.4(2.1)	50.3(1.0)	79.6(0.5)
GNN	PATCHYSAN	91.6(4.6)	58.9(3.7)	55.9(4.5)	75.1(3.3)	76.9(2.3)	62.9(3.9)	45.9(2.5)	73.1(2.7)
	GIN	90.1(4.4)	63.1(3.9)	62.2(3.6)	76.2(2.8)	82.2(0.8)	64.3(3.1)	50.9(1.7)	79.3(1.7)
	DropGIN	89.8(6.2)	62.3(6.8)	65.8(2.7)	76.9(4.3)	81.9(2.5)	66.3(4.5)	51.6(3.2)	80.1(2.8)
	PPGN	90.4(5.6)	65.6(6.0)	66.9(4.3)	77.1(4.0)	82.7(1.8)	67.2(4.1)	51.3(2.8)	81.0(2.1)
	DIFFPOOL	86.1(2.0)	45.0(5.2)	61.0(3.1)	71.7(1.4)	80.9(0.7)	61.1(2.0)	45.8(1.4)	80.8(1.6)
Kernels	FGW - ADJ	82.6(7.2)	55.3(8.0)	72.2(4.0)	72.4(4.7)	74.4(2.1)	70.8(3.6)	48.9(3.9)	80.6(1.5)
	FGW - SP	84.4(7.3)	55.5(7.0)	70.5(6.2)	74.3(3.3)	72.8(1.5)	65.0(4.7)	47.8(3.8)	77.8(2.4)
	WL	87.4(5.4)	56.0(3.9)	69.5(3.2)	74.4(2.6)	85.6(1.2)	67.5(4.0)	48.5(4.2)	78.5(1.7)
	WWL	86.3(7.9)	52.6(6.8)	71.4(5.1)	73.1(1.4)	85.7(0.8)	71.6(3.8)	52.6(3.0)	81.4(2.1)
	Gain with TFGW	**+4.3**	**+4.4**	**+2.9**	**+4.9**	**+2.4**	**+6.7**	**+4.2**	**+2.9**

- Comparison with state of the art approach from GNN and graph kernel methods.
- Systematic and significant gain of performance with GIN+TFGW.
- Gain independent of GNN architecture (GIN or GAT).
- 1 year after publication, world rankings of TFGW on "papers with code":
  #1 NCI1, #2 COLLAB ENZYMES IMDB-M, #3 MUTAG, PROTEIN.
- Experiments suggests that TFGW has expressivity beyond Weisfeiler-Lehman Isomorphism tests.







Gromov-Wasserstein family for graph modeling

- Graphs modelled as distributions, $\mathcal{GW}$ can measure their similarity.
- Extensions of GW for labeled graphs and Frechet means can be computed.
- Weights on the nodes are important but rarely available : relax the constraints [Séjourné et al., 2020] or even remove one of them [Vincent-Cuaz et al., 2022a].
- Many applications of FGW from brain imagery [Thual et al., 2022] to Graph Neural Networks [Vincent-Cuaz et al., 2022b].

Thank you

Python code available on GitHub:

https://github.com/PythonOT/POT

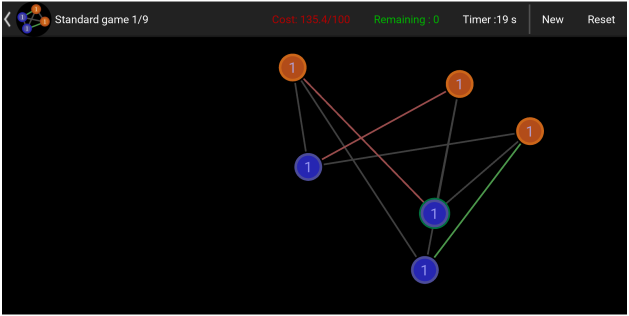
- OT LP solver, Sinkhorn (stabilized, $\epsilon-$scaling, GPU)
- Domain adaptation with OT.
- Barycenters, Wasserstein unmixing.
- Gromov Wasserstein.
- Differentiable solvers for Numpy/Pytorch/tensorflow/Cupy

For Jax : OTT-JAX at https://ott-jax.readthedocs.io/

Tutorial on OT for ML:
http://tinyurl.com/otml-isbi

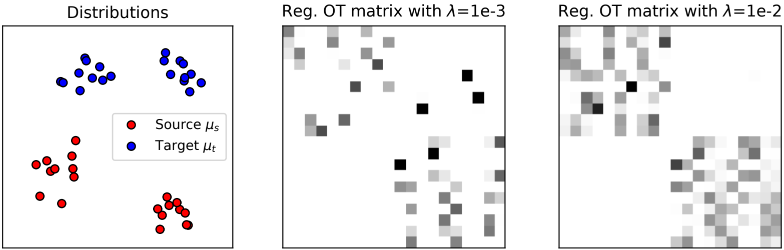
Papers available on my website:
https://remi.flamary.com/

OTGame



https://play.google.com/store/apps/details?id=com.flamary.otgame

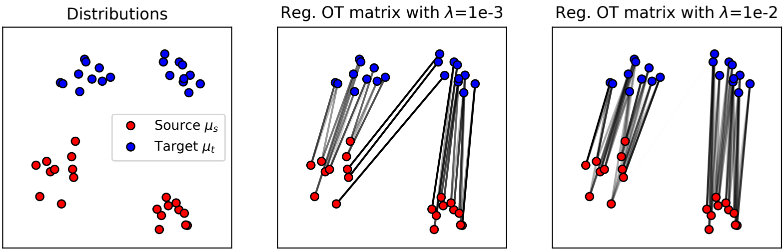
Entropic regularized optimal transport



Entropic regularization [Cuturi, 2013]

$$W_\epsilon(\mu_s, \mu_t) = \min_{\mathbf{T}\in\Pi(\mu_s,\mu_t)} \quad \langle \mathbf{T}, \mathbf{C}\rangle_F + \epsilon \sum_{i,j} T_{i,j} \log T_{i,j}$$

- Regularization with the negative entropy $-H(\mathbf{T})$.
- Looses sparsity, but strictly convex optimization problem [Benamou et al., 2015].
- Can be solved with the very efficient Sinkhorn-Knopp matrix scaling algorithm.
- Loss and OT matrix are differentiable and have better statistical properties [Genevay et al., 2018].



Entropic regularization [Cuturi, 2013]

$$W_\epsilon({\color{red}\mu_s}, {\color{blue}\mu_t}) = \min_{\mathbf{T}\in\Pi({\color{red}\mu_s},{\color{blue}\mu_t})} \quad \langle \mathbf{T}, \mathbf{C}\rangle_F + \epsilon \sum_{i,j} T_{i,j} \log T_{i,j}$$

- Regularization with the negative entropy $-H(\mathbf{T})$.
- Looses sparsity, but strictly convex optimization problem [Benamou et al., 2015].
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GW Upper bond [Vincent-Cuaz et al., 2021]
Let two graphs of order N in the linear embedding $\left(\sum_s w_s^{(1)}\overline{\boldsymbol{D}_s}\right)$ and $\left(\sum_s w_s^{(2)}\overline{\boldsymbol{D}_s}\right)$, the $\mathcal{GW}$ divergence can be upper bounded by

$$\mathcal{GW}_2\left(\sum_{s\in[S]} w_s^{(1)}\overline{\boldsymbol{D}_s}, \sum_{s\in[S]} w_s^{(2)}\overline{\boldsymbol{D}_s}\right) \leq \|\mathbf{w}^{(1)} - \mathbf{w}^{(2)}\|_{\boldsymbol{M}} \tag{1}$$

with $\boldsymbol{M}$ a PSD matrix of components $M_{p,q} = \left\langle \boldsymbol{D_h}\overline{\boldsymbol{D}_p}, \overline{\boldsymbol{D}_q}\boldsymbol{D_h}\right\rangle_F$, $\boldsymbol{D_h} = diag(\boldsymbol{h})$.

Discussion

- The upper bound is the value of GW for a transport $T = diag(\boldsymbol{h})$ assuming that the nodes are already aligned.
- The bound is exact when the weights $\mathbf{w}^{(1)}$ and $\mathbf{w}^{(2)}$ are close.
- Solving $\mathcal{GW}$ with FW si $O(N^3\log(N))$ at each iterations.
- Computing the Mahalanobis upper bound is $O(S^2)$: very fast alterative to GW for nearest neighbors retrieval.

Optimization problem

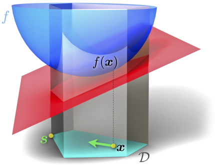
$$\mathcal{GW}_p^p(\mu_s,\mu_t) = \min_{\mathbf{T}\in\Pi(\mu_s,\mu_t)} \sum_{i,j,k,l} |D_{i,k} - D'_{j,l}|^p T_{i,j}\, T_{k,l}$$

with $\mu_s = \sum_i a_i \delta_{\mathbf{x}_i^s}$ and $\mu_t = \sum_j b_j \delta_{x_j^t}$ and $D_{i,k} = \|\mathbf{x}_i^s - \mathbf{x}_k^s\|, D'_{j,l} = \|\mathbf{x}_j^t - \mathbf{x}_l^t\|$

- Quadratic Program (Wasserstein is a linear program).
- Nonconvex, NP-hard, related to Quadratic Assignment Problem (QAP).
- Large problem and non convexity forbid standard QP solvers.

Optimization algorithms

- Local solution with conditional gradient algorithm (Frank-Wolfe) [Frank and Wolfe, 1956].
- Each FW iteration requires solving an OT problems.
- Gromov in 1D has a close form (solved in discrete with a sort) [Vayer et al., 2019b].
- With entropic regularization, one can use mirror descent [Peyré et al., 2016] or fast low rank approximations [Scetbon et al., 2021].



Optimization Problem

$$\mathcal{GW}_{p,\epsilon}^p(\mu_s,\mu_t) = \min_{\mathbf{T}\in\Pi(\mu_s,\mu_t)} \sum_{i,j,k,l} |D_{i,k} - D'_{j,l}|^p T_{i,j}\, T_{k,l} + \epsilon \sum_{i,j} T_{i,j} \log T_{i,j} \qquad (2)$$

with $\mu_s = \sum_i a_i \delta_{\mathbf{x}_i^s}$ and $\mu_t = \sum_j b_j \delta_{x_j^t}$ and $D_{i,k} = \|\mathbf{x}_i^s - \mathbf{x}_k^s\|, D'_{j,l} = \|\mathbf{x}_j^t - \mathbf{x}_l^t\|$

- Smoothing the original GW with a convex and smooth entropic term.

Solving the entropic $\mathcal{GW}$ [Peyré et al., 2016]

- Problem (2) can be solved using a KL mirror descent.
- This is equivalent to solving at each iteration t

$$\mathbf{T}^{(t+1)} = \min_{\mathbf{T}\in\mathcal{P}} \quad \left\langle \mathbf{T}, \mathbf{G}^{(t)} \right\rangle_F + \epsilon \sum_{i,j} T_{i,j} \log T_{i,j}$$

  Where $G_{i,j}^{(t)} = 2\sum_{k,l} |D_{i,k} - D'_{j,l}|^p T_{k,l}^{(t)}$ is the gradient of the GW loss at previous point $\mathbf{T}^{(k)}$.
- Problem above solved using a Sinkhorn-Knopp algorithm of entropic OT.
- Very fast approximation exist for low rank distances [Scetbon et al., 2021].

Optimization problem

$$\min_{\mathbf{w}\in\Sigma_S} \quad \mathcal{GW}_2^2\left(\sum_{s\in[S]} w_s\overline{\boldsymbol{D}_s}\ ,\ \boldsymbol{D}\right) - \lambda\|\mathbf{w}\|_2^2$$

- Non-convex Quadratic Program *w.r.t.* $\mathbf{T}$ and $\mathbf{w}$.
- GW for fixed $\mathbf{w}$ already have an existing Frank-Wolfe solver.
- We proposed a Block Coordinate Descent algorithm

BCD Algorithm for sparse GW unmixing [Tseng, 2001]

1: **repeat**
2: Compute OT matrix $\boldsymbol{T}$ of $\mathcal{GW}_2^2(\boldsymbol{D}, \sum_s w_s\overline{\boldsymbol{D}_s})$, with FW [Vayer et al., 2018].
3: Compute the optimal $\mathbf{w}$ given $\boldsymbol{T}$ with Frank-Wolfe algorithm.
4: **until** convergence

- Since the problem is quadratic optimal steps can be obtained for both FW.
- BCD convergence in practice in a few tens of iterations.

GDL on labeled graphs

- For datasets with labeled graphs, on can learn simultaneously a dictionary of the structure $\{\overline{\boldsymbol{D}}_s\}_{s\in[S]}$ and a dictionary on the labels/features $\{\overline{\mathbf{F}}_s\}_{s\in[S]}$.
- Data fitting is Fused Gromov-Wasserstein distance $\mathcal{FGW}$, same stochastic algorithmm.

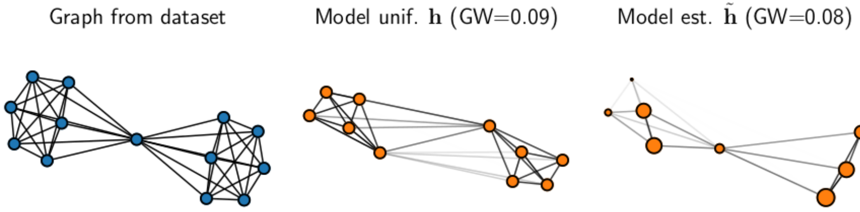
Dictionary on weights

$$\min_{\substack{\{(\mathbf{w}^{(k)},\mathbf{v}^{(k)})\}_k \\ \{(\overline{\boldsymbol{D}}_s,\overline{\boldsymbol{h}_s})\}_s}} \sum_{k=1}^{K} \mathcal{GW}_2^2\left(\boldsymbol{D}^{(k)}, \sum_s w_s^{(k)}\overline{\boldsymbol{D}_s}, \boldsymbol{h}^{(k)}, \sum_s v_s^{(k)}\overline{\boldsymbol{h}_s}\right) - \lambda\|\mathbf{w}^{(k)}\|_2^2 - \mu\|\mathbf{v}^{(k)}\|_2^2$$

- We model the graphs as a linear model on the structure and the node weights

$$(\boldsymbol{D}^{(k)}, \boldsymbol{h}^{(k)}) \longrightarrow \quad \left(\sum_s w_s^{(k)}\boldsymbol{D}_s, \sum_s v_s^{(k)}\overline{\boldsymbol{h}_s}\right)$$

- This allows for sparse weights $\boldsymbol{h}$ so embedded graphs with different order.
- We provide in [Vincent-Cuaz et al., 2021] subgradients of GW *w.r.t.* the mass $\boldsymbol{h}$.



Comparison of fixed and learned weights dictionaries

- Graph taken from the IMBD dataset.
- Show original graph and representation after projection on the embedding.
- Uniform weight $\boldsymbol{h}$ has a hard time representing a central node.
- Estimated weights $\tilde{\boldsymbol{h}}$ recover a central node.
- In addition some nodes are discarded with 0 weight (graphs can change order).

Table 1. Clustering: Rand Index computed for benchmarked approaches on real datasets.

	no attribute		discrete attributes		real attributes			
models	IMDB-B	IMDB-M	MUTAG	PTC-MR	BZR	COX2	ENZYMES	PROTEIN
GDL(ours)	**51.64(0.59)**	55.41(0.20)	**70.89(0.11)**	**51.90(0.54)**	**66.42(1.96)**	**59.48(0.68)**	66.97(0.93)	**60.49(0.71)**
GWF-r	51.24 (0.02)	**55.54(0.03)**	-	-	52.42(2.48)	56.84(0.41)	**72.13(0.19)**	59.96(0.09)
GWF-f	50.47(0.34)	54.01(0.37)	-	-	51.65(2.96)	52.86(0.53)	71.64(0.31)	58.89(0.39)
GW-k	50.32(0.02)	53.65(0.07)	57.56(1.50)	50.44(0.35)	56.72(0.50)	52.48(0.12)	66.33(1.42)	50.08(0.01)
SC	50.11(0.10)	54.40(9.45)	50.82(2.71)	50.45(0.31)	42.73(7.06)	41.32(6.07)	70.74(10.60)	49.92(1.23)

Clustering Experiments on real datasets

- Different data fitting losses:
  - Graphs without node attributes : Gromov-Wasserstein.
  - Graphs with node attributes (discrete and real): Fused Gromov-Wasserstein.
- We learn a dictionary on the dataset and perform K-means in the embedding using the Mahalanobis distance approximation.
- Compared to GW Factorization (GWF) [Xu, 2020] and spectral clustering.
- Similar performance for supervised classification (using GW in a kernel).

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