Optimal Transport for graph representation

From unsupervised learning to graph prediction

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Uncertainty in multivariate, non-Euclidean, and functional spaces: theory and practice.

Collaborators about OT on graphs


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P. Krzakala


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G. Gasso


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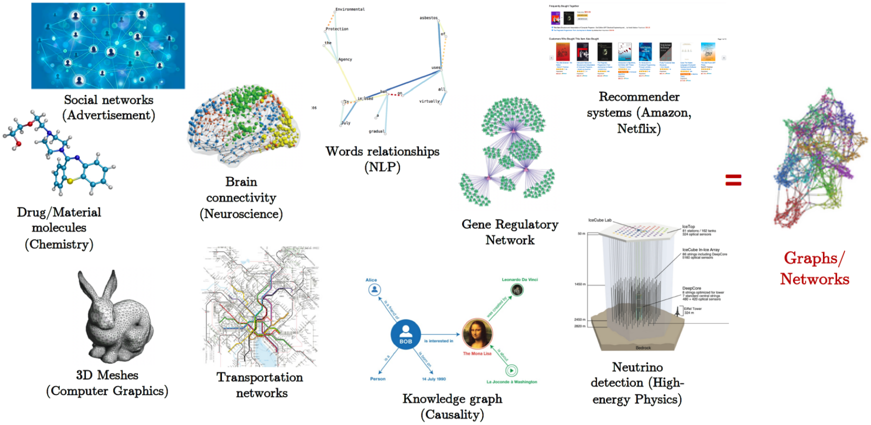
B. Thirion


F. d'Alché-Buc


L. Brogat-Motte


C. Laclau

Graphs are everywhere



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

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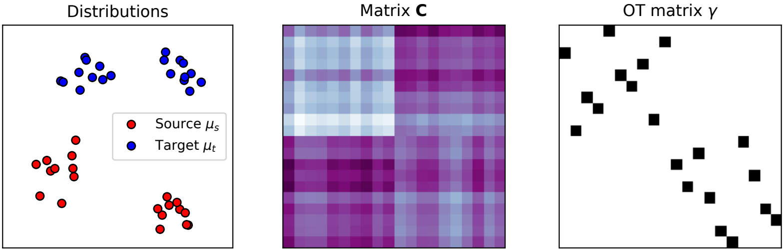
Optimal Transport and divergences between graphs



Kantorovitch formulation : OT Linear Program

When $\mu_s = \sum_{i=1}^{n_s} a_i \delta_{\mathbf{x}_i^s}$ and $\mu_t = \sum_{i=1}^{n_t} b_i \delta_{\mathbf{x}_i^t}$

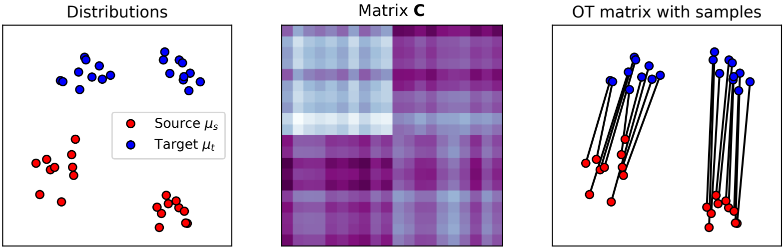
$$W_p^p(\mu_s, \mu_t) = \min_{\mathbf{T} \in \Pi(\mu_s, \mu_t)} \left\{ \langle \mathbf{T}, \mathbf{C} \rangle_F = \sum_{i,j} T_{i,j} c_{i,j} \right\}$$

where $\mathbf{C}$ is a cost matrix with $c_{i,j} = c(\mathbf{x}_i^s, \mathbf{x}_j^t) = \|\mathbf{x}_i^s - \mathbf{x}_j^t\|^p$ and the constraints are

$$\Pi(\mu_s, \mu_t) = \left\{ \mathbf{T} \in (\mathbb{R}^+)^{n_s \times n_t} | \, \mathbf{T}\mathbf{1}_{n_t} = \mathbf{a}, \mathbf{T}^T \mathbf{1}_{n_s} = \mathbf{b} \right\}$$

- $W_p(\mu_s, \mu_t)$ is called the Wasserstein distance (EMD for $p = 1$).
- Entropic regularization solved efficiently with Sinkhorn [Cuturi, 2013].
- Classical OT needs distributions lying in the same space → Gromov-Wasserstein.

Optimal transport between discrete distributions (recap)



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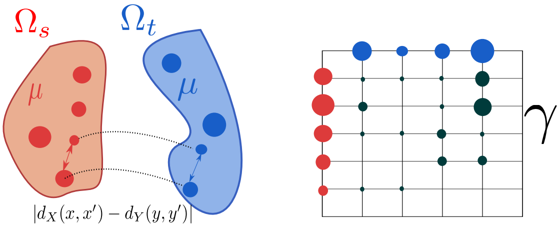


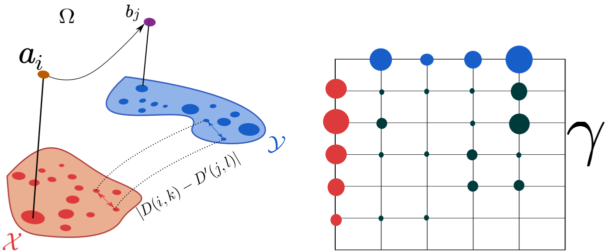
Inspired from Gabriel Peyré

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]

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

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

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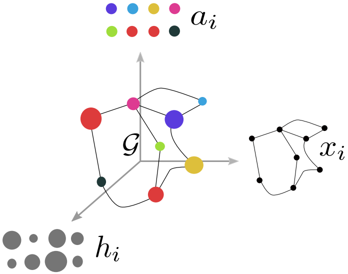


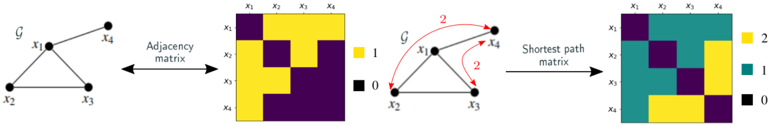
$$\mu = \sum_i h_i \delta_{(x_i, a_i)}$$

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

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

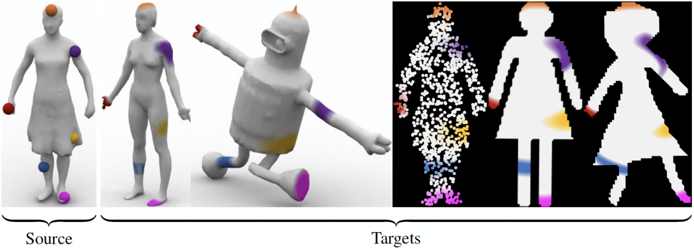
Graph as a distribution $(\boldsymbol{D}, \mathbf{F}, \boldsymbol{h})$

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

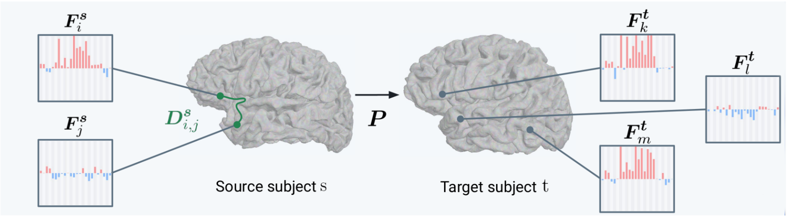


- The node features can be compared between graphs and stored in $\mathbf{F}$.
- h_i are the masses on the nodes of the graphs (uniform by default).

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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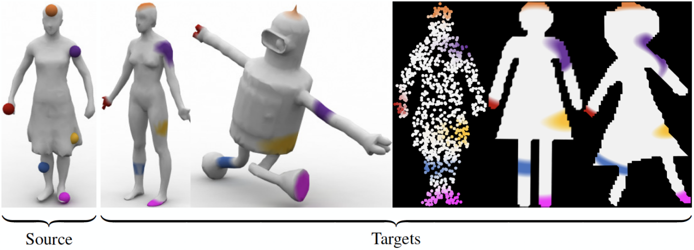

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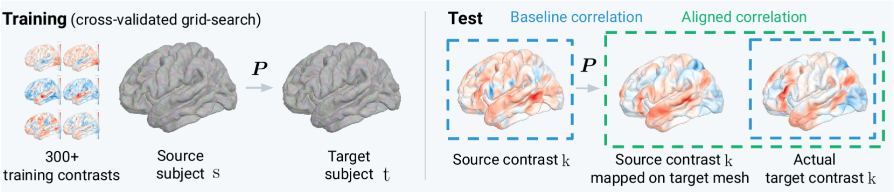

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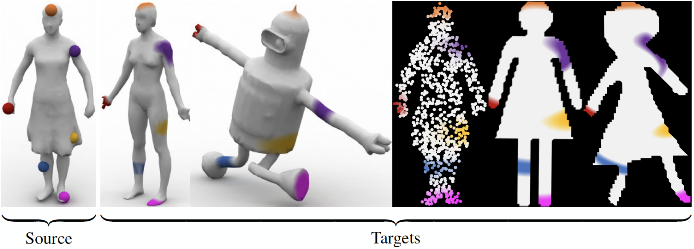

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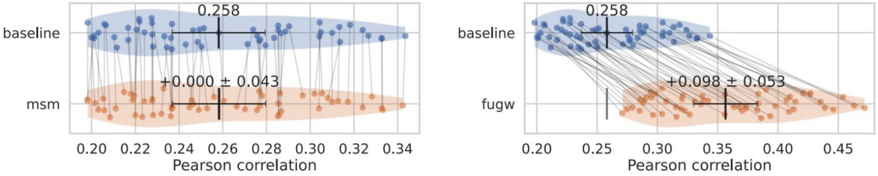


Unbalanced Gromov-Wasserstein [Séjourné et al., 2020]

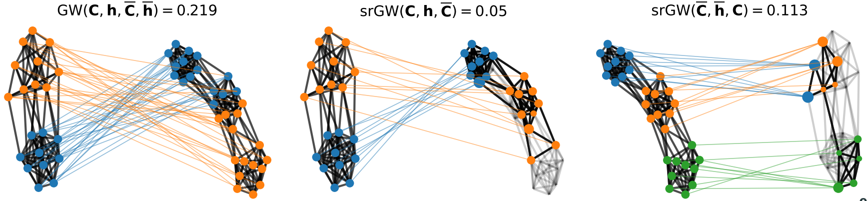
$$\min_{T\in\Pi(\mu_s,\mu_t)} \sum_{i,j,k,l} |D_{i,k} - D'_{j,l}|^p T_{i,j}\, T_{k,l} + \lambda^u D_\varphi(\mathbf{T1}_m, \mathbf{a}) + \lambda^u D_\varphi(\mathbf{T}^\top \mathbf{1}_n, \mathbf{b})$$

- 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].

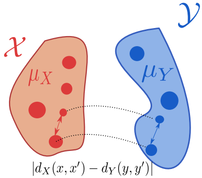
Semi-relaxed (F)GW [Vincent-Cuaz et al., 2022a]

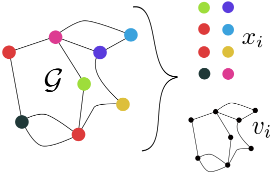
$$\min_{T\geq 0, \mathbf{T1}_m=\mathbf{a}} \sum_{i,j,k,l} |D_{i,k} - D'_{j,l}|^p T_{i,j}\, T_{k,l}$$

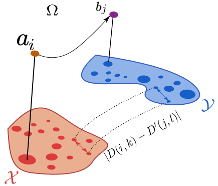
- Second marginal constraint relaxed: optimal weights $\mathbf{b}$ w.r.t. GW.
- Very fast solver (Frank-Wolfe) because constraints are separable



Learning graph representation with optimal transport







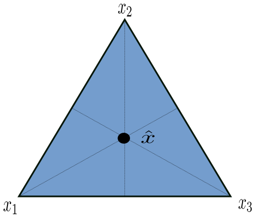
GW and extensions

- 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

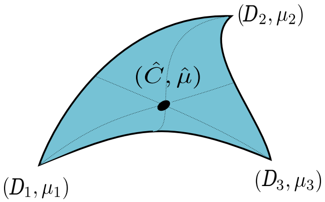
- OT plan gives interpretable alignment between graphs.
- GW geometry allows barycenter and interpolation between graphs.
- GW provides similarity between graphs (data fitting).

Euclidean barycenter



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

FGW barycenter

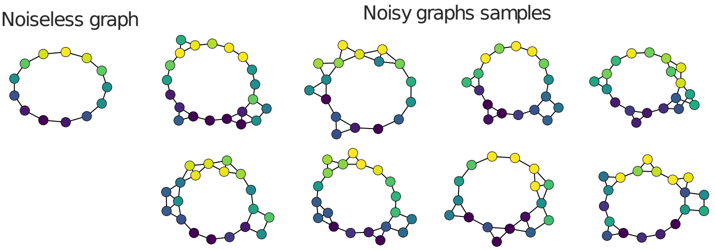


$$\min_{D \in \mathbb{R}^{n \times n}, \mu} \sum_i \lambda_i \mathcal{FGW}(D_i, D, \mu_i, \mu)$$

FGW barycenter

- Estimate FGW barycenter using Fréchet means ([Peyré et al., 2016] for GW).
- Barycenter optimization solved via block coordinate descent (on $\mathbf{T}, \mathbf{D}, \mu$).
- Extention of K-means clustering to FGW [Vayer et al., 2019a].
- Use for data augmentation /mixup in [Ma et al., 2023].

(F)GW barycenter



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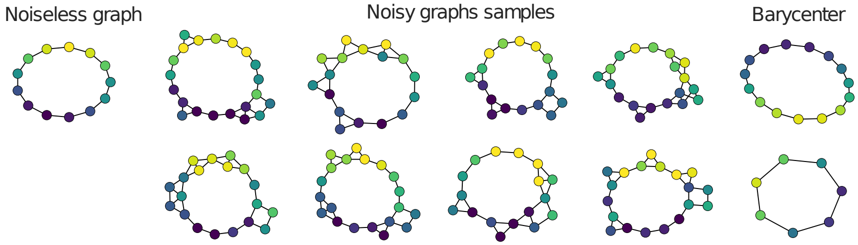

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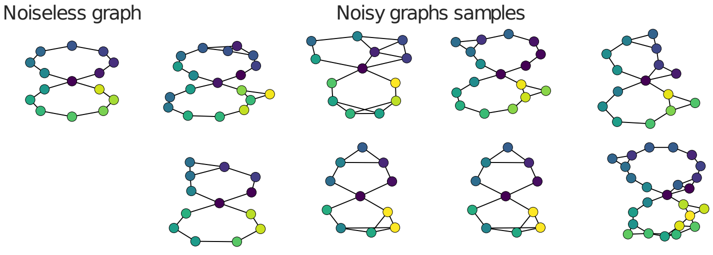

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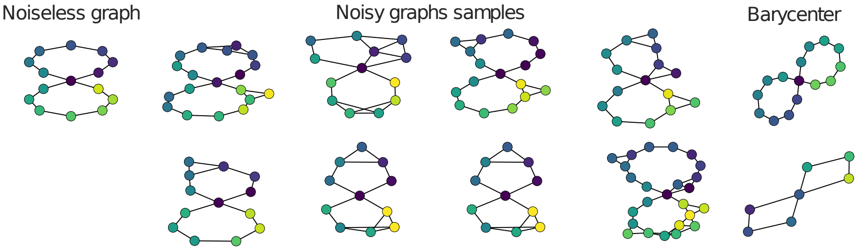

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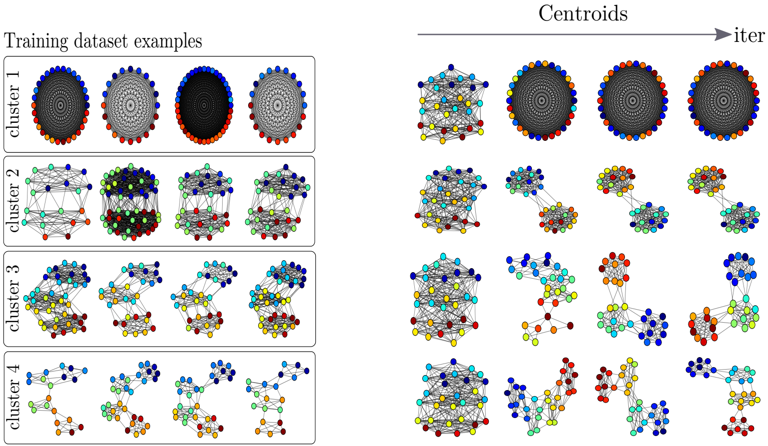
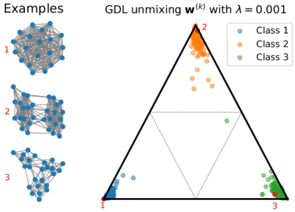
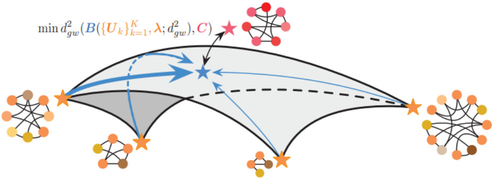
FGW for graphs based clustering



- 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





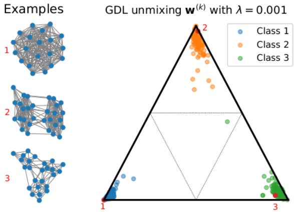
Representation learning for graphs

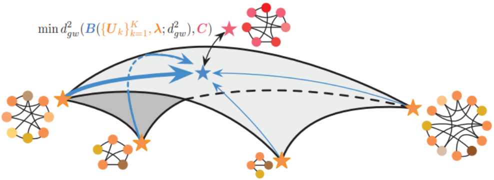
$$\min_{\{\overline{\mathbf{C}_k}\}_k, \{\mathbf{w}_i\}_i} \frac{1}{N} \sum_i GW(\mathbf{C}_i, \widehat{\mathbf{C}}(\mathbf{w}_i))$$

- 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].





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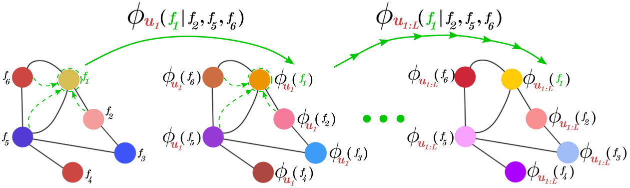
Supervised learning with OT on graphs

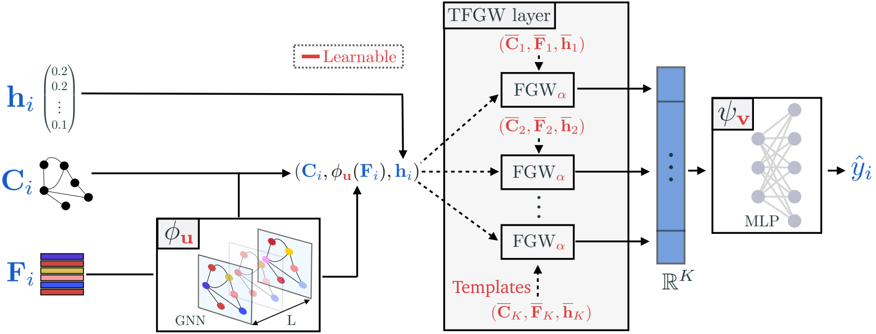
Graph kernels and FGW

- Graph kernels still SOTA on many datasets : WWL [Togninalli et al., 2019].
- FGW can be used in a non-positive "kernel" [Vayer et al., 2019b].
- 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?



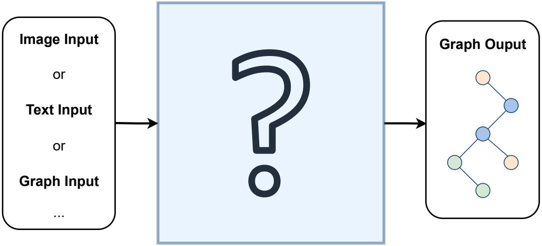
Template based FGW layer (TFGW) [Vincent-Cuaz et al., 2022b]

- 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.

TFGW benchmark

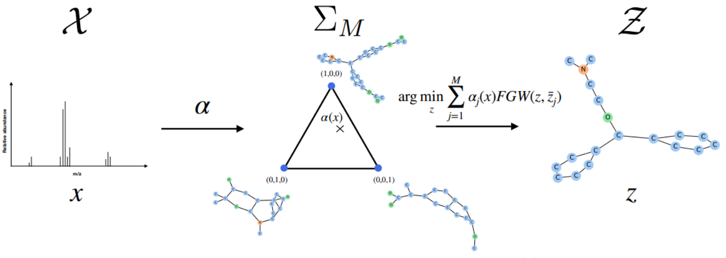
category	model	MUTAG	PTC	ENZYMES	PROTEIN	NCI1	IMDB-B	IMDB-M	COLLAB
Ours	TFGW ADJ (L=2)	**96.4(3.3)**	**72.4(5.7)**	73.8(4.6)	**82.9(2.7)**	**88.1(2.5)**	**78.3(3.7)**	**56.8(3.1)**	**84.3(2.6)**
($\phi_{\mathbf{u}}$ = GIN)	TFGW SP (L=2)	94.8(3.5)	70.8(6.3)	**75.1(5.0)**	82.0(3.0)	86.1(2.7)	74.1(5.4)	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).
- 3 year after publication, rankings of TFGW on "papers with code":
  #1 NCI1, #2 COLLAB, IMDB-M, #3 MUTAG, PROTEIN.
- Experiments suggests that TFGW has expressivity beyond Weisfeiler-Lehman Isomorphism tests.



Supervised graph prediction (a.k.a graph regression)

- Objective : learn a function f predicting a graph g from an input x.
- Applications of SGP:
  - knowledge graph extraction [Melnyk et al., 2022]
  - Natural language processing [Dozat and Manning, 2017]
  - Molecule identification in chemistry [Brouard et al., 2016]
- Surrogate based methods [Brouard et al., 2016, El Ahmad et al., 2024]:
  - Represent graph as a vector in a high dimensional space (RKHS).
  - Learn a mapping from input to this space.
  - Decode the vector to a graph (e.g. search among finite candidates).
- Linear regression of Adjacency matrix [Calissano et al., 2022].



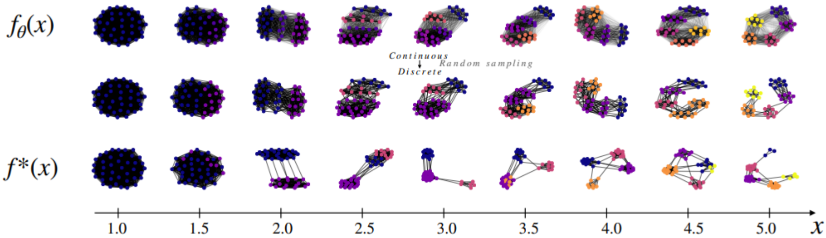
Structured prediction with GW barycenter [Brogat-Motte et al., 2022]

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

- 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].
- Very powerful but slow at training and prediction due to barycenter computation.



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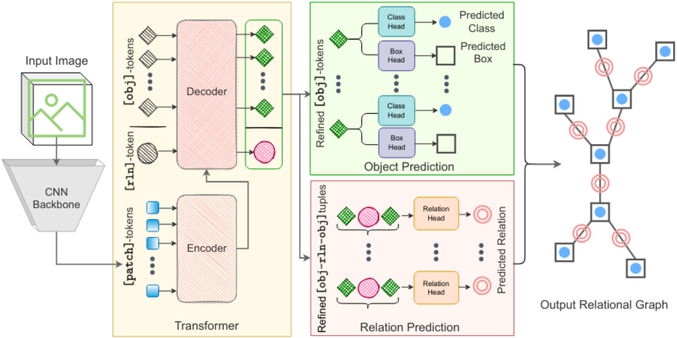
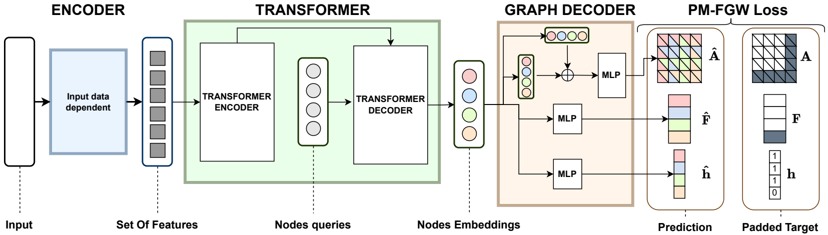
Graph prediction with deep learning



Relationformer [Shit et al., 2022]

- Predict a graph of max size M and activation scores for nodes to keep.
- Encoder-Decoder Transformer to predict node embeddings.
- Loss solves linear assignment problem (Hungarian) and uses assignment in quadratic loss between graphs of same size (padding the target).
- Fast prediction (thresholding) of graphs but focused on Image2Graph.



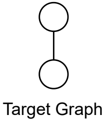
Principle [Krzakala et al., 2024]

- End-to-end supervised graph prediction with a deep learning framework.
- Learning optimization problem:

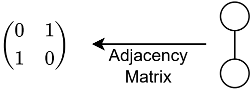
$$\min_{\theta} \quad \frac{1}{n}\sum_{i=1}^{n}\mathcal{L}(f_\theta(x_i), \mathcal{P}(g_i)). \tag{1}$$

- $\{x_i, g_i\}$ are the input/output training data and $\mathcal{P}$ is a padding operator.
- f_θ is a transformer neural network with fixed max number of nodes M.
- f_θ also predicts is a padding vector $\hat{\boldsymbol{h}}$ (selection of subset of nodes).
- $\mathcal{L}$ is an optimal transport based loss for permutation invariant prediction.

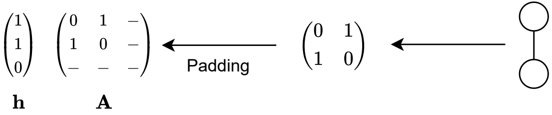
End-to-end SGP pipeline



End-to-end SGP pipeline



End-to-end SGP pipeline

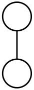


- Pad target graphs to have same size M.

Input

$\mathbf{x}$

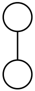
$$\underset{\mathbf{h}}{\begin{pmatrix}1\\1\\0\end{pmatrix}} \quad \underset{\mathbf{A}}{\begin{pmatrix}0 & 1 & -\\1 & 0 & -\\- & - & -\end{pmatrix}} \longleftarrow \begin{pmatrix}0 & 1\\1 & 0\end{pmatrix} \longleftarrow$$



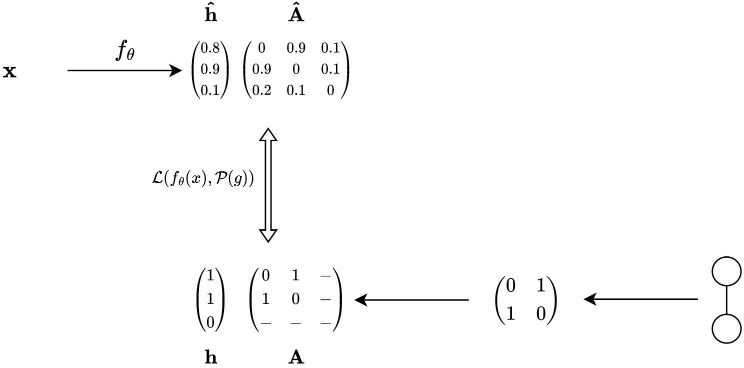
- Pad target graphs to have same size M.

$$\mathbf{x} \xrightarrow{f_\theta} \underbrace{\begin{pmatrix}0.8\\0.9\\0.1\end{pmatrix}}_{\hat{\mathbf{h}}} \underbrace{\begin{pmatrix}0 & 0.9 & 0.1\\0.9 & 0 & 0.1\\0.2 & 0.1 & 0\end{pmatrix}}_{\hat{\mathbf{A}}}$$

$$\underbrace{\begin{pmatrix}1\\1\\0\end{pmatrix}}_{\mathbf{h}} \underbrace{\begin{pmatrix}0 & 1 & -\\1 & 0 & -\\- & - & -\end{pmatrix}}_{\mathbf{A}} \longleftarrow \begin{pmatrix}0 & 1\\1 & 0\end{pmatrix} \longleftarrow$$



- Pad target graphs to have same size M.
- Predict with f_θ (continuous) size M graph with padding vector $\hat{\boldsymbol{h}}$.



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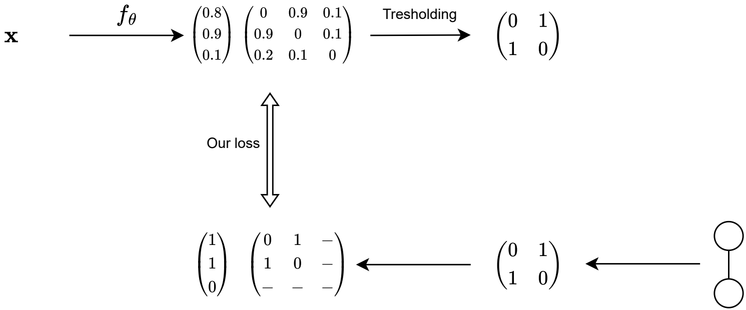
End-to-end SGP pipeline



- Pad target graphs to have same size M.
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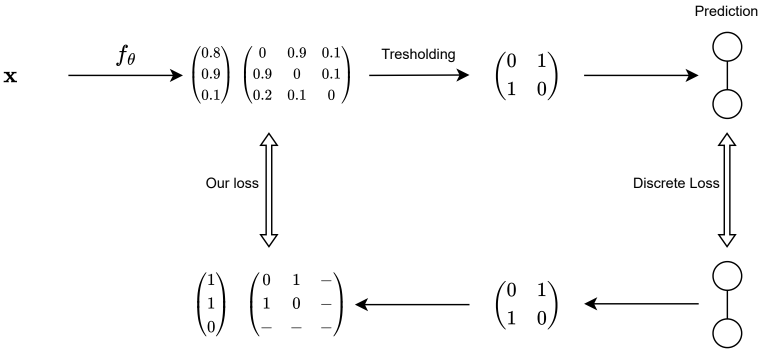
- Minimize OT loss L between predicted and padded target graphs.



- Pad target graphs to have same size M.
- Predict with f_θ (continuous) size M graph with padding vector $\hat{\boldsymbol{h}}$.
- Minimize OT loss L between predicted and padded target graphs.
- At test time, thresholding recovers discrete graph.

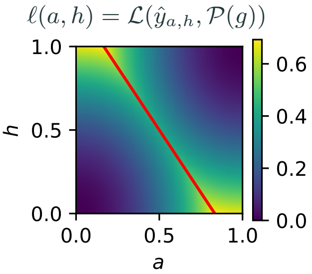
Partially-Masked Fused Gromov-Wasserstein (PM-FGW)

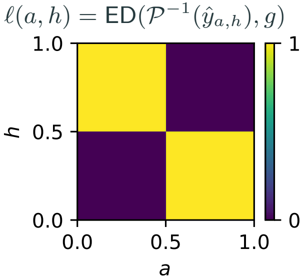
Definition of PM-FGW

$$\text{PM-FGW}(\hat{y}, y) = \min_{\mathbf{T} \in \Pi_M} \mathcal{L}_{\mathbf{T}}(\hat{y}, y)$$

$$\begin{aligned} \text{with } \mathcal{L}_{\mathbf{T}}(\hat{y}, y) = & \frac{\alpha_{\mathsf{h}}}{M} \sum_{i,j} T_{i,j} \ell_h(\hat{h}_i, h_j) && \text{Padding loss} \\ & + \frac{\alpha_{\mathsf{f}}}{m} \sum_{i,j} T_{i,j} \ell_f(\hat{\mathbf{f}}_i, \mathbf{f}_j) h_j && \text{Feature loss} \\ & + \frac{\alpha_{\mathsf{A}}}{m^2} \sum_{i,j,k,l} T_{i,j} T_{k,l} \ell_A(\hat{A}_{i,k}, A_{j,l}) h_j h_l. && \text{Structure loss} \end{aligned}$$

- ℓ_h, ℓ_f and ℓ_A are loss functions for node, feature and adjacency matrix discrepancies (Kullback-Leibler when target discrete, Squared loss when continuous feature).
- α_{h}, α_{f} and α_{A} are hyperparameters on the simplex.
- Loss is highly asymmetric due to the right masking by $\mathbf{h}$.
- Can be solved by Conditional Gradient with $O(M^3 \log M)$ iteration.





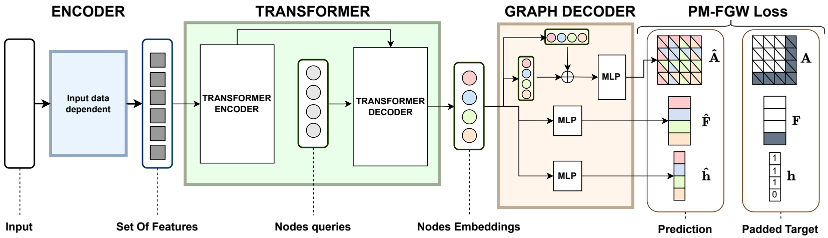
- The target graph is $g = (\mathbf{F}, \mathbf{A})$ with

$$\mathbf{F} = \begin{pmatrix} \mathbf{f}_1 \\ \mathbf{f}_2 \end{pmatrix}; \mathbf{A} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

- The prediction $\hat{y}_{a,h} = (\hat{\mathbf{h}}, \hat{\mathbf{F}}, \hat{\mathbf{A}})$ is

$$\hat{\mathbf{h}} = \begin{pmatrix} 1 \\ h \\ 1-h \end{pmatrix}; \hat{\mathbf{F}} = \begin{pmatrix} \mathbf{f}_1 \\ \mathbf{f}_2 \\ \mathbf{f}_2 \end{pmatrix}; \hat{\mathbf{A}} = \begin{pmatrix} 0 & a & 1-a \\ a & 0 & 0 \\ 1-a & 0 & 0 \end{pmatrix}$$

Neural network architecture



- The **encoder** extract a set of features $x \to (\mathbf{V}_1, ..., \mathbf{V}_k) \in \mathbb{R}^{k \times d}$
- The **transformer** translate them into M nodes embedding $(\mathbf{Z}_1, ..., \mathbf{Z}_M) \to \in \mathbb{R}^{M \times d}$
- The **decoder** produce the graph following

$$\hat{h}_i = \sigma(\text{MLP}_m(\mathbf{z}_i)) \qquad \forall i \in \{1, \dots, M\}$$
$$\hat{F}_i = \text{MLP}_f(\mathbf{z}_i) \qquad \forall i \in \{1, \dots, M\}$$
$$\hat{A}_{i,j} = \sigma(\text{MLP}_s(\mathbf{z}_i + \mathbf{z}_j)) \qquad \forall i, j \in \{1, \dots, M\}^2$$

- Similar to Relationformer [Shit et al., 2022] but with symmetric adjacency matrix.

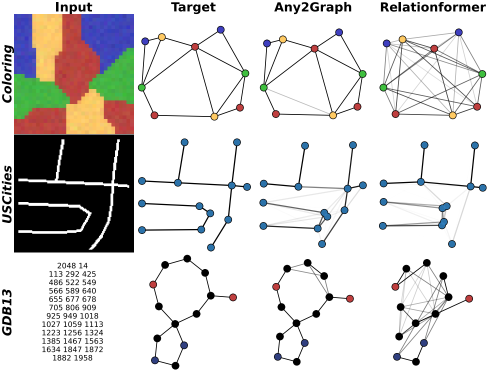
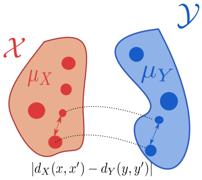
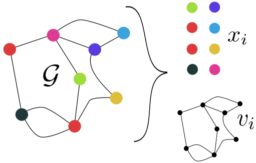


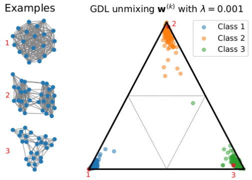
Figure 1: Qualitative comparison of Any2Graph (ours) and Relationformer.

Datasets	Model	Edit Distance ↓
Coloring	FGWBary-NN*	6.73
	Relationformer	5.47
	Any2Graph (Ours)	**0.20**
Toulouse	FGWBary-NN*	8.11
	Relationformer	**0.13**
	Any2Graph (Ours)	**0.13**
USCities	Relationformer	2.09
	Any2Graph (Ours)	**1.86**
QM9	FGWBary-ILE*	2.84
	Relationformer	3.80
	Any2Graph (Ours)	**2.13**
GDB13	Relationformer	8.83
	Any2Graph (Ours)	**3.63**

Table 1: Prediction performances measured with (test) edit distance.







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].
- OT is a powerful tool for (deep) graph structured prediction models [Brogat-Motte et al., 2022, Krzakala et al., 2024].

Thank you

Python code available on GitHub:

https://github.com/PythonOT/POT

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

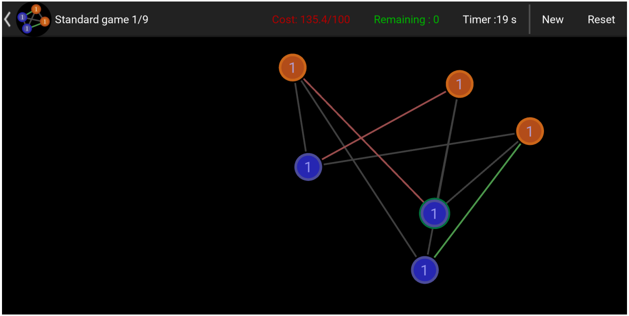
For Jax : OTT-JAX at https://ott-jax.readthedocs.io/

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

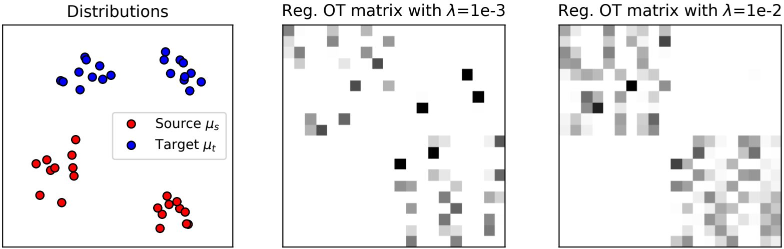
Papers available on my website:
https://remi.flamary.com/

OTGame (OT Puzzle game on android)

OTGame



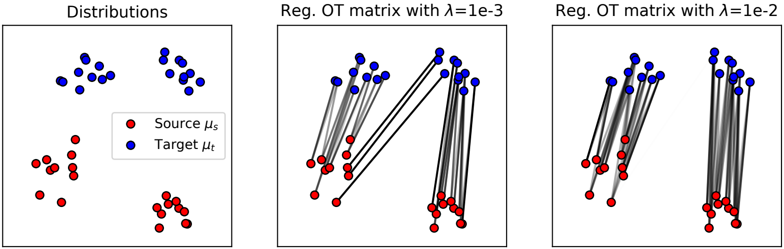
https://play.google.com/store/apps/details?id=com.flamary.otgame



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].



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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

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

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

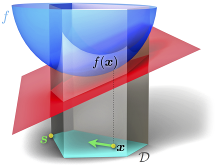
$$\mathcal{GW}_p^p(\mu_s,\mu_t) = \min_{\mathbf{T}\in\Pi(\mu_s,\mu_t)} \sum_{i,j,k,l} |D_{i,k} - D'_{j,l}|^p T_{i,j}\, T_{k,l}$$

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., 2019c].
- With entropic regularization, one can use mirror descent [Peyré et al., 2016] or fast low rank approximations [Scetbon et al., 2021].



Optimization Problem

$$\mathcal{GW}_{p,\epsilon}^{p}(\mu_s, \mu_t) = \min_{\mathbf{T}\in\Pi(\mu_s,\mu_t)} \sum_{i,j,k,l} |D_{i,k} - D'_{j,l}|^p T_{i,j}\, T_{k,l} + \epsilon \sum_{i,j} T_{i,j} \log T_{i,j} \qquad (3)$$

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 (3) 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.

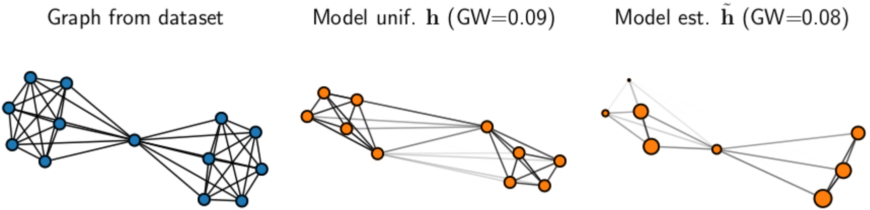
Dictionary on weights

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

- 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

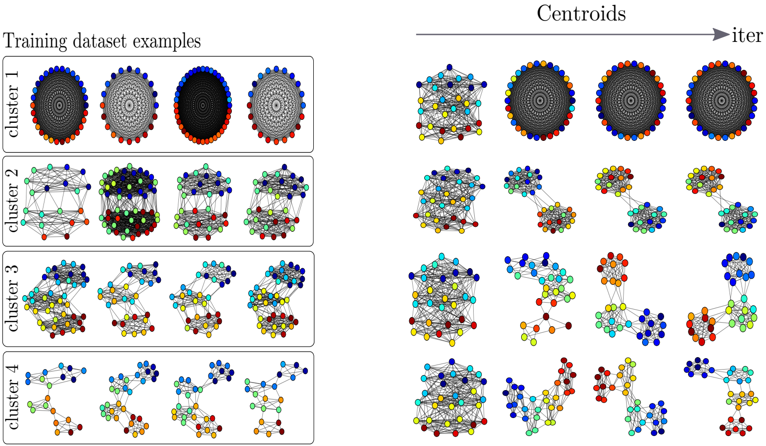
- Graph taken from the IMBD dataset.
- Show original graph and representation after projection on the embedding.
- Uniform weight $\boldsymbol{h}$ has a hard time representing a central node.
- Estimated weights $\tilde{\boldsymbol{h}}$ recover a central node.
- In addition some nodes are discarded with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

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

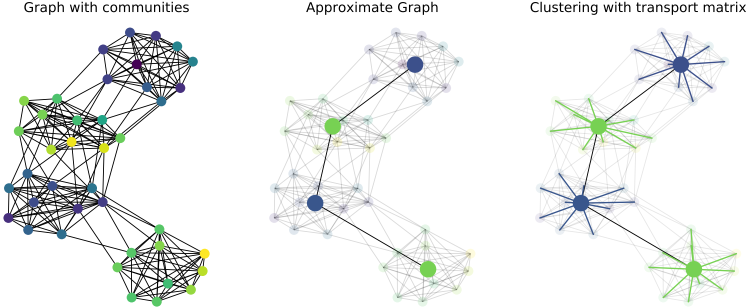
	no attribute		discrete attributes		real attributes			
models	IMDB-B	IMDB-M	MUTAG	PTC-MR	BZR	COX2	ENZYMES	PROTEIN
GDL(ours)	**51.64(0.59)**	55.41(0.20)	**70.89(0.11)**	**51.90(0.54)**	**66.42(1.96)**	**59.48(0.68)**	66.97(0.93)	**60.49(0.71)**
GWF-r	51.24 (0.02)	**55.54(0.03)**	-	-	52.42(2.48)	56.84(0.41)	**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).



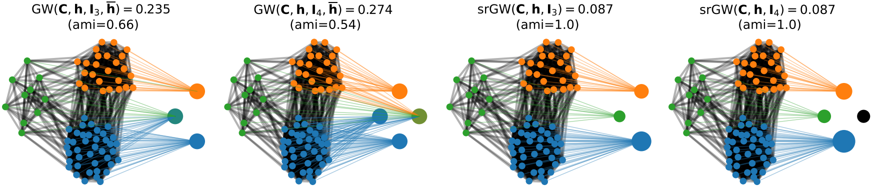
- Clustering of multiple real-valued graphs. Dataset composed of 40 graphs (10 graphs $\times$ 4 types of communities)
- k-means clustering using the FGW barycenter



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].



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Benamou, J.-D., Carlier, G., Cuturi, M., Nenna, L., and Peyré, G. (2015).
Iterative Bregman projections for regularized transportation problems.
SISC.

Brogat-Motte, L., Flamary, R., Brouard, C., Rousu, J., and d'Alché Buc, F. (2022).
Learning to predict graphs with fused gromov-wasserstein barycenters.
In *International Conference in Machine Learning (ICML)*.

Bronstein, M. M., Bruna, J., LeCun, Y., Szlam, A., and Vandergheynst, P. (2017).
Geometric deep learning: going beyond euclidean data.
IEEE Signal Processing Magazine, 34(4):18–42.

Brouard, C., Shen, H., Dührkop, K., d'Alché-Buc, F., Böcker, S., and Rousu, J. (2016).
Fast metabolite identification with input output kernel regression.
Bioinformatics, 32(12):i28–i36.

Calissano, A., Feragen, A., and Vantini, S. (2022).
Graph-valued regression: Prediction of unlabelled networks in a non-euclidean graph space.
Journal of Multivariate Analysis, 190:104950.

Chapel, L., Alaya, M. Z., and Gasso, G. (2020).
Partial optimal tranport with applications on positive-unlabeled learning.
Advances in Neural Information Processing Systems, 33:2903–2913.

Chowdhury, S. and Needham, T. (2021).
Generalized spectral clustering via gromov-wasserstein learning.
In *International Conference on Artificial Intelligence and Statistics*, pages 712–720. PMLR.

Cuturi, M. (2013).
Sinkhorn distances: Lightspeed computation of optimal transportation.
In *Neural Information Processing Systems (NIPS)*, pages 2292–2300.

Dozat, T. and Manning, C. D. (2017).
Deep biaffine attention for neural dependency parsing.
In *International Conference on Learning Representations, ICLR*. OpenReview.net.

El Ahmad, T., Brogat-Motte, L., Laforgue, P., and d'Alché Buc, F. (2024).
Sketch in, sketch out: Accelerating both learning and inference for structured prediction with kernels.
In *International Conference on Artificial Intelligence and Statistics*, pages 109–117. PMLR.

Frank, M. and Wolfe, P. (1956).
An algorithm for quadratic programming.
Naval research logistics quarterly, 3(1-2):95–110.

Genevay, A., Chizat, L., Bach, F., Cuturi, M., and Peyré, G. (2018).
Sample complexity of sinkhorn divergences.
arXiv preprint arXiv:1810.02733.

Krzakala, P., Yang, J., Flamary, R., d'Alché Buc, F., Laclau, C., and Labeau, M. (2024).

Any2graph: Deep end-to-end supervised graph prediction with an optimal transport loss.

Ma, X., Chu, X., Wang, Y., Lin, Y., Zhao, J., Ma, L., and Zhu, W. (2023).

Fused gromov-wasserstein graph mixup for graph-level classifications.

In *Thirty-seventh Conference on Neural Information Processing Systems*.

Melnyk, I., Dognin, P., and Das, P. (2022).

Knowledge graph generation from text.

In Goldberg, Y., Kozareva, Z., and Zhang, Y., editors, *Findings of the Association for Computational Linguistics: EMNLP 2022*, pages 1610–1622.

Memoli, F. (2011).

Gromov wasserstein distances and the metric approach to object matching.

Foundations of Computational Mathematics, pages 1–71.

Peyré, G., Cuturi, M., and Solomon, J. (2016).
Gromov-wasserstein averaging of kernel and distance matrices.
In *ICML*, pages 2664–2672.

Scetbon, M., Klein, M., Palla, G., and Cuturi, M. (2023).
Unbalanced low-rank optimal transport solvers.
arXiv preprint arXiv:2305.19727.

Scetbon, M., Peyré, G., and Cuturi, M. (2021).
Linear-time gromov wasserstein distances using low rank couplings and costs.
arXiv preprint arXiv:2106.01128.

Séjourné, T., Vialard, F.-X., and Peyré, G. (2020).
The unbalanced gromov wasserstein distance: Conic formulation and relaxation.
arXiv preprint arXiv:2009.04266.

Shit, S., Koner, R., Wittmann, B., Paetzold, J., Ezhov, I., Li, H., Pan, J., Sharifzadeh, S., Kaissis, G., Tresp, V., et al. (2022).
Relationformer: A unified framework for image-to-graph generation.
In *European Conference on Computer Vision*, pages 422–439. Springer.

Solomon, J., Peyré, G., Kim, V. G., and Sra, S. (2016).
Entropic metric alignment for correspondence problems.
ACM Transactions on Graphics (TOG), 35(4):72.

Thual, A., Tran, H., Zemskova, T., Courty, N., Flamary, R., Dehaene, S., and Thirion, B. (2022).
Aligning individual brains with fused unbalanced gromov-wasserstein.
In *Neural Information Processing Systems (NeurIPS)*.

Togninalli, M., Ghisu, E., Llinares-López, F., Rieck, B., and Borgwardt, K. (2019).
Wasserstein weisfeiler-lehman graph kernels.
Advances in neural information processing systems, 32.

Tseng, P. (2001).
Convergence of a block coordinate descent method for nondifferentiable minimization.
Journal of optimization theory and applications, 109(3):475–494.

Van Assel, H., Vincent-Cuaz, C., Vayer, T., Flamary, R., and Courty, N. (2023).
Interpolating between clustering and dimensionality reduction with gromov-wasserstein.

Vayer, T., Chapel, L., Flamary, R., Tavenard, R., and Courty, N. (2018).
Fused gromov-wasserstein distance for structured objects: theoretical foundations and mathematical properties.

Vayer, T., Chapel, L., Flamary, R., Tavenard, R., and Courty, N. (2019a).
Optimal transport for structured data with application on graphs.
In *International Conference on Machine Learning (ICML)*.

Vayer, T., Courty, N., Tavenard, R., and Flamary, R. (2019b).
Optimal transport for structured data with application on graphs.
In *International Conference on Machine Learning*, pages 6275–6284. PMLR.

Vayer, T., Flamary, R., Tavenard, R., Chapel, L., and Courty, N. (2019c).
Sliced gromov-wasserstein.
In *Neural Information Processing Systems (NeurIPS)*.

Vincent-Cuaz, C., Flamary, R., Corneli, M., Vayer, T., and Courty, N. (2022a).
Semi-relaxed gromov wasserstein divergence with applications on graphs.
In *International Conference on Learning Representations (ICLR)*.

Vincent-Cuaz, C., Flamary, R., Corneli, M., Vayer, T., and Courty, N. (2022b).
Template based graph neural network with optimal transport distances.
In *Neural Information Processing Systems (NeurIPS)*.

Vincent-Cuaz, C., Vayer, T., Flamary, R., Corneli, M., and Courty, N. (2021).
Online graph dictionary learning.
In *International Conference on Machine Learning (ICML)*.

Xu, H. (2020).
Gromov-wasserstein factorization models for graph clustering.
In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 34, pages 6478–6485.