Introduction to (Python) Optimal Transport

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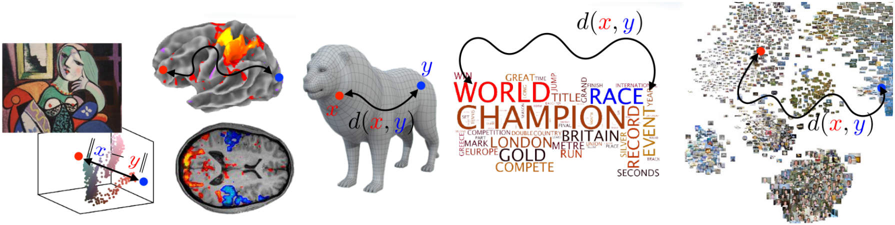
CentraleSupelec, Gif-sur-Yvette

Distributions are everywhere in machine learning

- Images, vision, graphics, Time series, text, genes, proteins.
- Many datum and datasets can be seen as distributions.
- Important questions:
  - How to compare distributions?
  - How to use the geometry of distributions?
- Optimal transport provides many tools that can answer those questions.

Illustration from the slides of Gabriel Peyré.

Distributions are everywhere



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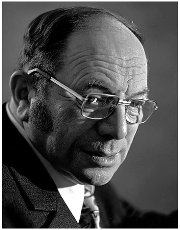
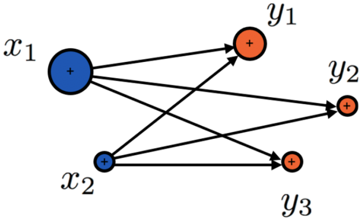
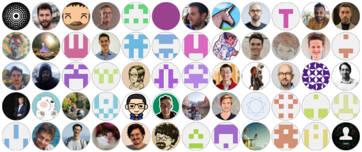
Optimal transport

- Problem introduced by Gaspard Monge in his memoire [Monge, 1781].
- How to move mass while minimizing a cost (mass + cost)
- Monge formulation seeks for a mapping between two mass distribution.
- Reformulated by Leonid Kantorovich (1912–1986), Economy nobelist in 1975
- Focus on where the mass goes, allow splitting [Kantorovich, 1942].
- Applications originally for resource allocation problems

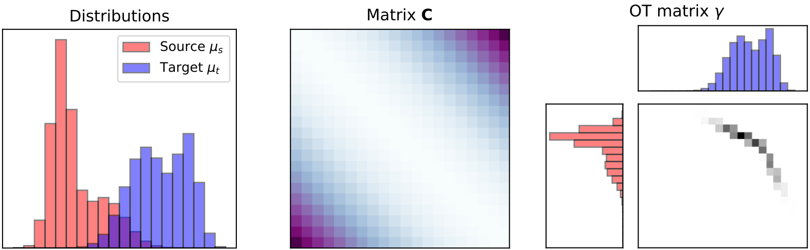
Python Optimal Transport (PO)



The toolbox

- Website/documentation: `https://pythonot.github.io/`
- Github: `https://github.com/PythonOT/POT`
- Activity: 65 contributors, 2k stars, 1.2 M PyPI downloads, 600 citations.
- Features: OT solvers from 57 papers, 58 examples in gallery.
- Geek features: 95% test coverage, 100% PEP8 compliant.
- Deep learning features: Pytorch/Tensorflow/Jax support with autodiff.

Optimal transport between discrete distributions



Kantorovitch formulation : OT Linear Program

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

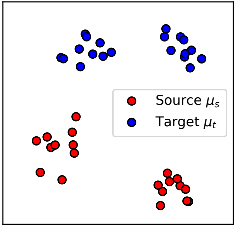
$$W_p^p(\mu_s, \mu_t) = \min_{\boldsymbol{T} \in \Pi(\mu_s, \mu_t)} \left\{ \langle \boldsymbol{T}, \mathbf{C} \rangle_F = \sum_{i,j} T_{i,j} c_{i,j} \right\}$$

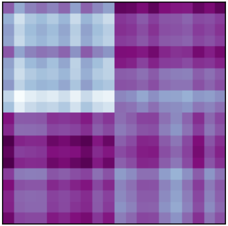
where $\mathbf{C}$ is a cost matrix with $c_{i,j} = c(\mathbf{x}_i^s, \mathbf{x}_j^t) = \|\mathbf{x}_i^s - \mathbf{x}_j^t\|^p$ and the constraints are

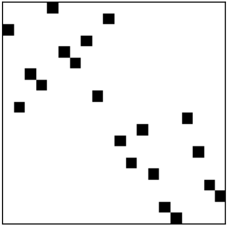
$$\Pi(\mu_s, \mu_t) = \left\{ \boldsymbol{T} \in (\mathbb{R}^+)^{n_s \times n_t} | \, \boldsymbol{T} \mathbf{1}_{n_t} = \mathbf{a}, \boldsymbol{T}^T \mathbf{1}_{n_s} = \mathbf{b} \right\}$$

- Solving the OT problem with network simplex is $O(n^3 \log(n))$ for $n = n_s = n_t$.
- $W_p(\mu_s, \mu_t)$ is called the Wasserstein distance (EMD for $p = 1$).

Optimal transport between discrete distributions







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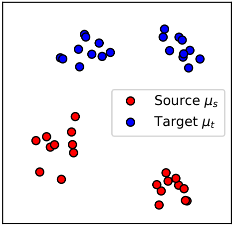
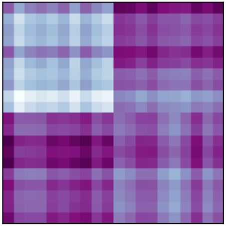
Optimal transport between discrete distributions

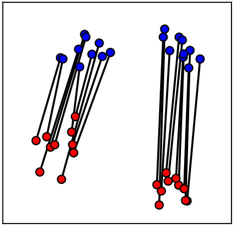
Distributions



Matrix **C**



OT matrix with samples



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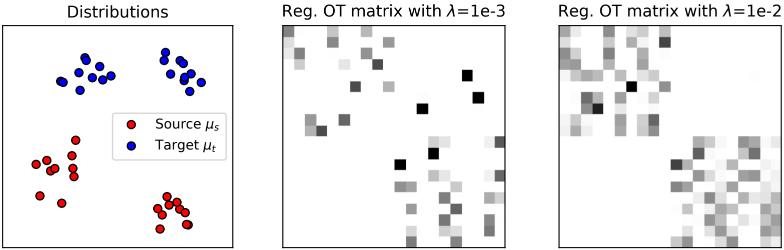
Entropic regularized optimal transport



Entropic regularization [Cuturi, 2013]

$$\mathbf{T}_0^\lambda = \underset{\mathbf{T}\in\Pi(\mu_s,\mu_t)}{\arg\min} \quad \langle \mathbf{T}, \mathbf{C}\rangle_F + \lambda \sum_{i,j} T_{i,j}(\log T_{i,j} - 1)$$

- Regularization with the negative entropy of $\boldsymbol{T}$.
- Looses sparsity but smooth and strictly convex optimization problem.
- Can be solved efficiently with Sinkhorn's matrix scaling algorithm with $\mathbf{u}^{(0)} = \mathbf{1}, \mathbf{K} = \exp(-\mathbf{C}/\lambda)$ and $\mathbf{T} = \text{diag}(\mathbf{u}^\star)\mathbf{K}\text{diag}(\mathbf{v}^\star)$

$$\mathbf{v}^{(k)} = \mathbf{b} \oslash \mathbf{K}^\top \mathbf{u}^{(k-1)}, \quad \mathbf{u}^{(k)} = \mathbf{a} \oslash \mathbf{K}\mathbf{v}^{(k)}$$

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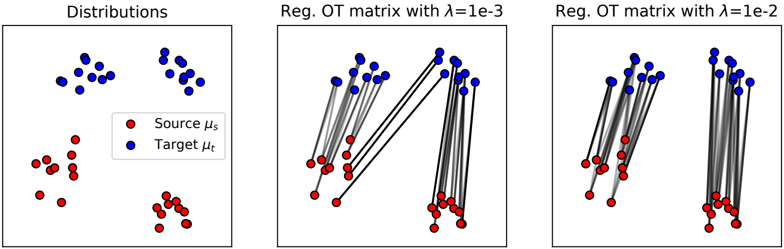

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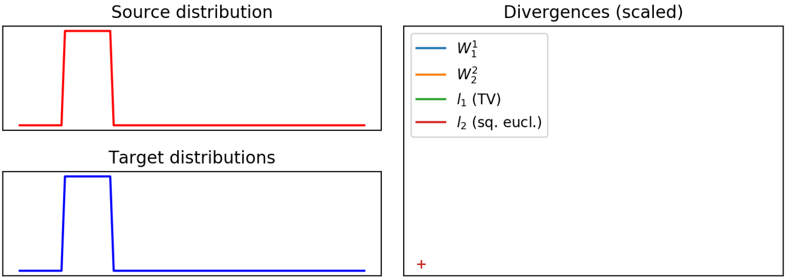
Wasserstein distance



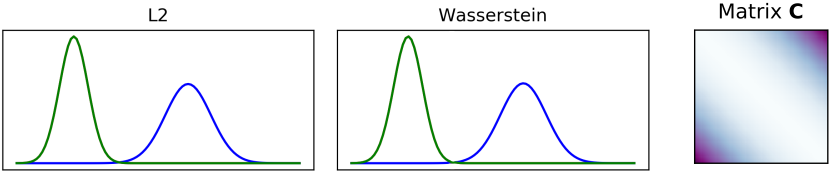
Wasserstein distance

$$W_p^p(\mu_s, \mu_t) = \min_{\gamma \in \mathcal{P}} \int_{\Omega_s \times \Omega_t} \|\mathbf{x} - \mathbf{y}\|^p \gamma(\mathbf{x}, \mathbf{y}) d\mathbf{x} d\mathbf{y} = \mathbb{E}_{(\mathbf{x},\mathbf{y}) \sim \gamma}[\|\mathbf{x} - \mathbf{y}\|^p] \quad (1)$$

In this case we have $c(\mathbf{x}, \mathbf{y}) = \|\mathbf{x} - \mathbf{y}\|^p$

- A.K.A. Earth Mover's Distance (W_1^1) [Rubner et al., 2000].
- Useful between discrete distribution even without overlapping support.
- Smooth approximation can be computed with Sinkhorn [Cuturi, 2013].
- **Wasserstein barycenter**: $\overline{\mu} = \arg\min_\mu \sum_i w_i W_p^p(\mu, \mu_i)$

Wasserstein distance



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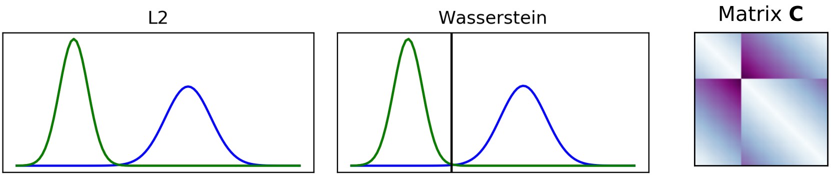

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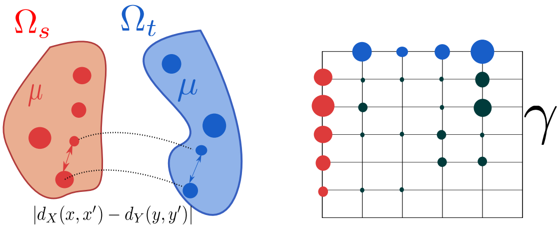


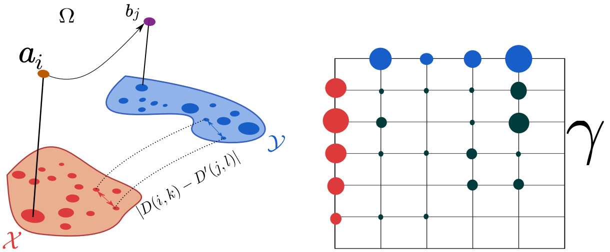
Inspired from Gabriel Peyré

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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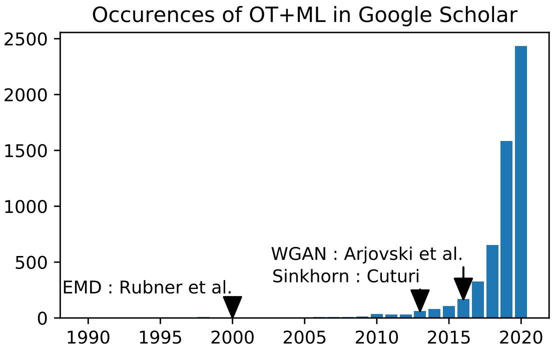
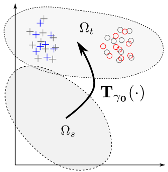


Short history of OT for ML

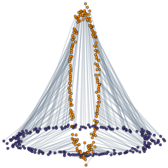
- Proposed in in image processing by [Rubner et al., 2000] (EMD).
- Entropic regularized OT allows fast approximation [Cuturi, 2013].
- Deep learning/ stochastic optimization [Arjovsky et al., 2017].
- Generative models with diffusion/Schrödinger bridges.

Three aspects of optimal transport



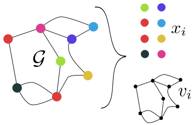
Transporting with optimal transport

- Learn to map between distributions.
- Estimate a smooth mapping from discrete distributions.
- Applications in domain adaptation.



Divergence between histograms/empirical distributions

- Use the ground metric to encode complex relations between the bins of histograms for data fitting.
- OT losses are non-parametric divergences between non overlapping distributions.
- Used to train minimal Wasserstein estimators.



Divergence between structured objects and spaces

- Modeling of structured data and graphs as distribution.
- OT losses (Wass. or (F)GW) measure similarity between distributions/objects.
- OT find correspondance across spaces for adaptation.

Collaborators


N. Courty


A. Rakotomamonjy


D. Tuia


A. Habrard


M. Perrot


M. Ducoffe


M. Cuturi


K. Lounici


A. Férrari


C. Févotte


V. Emiya


V. Seguy


B. Damodaran

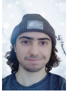

T. Vayer


L. Chapel


R. Tavenard


K. Fatras


I. Redko


H. Janati


T. Séjourné


H. Tran


G. Gasso


M. Corneli


C. Vincent-Cuaz

+ H. Van Assel, Th. Gnassounou, A. Gramfort

Thank you

Python code available on GitHub:

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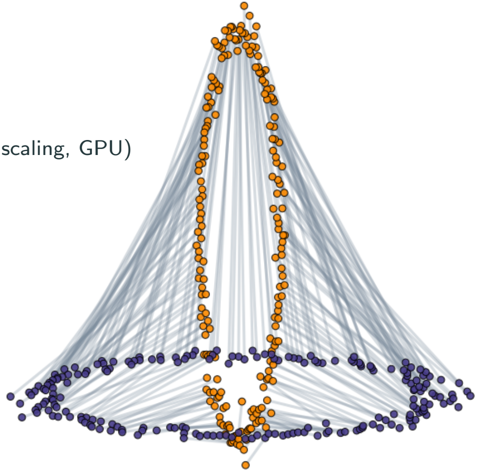
`https://github.com/PythonOT/POT`

- OT LP solver, Sinkhorn (stabilized, $\epsilon-$scaling, GPU)
- Domain adaptation with OT.
- Barycenters, Wasserstein unmixing.
- Wasserstein Discriminant Analysis.



Tutorial on OT for ML:

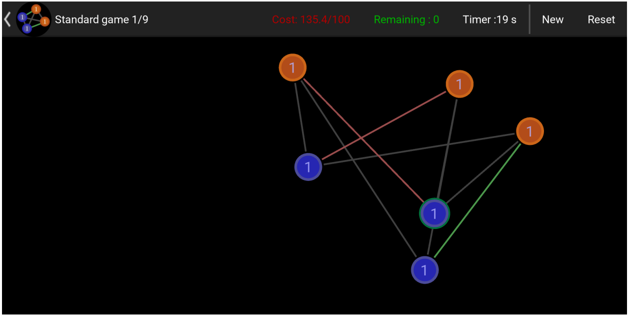
`http://tinyurl.com/otml-isbi`

Papers available on my website:

`https://remi.flamary.com/`

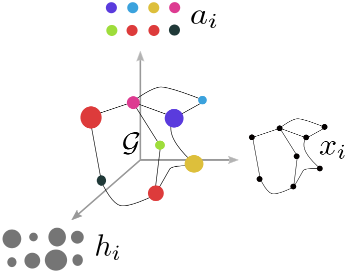
OTGame (OT Puzzle game on android)

OTGame



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

References and supplementary material



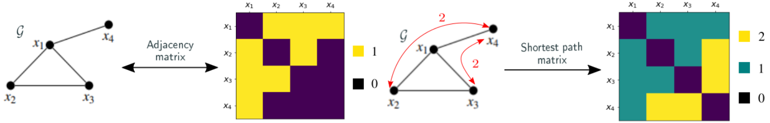
$$\mu = \sum_i h_i \delta_{(x_i, a_i)}$$

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

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

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

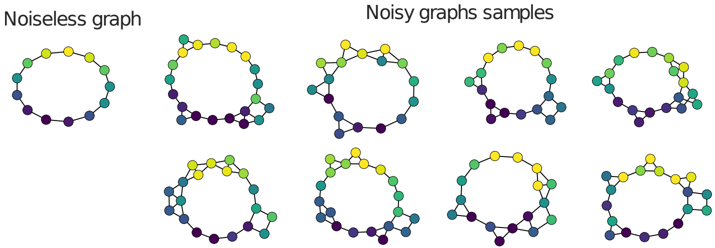
- The positions x_i are implicit and represented as the pairwise matrix $\boldsymbol{D}$.
- Possible choices for $\boldsymbol{D}$: Adjacency matrix, Laplacian, Shortest path, ...



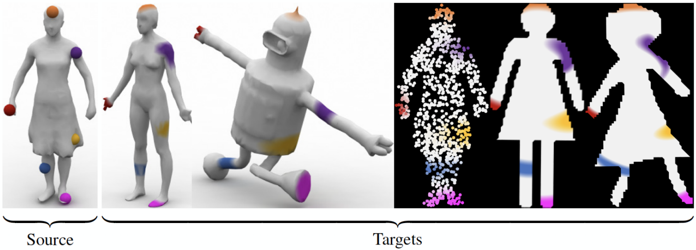
- The node features can be compared between graphs and stored in $\mathbf{F}$.
- h_i are the masses on the nodes of the graphs (uniform by default).

Applications of (F)GW

Barycenter/averaging of labeled graphs [Vayer et al., 2018]



Shape matching between surfaces [Solomon et al., 2016, Thual et al., 2022]



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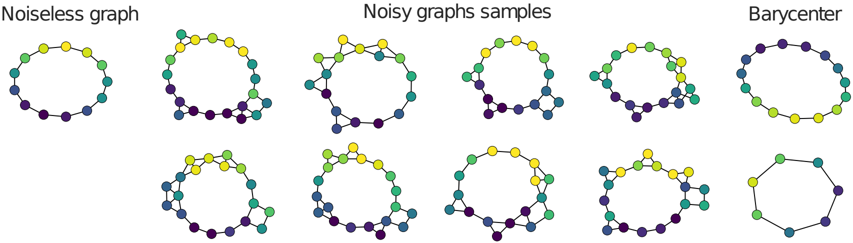

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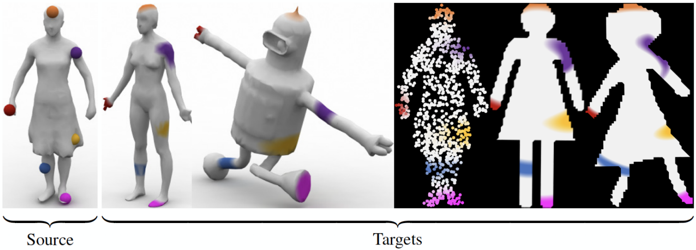

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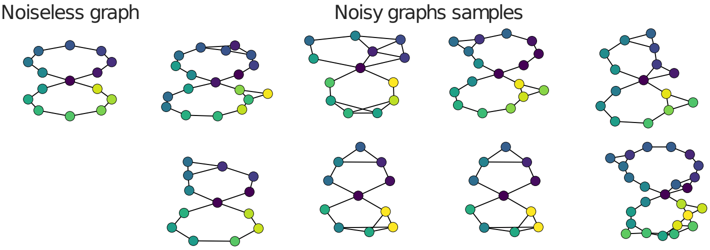

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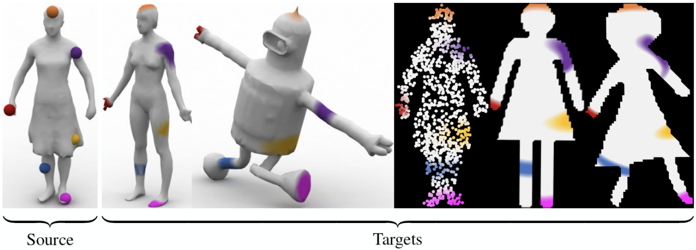

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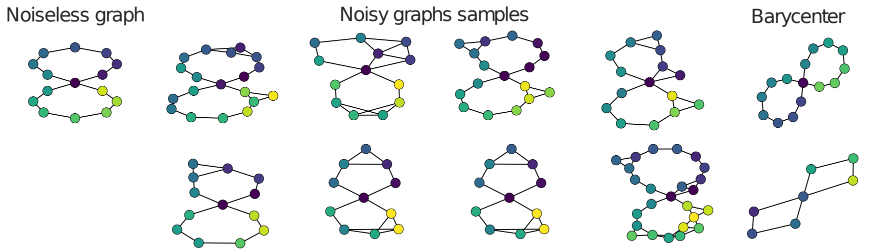

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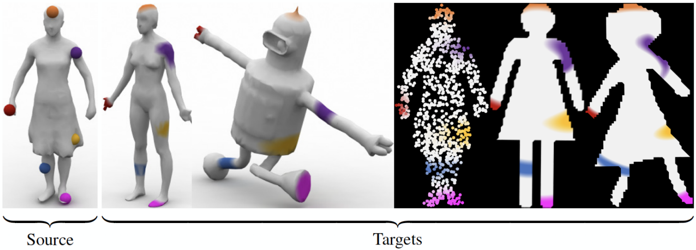
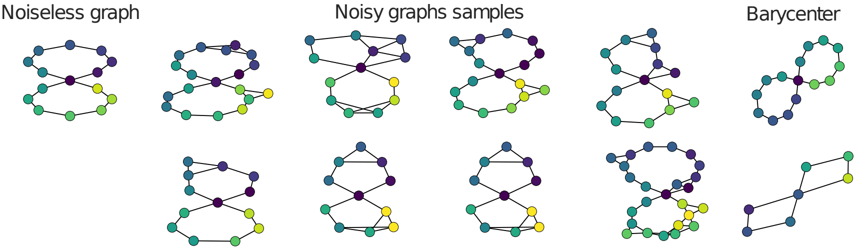
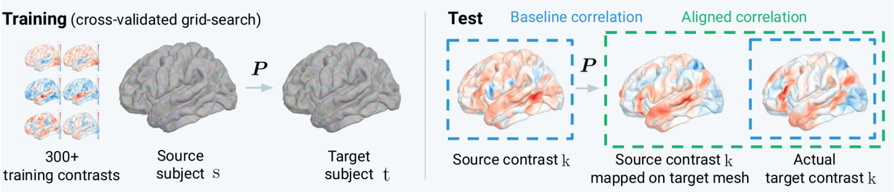


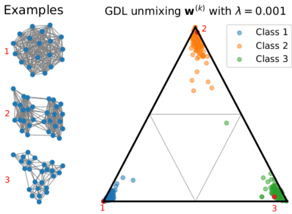
Applications of (F)GW

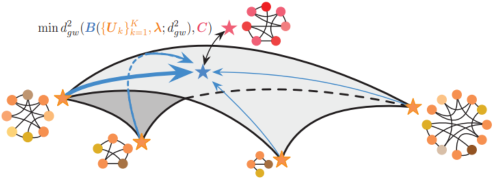
Barycenter/averaging of labeled graphs [Vayer et al., 2018]



Shape matching between surfaces [Solomon et al., 2016, Thual et al., 2022]







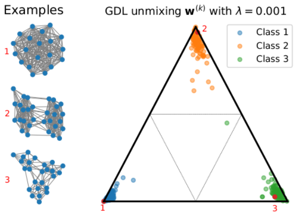
Representation learning for graphs

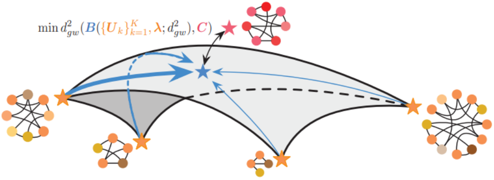
- Learn a dictionary $\{\overline{\mathbf{C}_i}\}_i$ of graph templates to describe a continuous manifold.
- The representation is learned by minimizing the (F)GW distance between the graph reconstruction from the embedding in the dictionary.
- Online Graph Dictionary learning : Linear model [Vincent-Cuaz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

$$\widehat{\mathbf{C}} = \sum_i w_i \overline{\mathbf{C}_i}$$

- GW Factorization : Nonlinear (GW barycenter) model [Xu, 2020].
- Dictionary for structured prediction with GW bary. [Brogat-Motte et al., 2022].

Graph Dictionary Learning





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$$\widehat{\mathbf{C}} = \arg\min_{\mathbf{C}} \sum_i w_i GW(\mathbf{C}, \overline{\mathbf{C}_i})$$

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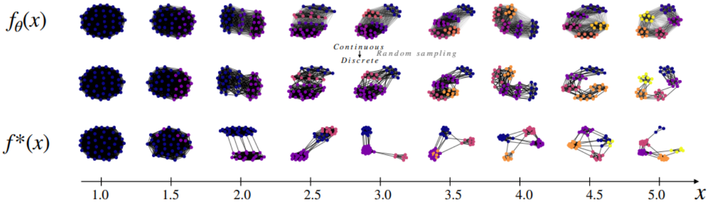
Graph Dictionary Learning



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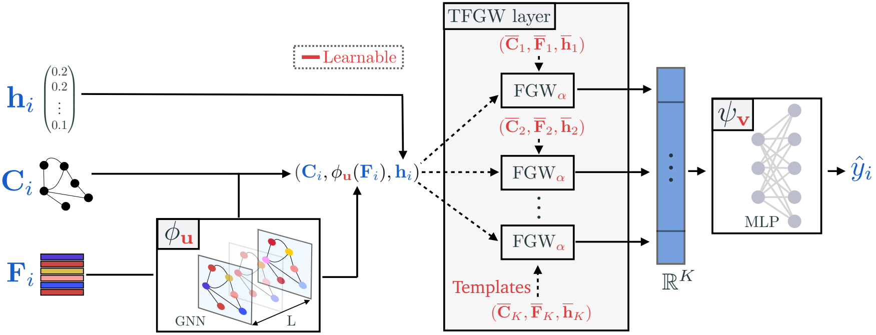
$$f(\mathbf{x}) = \widehat{\mathbf{C}}(\mathbf{x}) = \arg\min_{\mathbf{C}} \sum_i w_i(\mathbf{x}) GW(\mathbf{C}, \overline{\mathbf{C}_i})$$

FGW for a pooling layer in GNN



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

- Principle: represent a graph through its distances to learned templates.
- Learnable parameters are illustrated in red above.
- New end-to-end GNN models for graph-level tasks.
- Sate-of-the-art (still!) on graph classification (1×#1, 3×#2 on paperwithcode).

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