



INSTITUT
POLYTECHNIQUE
DE PARIS

Optimal Transport for Machine Learning

10 years of least effort

Rémi Flamary, École polytechnique

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Mathematical Foundations of AI, 2023, Paris

Distributions are everywhere

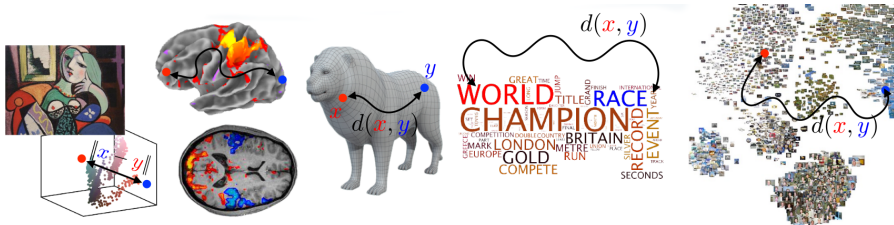


Distributions are everywhere in machine learning

- 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.

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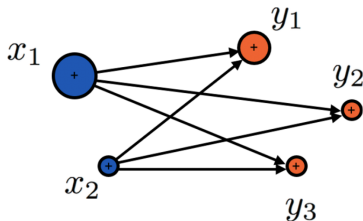
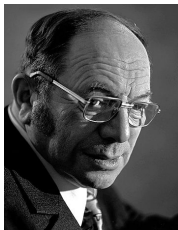
Optimal Transport between spaces and structures

- Gromov-Wasserstein and extensions

- Applications of OT between graphs

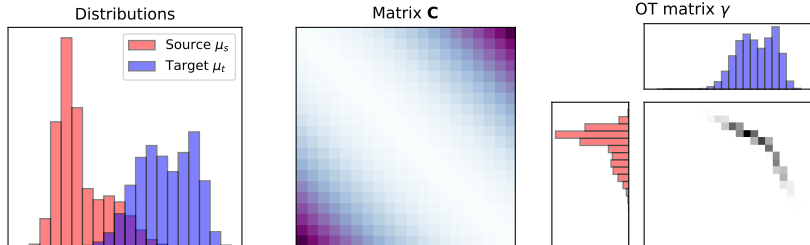
Conclusion

Optimal transport



- Problem introduced by Gaspard Monge in his memoir [Monge, 1781].
- How to move mass while minimizing a cost (mass + cost)
- Monge formulation seeks for a mapping between two mass distributions.
- 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

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 $\mu_t = \sum_{i=1}^{n_t} b_i \delta_{\mathbf{x}_i^t}$

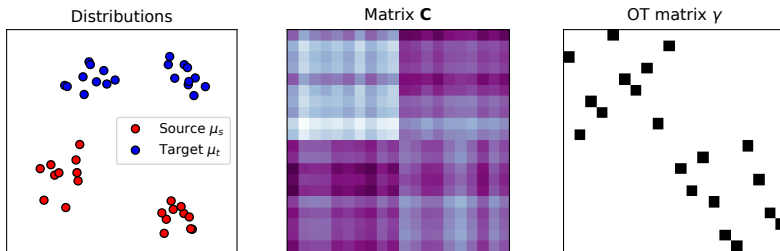
$$W_p^p(\mu_s, \mu_t) = \min_{\mathbf{T} \in \Pi(\mu_s, \mu_t)} \left\{ \langle \mathbf{T}, \mathbf{C} \rangle_F = \sum_{i,j} T_{i,j} c_{i,j} \right\}$$

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

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

- 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 $p = 1$).

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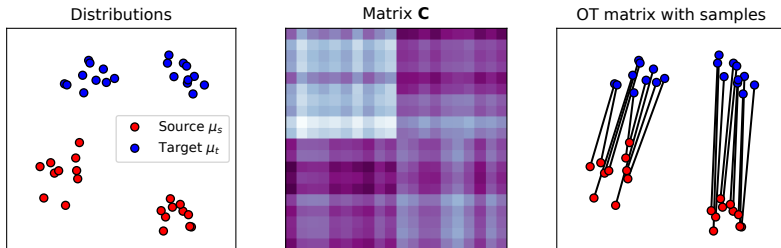
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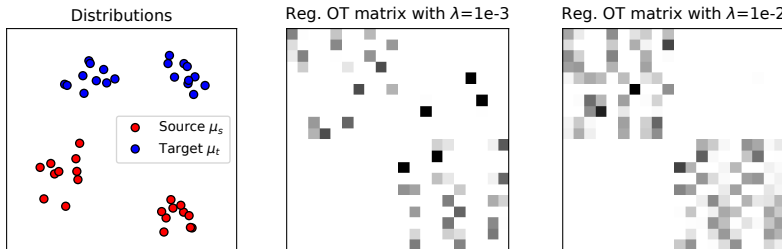
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Entropic regularized optimal transport



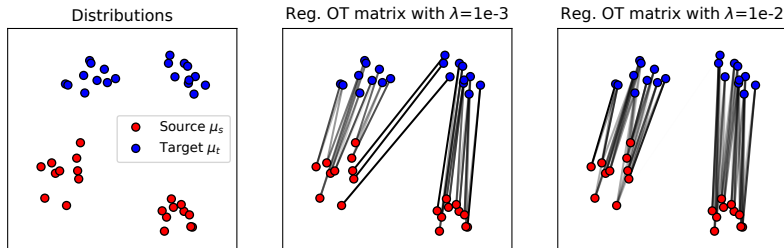
Entropic regularization [Cuturi, 2013]

$$\mathbf{T}_0^\lambda = \arg \min_{\mathbf{T} \in \Pi(\boldsymbol{\mu}_s, \boldsymbol{\mu}_t)} \langle \mathbf{T}, \mathbf{C} \rangle_F + \lambda \sum_{i,j} T_{i,j} (\log T_{i,j} - 1)$$

- Regularization with the negative entropy of $\mathbf{T}$.
- 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 $\mathbf{T} = \text{diag}(\mathbf{u}^*) \mathbf{K} \text{diag}(\mathbf{v}^*)$

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

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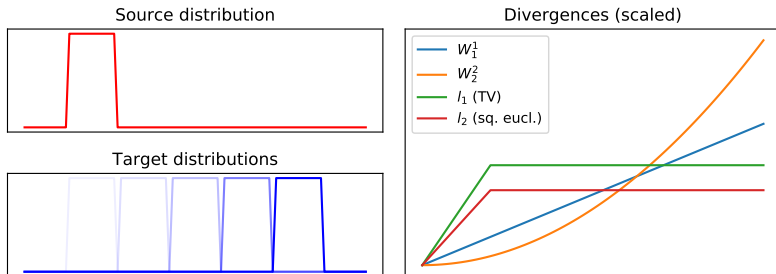
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Wasserstein distance



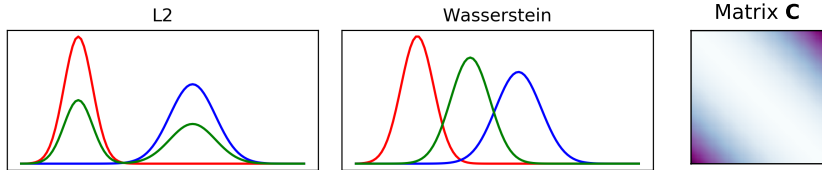
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$$W_p^p(\mu_s, \mu_t) = \min_{\gamma \in \mathcal{P}} \int_{\Omega_s \times \Omega_t} \|\mathbf{x} - \mathbf{y}\|^p \gamma(\mathbf{x}, \mathbf{y}) d\mathbf{x} d\mathbf{y} = \mathbb{E}_{(\mathbf{x}, \mathbf{y}) \sim \gamma} [\|\mathbf{x} - \mathbf{y}\|^p]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

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:** $\bar{\mu} = \arg \min_{\mu} \sum_i w_i W_p^p(\mu, \mu_i)$

Wasserstein distance



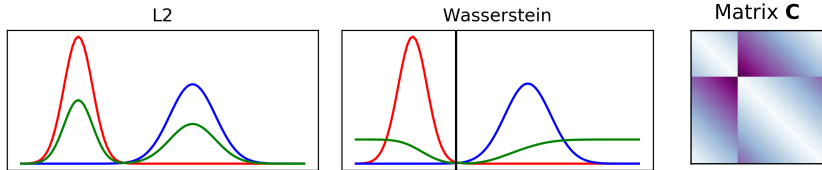
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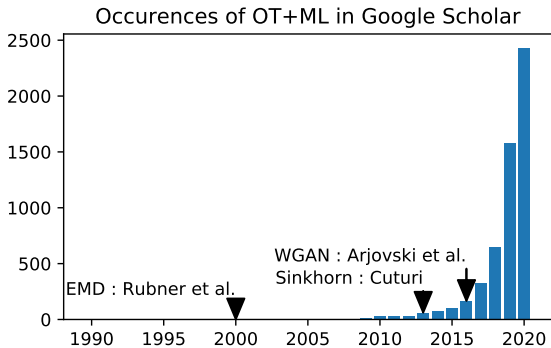
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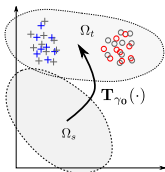
Optimal transport for machine learning



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

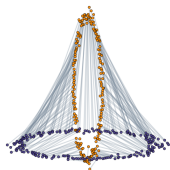


Transporting with optimal transport

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

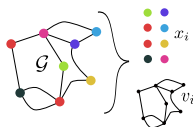
Divergence between histograms/empirical distributions

- 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.



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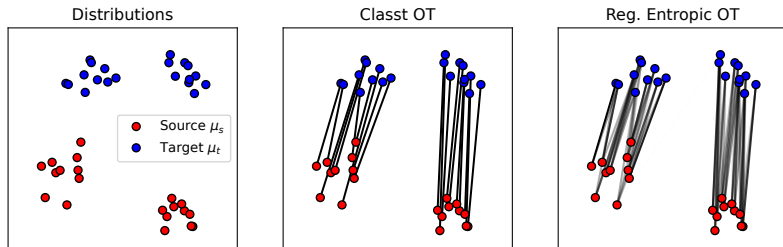
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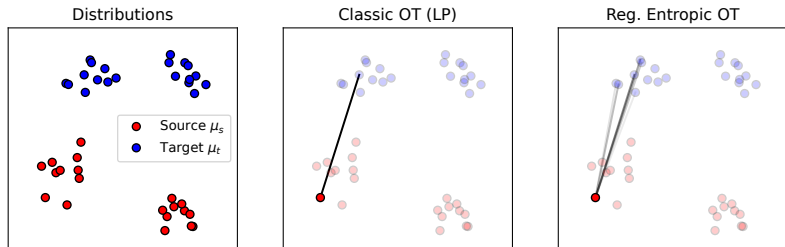
Mapping estimation

- Barycentric mapping using the OT matrix T [Ferradans et al., 2014].

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Mapping with optimal transport



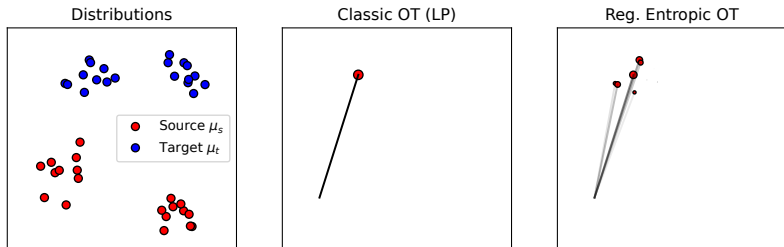
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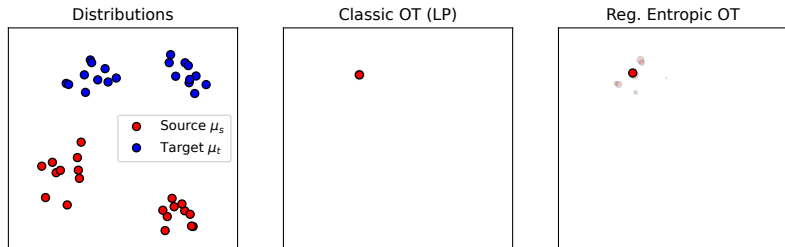
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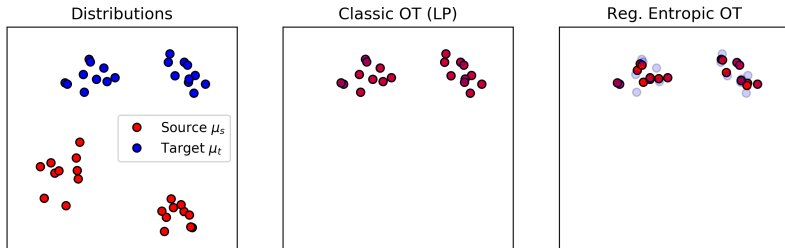
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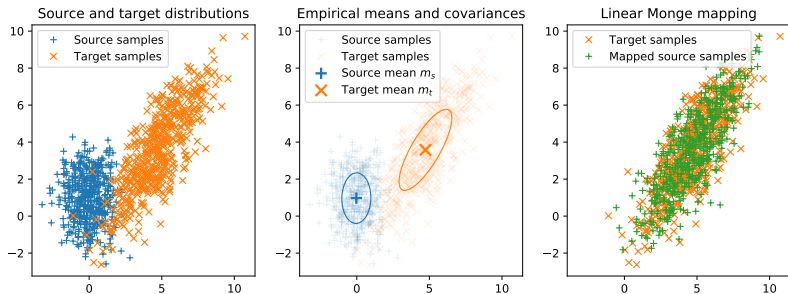
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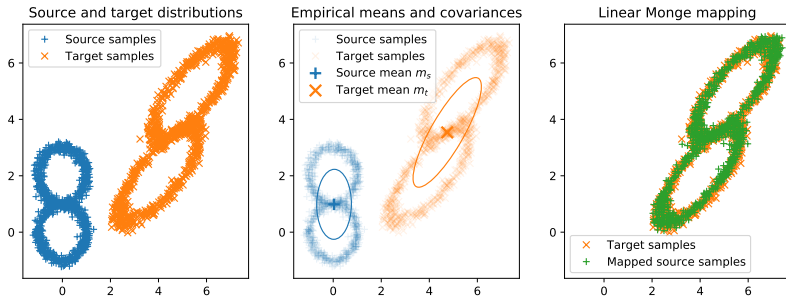
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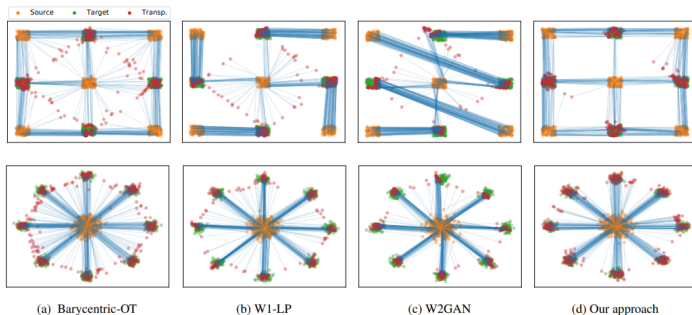
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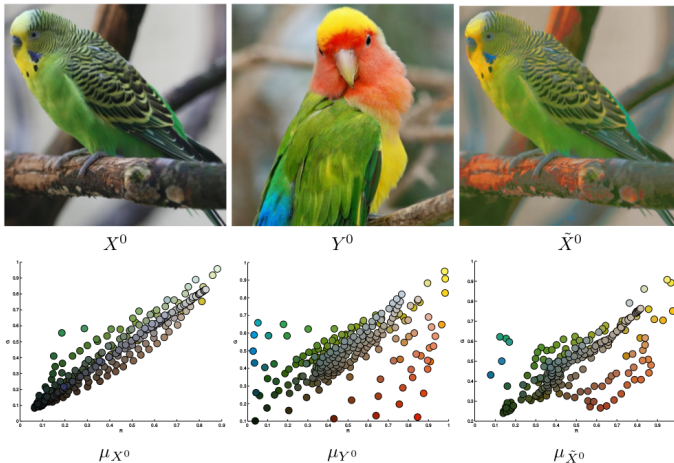


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Histogram matching in images

Pixels as empirical distribution [Ferradans et al., 2014]



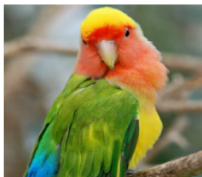
Histogram matching in images

Image colorization [Ferradans et al., 2014]

Original X^0



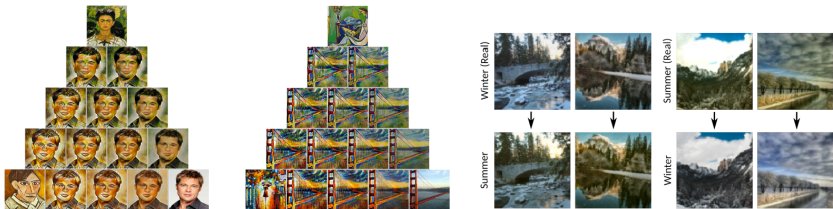
Original Y^0



Proposed method



OT mapping for Image-to-Image translation



Principle

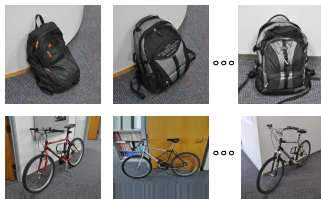
- Encode image as a distribution in a DNN embedding.
- Transform between images using estimated Monge mapping.
- Linear Monge Mapping (Wasserstein Style Transfer [Mroueh, 2019]).
- Nonlinear Monge Mapping using input Convex Neural Networks [Korotin et al., 2019].
- Allows for transformation between two images but also style interpolation with Wasserstein barycenters.

Domain Adaptation problem

Amazon



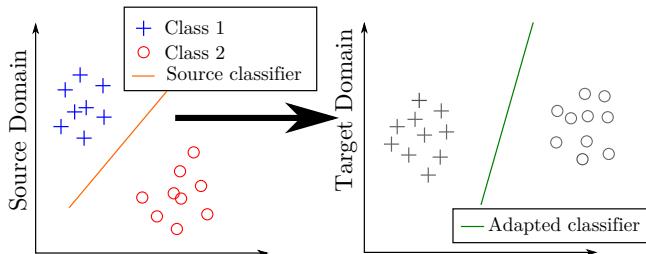
DLSR



Domain Adaptation

- Classification problem with data coming from different sources (domains).
- Distributions are different but related.
- Labels only available in the **source domain**, but prediction is conducted in the **target domain**.
- Objective : Train a classifier that performs well in the target domain

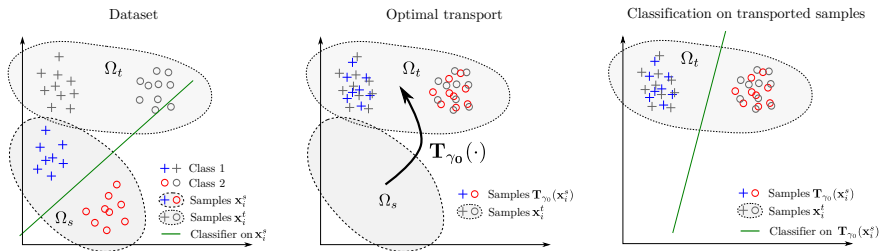
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Optimal transport for domain adaptation



Assumptions

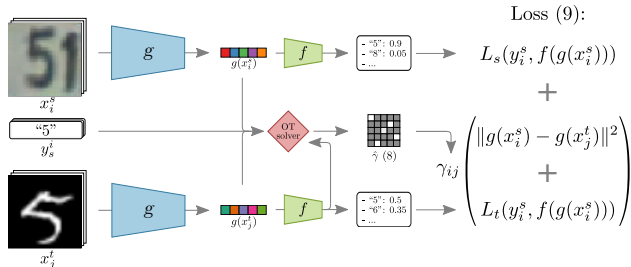
1. There exist an OT mapping m in the feature space between the two domains.
2. The transport preserves the joint distributions:

$$P^s(\mathbf{x}, y) = P^t(m(\mathbf{x}), y).$$

3-step strategy [Courty et al., 2014, Courty et al., 2016]

1. Estimate optimal transport between distributions (use regularization).
2. Transport the training samples on target domain.
3. Learn a classifier on the transported training samples.

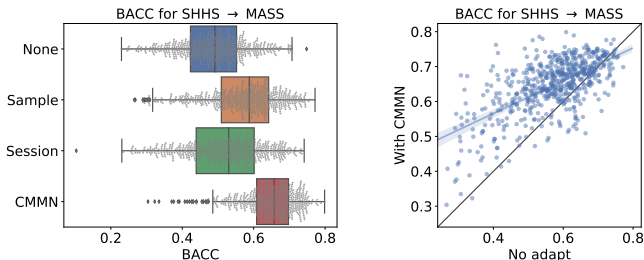
Domain adaptation with optimal transport



Extensions and related works

- JDOT [Courty et al., 2017b] : Joint OT and target predictor estimation.
- [Shen et al., 2018] : Wasserstein Distance Guided Representation Learning.
- DeepJDOT [Damodaran et al., 2018, Fatras et al., 2021] : Deep learning JDOT.
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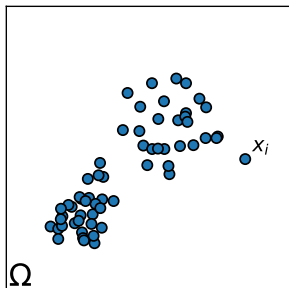
Applications of OT between graphs

Conclusion

Discrete distributions: Empirical vs Histogram

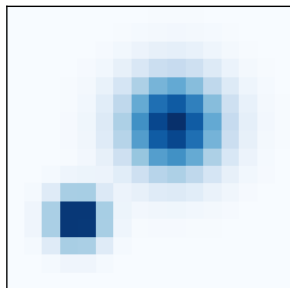
Discrete measure: $\mu = \sum_{i=1}^n a_i \delta_{\mathbf{x}_i}, \quad \mathbf{x}_i \in \Omega, \quad \sum_{i=1}^n a_i = 1$

Lagrangian (point clouds)



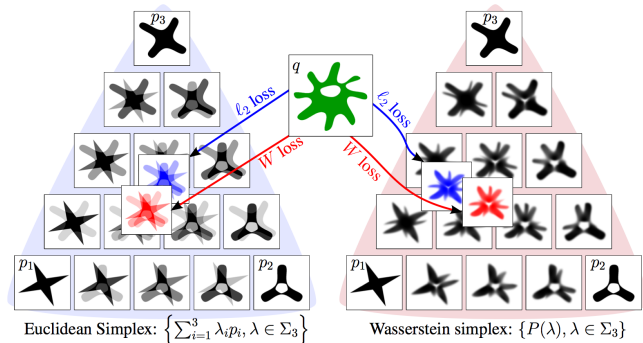
- Constant weight: $a_i = \frac{1}{n}$
- Quotient space: Ω^n, Σ_n

Eulerian (histograms)



- Fixed positions $\mathbf{x}_i$ e.g. grid
- Convex polytope Σ_n (simplex):
 $\{(a_i)_i \geq 0; \sum_i a_i = 1\}$

Dictionary Learning and Principal Geodesics Analysis



Unsupervised learning on histogram data

- DL with Wasserstein distance [Sandler and Lindenbaum, 2011, Rolet et al., 2016]
- Nonlinear DL with Wasserstein barycenter [Schmitz et al., 2017]
- Geodesic PCA in Wasserstein space [Seguy and Cuturi, 2015, Bigot et al., 2017].
- Approximation using Wasserstein embedding [Courty et al., 2017a].

Dictionary Learning and Principal Geodesics Analysis

Class 0						Class 1						Class 4					
PCA			PGA			PCA			PGA			PCA			PGA		
1	2	3	1	2	3	1	2	3	1	2	3	1	2	3	1	2	3
																	
																	
																	
																	
																	
																	
																	

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Multi-label learning with Wasserstein Loss



Siberian husky



Eskimo dog



Flickr : street, parade, dragon
Prediction : people, protest, parade



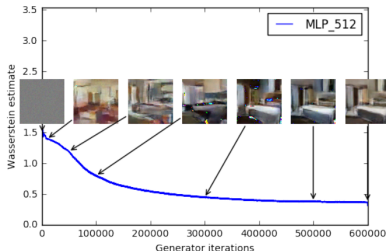
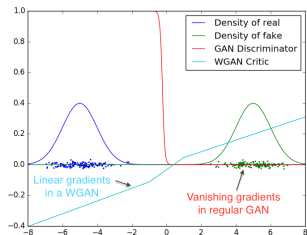
Flickr : water, boat, ref ection, sun-shine
Prediction : water, river, lake, summer;

Learning with a Wasserstein Loss [Frognier et al., 2015]

$$\min_f \sum_{k=1}^N W_1^1(f(\mathbf{x}_i), \mathbf{l}_i)$$

- Empirical loss minimization with Wasserstein loss.
- Multi-label prediction (labels $\mathbf{l}$ seen as histograms, f output softmax).
- Cost between labels can encode semantic similarity between classes.
- Good performances in image tagging.

Wasserstein Generative Adversarial Networks (WGAN)



Wasserstein GAN [Arjovsky et al., 2017]

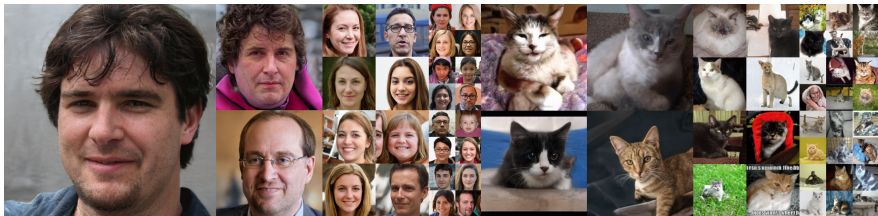
$$\min_G W_1^1(G\#\mu_z, \mu_d), \quad \text{s.t. } \mathbf{z} \sim \mathcal{N}(0, \mathbf{I}) \quad (2)$$

- Minimizes the distance between the true μ_d and generated data $G\#\mu_z$.
- Better convergence in practice than classical GANs [Goodfellow et al., 2014].
- Wasserstein in the dual (separable w.r.t. the samples).

$$\min_G \sup_{\phi \in \text{Lip}^1} \mathbb{E}_{\mathbf{x} \sim \mu_d} [\phi(\mathbf{x})] - \mathbb{E}_{\mathbf{z} \sim \mu_z} [\phi(G(\mathbf{z}))]$$

- Lipschitzness constrained or penalized [Gulrajani et al., 2017].
- State of the art for image generation with [Karras et al., 2019] (before diffusion)

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- OT problem and mathematical tools

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Mapping with optimal transport

- Mapping with optimal transport from discrete samples

- Optimal transport for domain adaptation

Optimal Transport as a distance between distributions

- OT between histogram data

- OT between empirical distributions

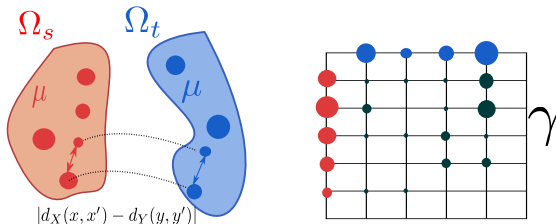
Optimal Transport between spaces and structures

- Gromov-Wasserstein and extensions

- Applications of OT between graphs

Conclusion

Gromov-Wasserstein and extensions



Inspired from Gabriel Peyré

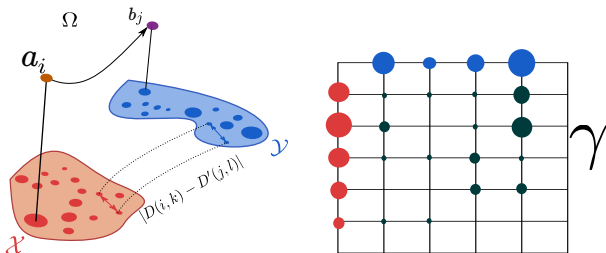
GW for discrete distributions [Memoli, 2011]

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

with $\mu_s = \sum_i a_i \delta_{\mathbf{x}_i^s}$ and $\mu_t = \sum_j b_j \delta_{\mathbf{x}_j^t}$ 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].

Gromov-Wasserstein and extensions



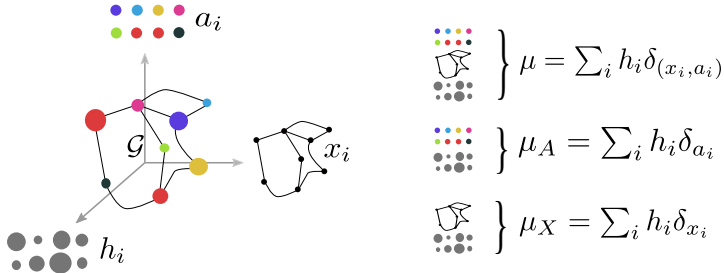
FGW for discrete distributions [Vayer et al., 2018]

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

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

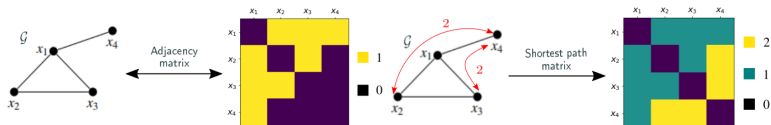
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Gromov-Wasserstein between graphs



Graph as a distribution (D, F, h)

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



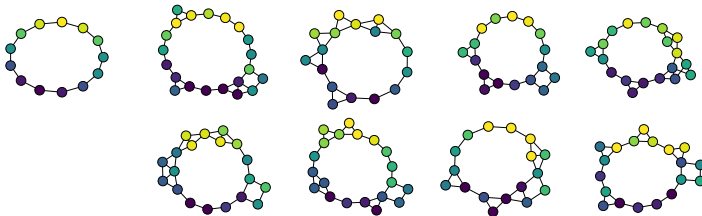
- The node features can be compared between graphs and stored in F .
- h_i are the masses on the nodes of the graphs (uniform by default).

Applications of (F)GW

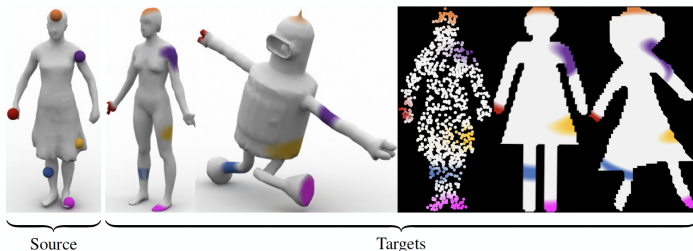
Barycenter/averaging of labeled graphs [Vayer et al., 2018]

Noiseless graph

Noisy graphs samples



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



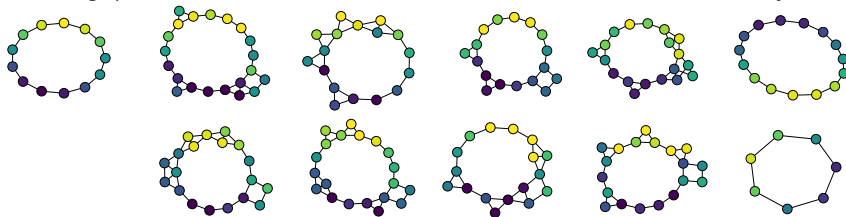
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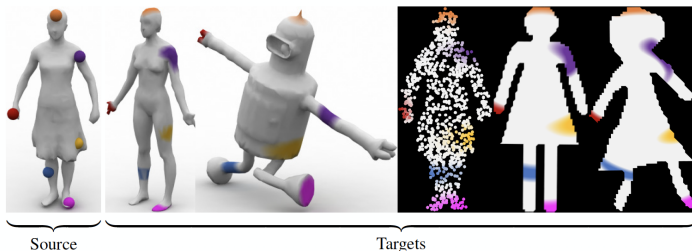
Noiseless graph

Noisy graphs samples

Barycenter



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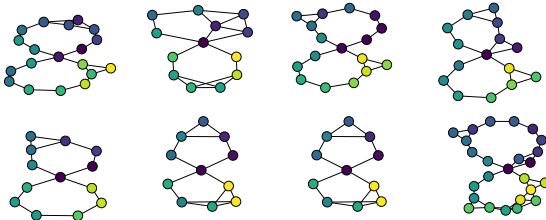
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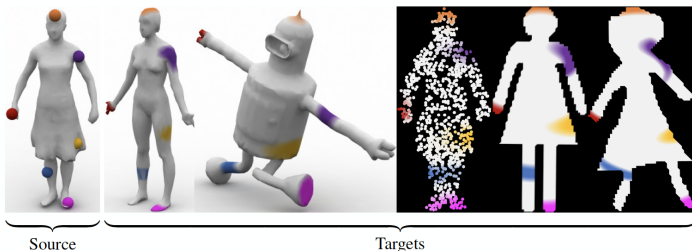
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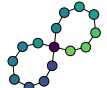
Noiseless graph



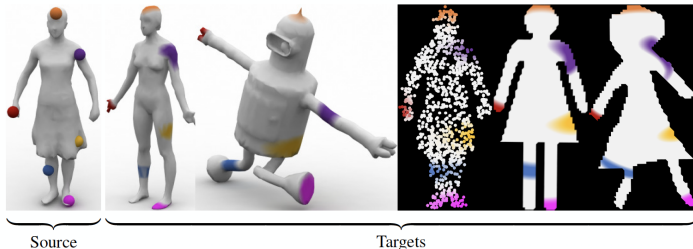
Noisy graphs samples



Barycenter



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



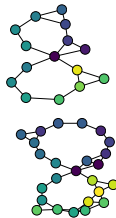
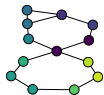
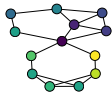
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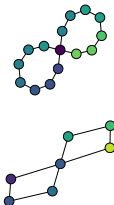
Noiseless graph



Noisy graphs samples

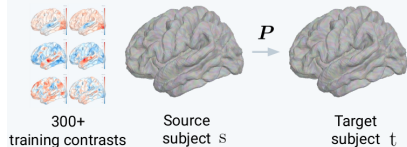


Barycenter



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

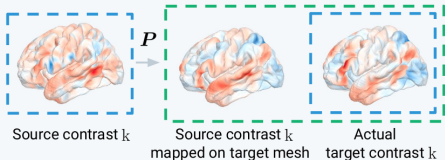
Training (cross-validated grid-search)



Test

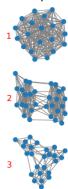
Baseline correlation

Aligned correlation

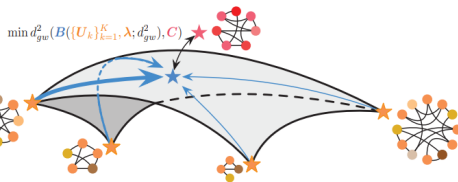
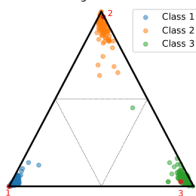


Graph Dictionary Learning

Examples



GDL unmixing $\mathbf{w}^{(k)}$ with $\lambda = 0.001$



Representation learning for graphs

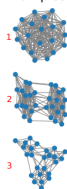
- Learn a dictionary $\{\overline{\mathbf{C}}_i\}_i$ of graph templates to describe a continuous manifold.
- The representation is learned by minimizing the (F)GW distance between the graph reconstruction from the embedding in the dictionary.
- Online Graph Dictionary learning : Linear model [Vincent-Cuaz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

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

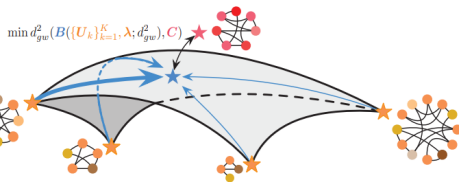
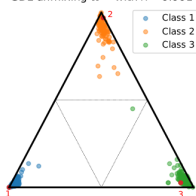
- GW Factorization : Nonlinear (GW barycenter) model [Xu, 2020].
- Dictionary for structured prediction with GW bary. [Brogat-Motte et al., 2022].

Graph Dictionary Learning

Examples



GDL unmixing $\mathbf{w}^{(k)}$ with $\lambda = 0.001$



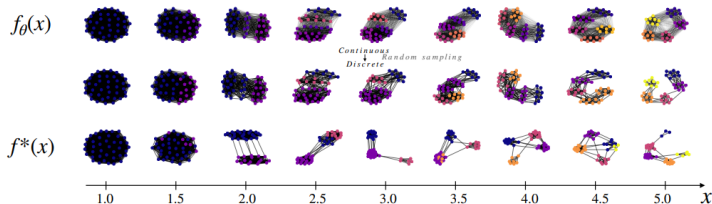
Representation learning for graphs

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

- Dictionary for structured prediction with GW bary. [Brogat-Motte et al., 2022].

Graph Dictionary Learning

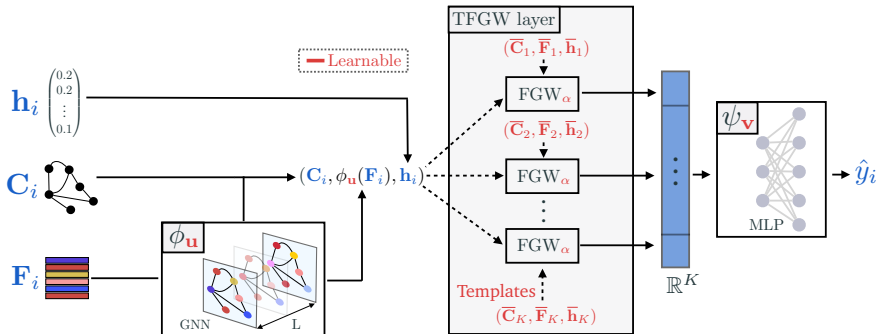


Representation learning for graphs

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

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.
- State-of-the-art (still!) on graph classification ($1 \times \#1$, $3 \times \#2$ on paperwithcode).

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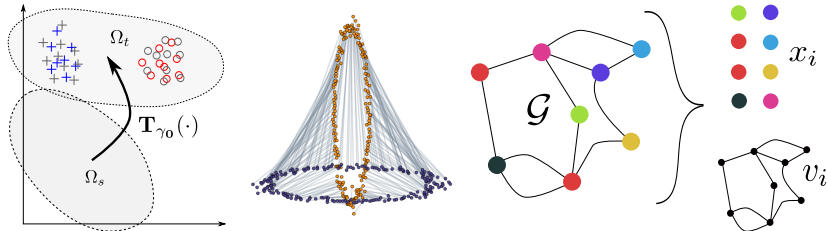
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Ten years of least effort



Optimal Transport for Machine Learning

- Very dynamic community (NeurIPS OTML workshop every 2 years).
- Distributions are everywhere, and geometry can help.
- OT can be used to map, find correspondances and measure similarity.
- Many extensions: sliced, unbalanced, multi-marginal, ...

What about the next ten years ?

- OT is here to stay, it is a tool that can be adapted/relaxed.
- We need better solvers (faster, more scalable, more robust).

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

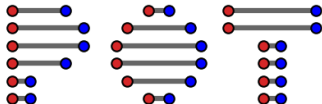


C. Vincent-Cuaz

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

Thank you

Python code available on GitHub:



Python code available on GitHub:

<https://github.com/PythonOT/POT>

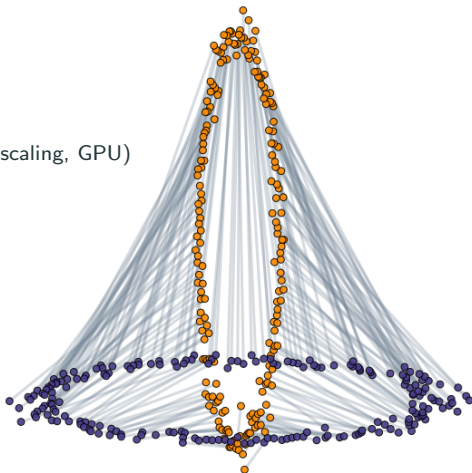
- OT LP solver, Sinkhorn (stabilized, ϵ -scaling, GPU)
- Domain adaptation with OT.
- Barycenters, Wasserstein unmixing.
- Wasserstein Discriminant Analysis.

Tutorial on OT for ML:

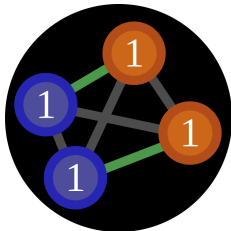
<http://tinyurl.com/otml-isbi>

Papers available on my website:

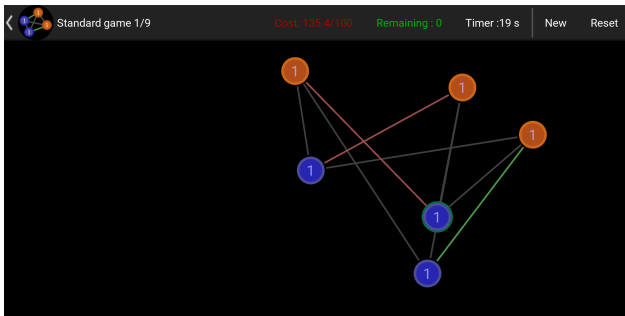
<https://remi.flamary.com/>



OTGame (OT Puzzle game on android)



OTGame



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