Any2Graph: Deep end-to-end supervised graph prediction with an optimal transport loss

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Learning and Optimization in Luminy (LOL 24)


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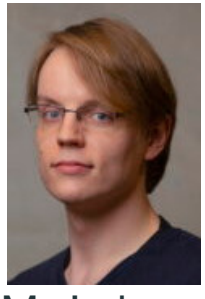
M. Labeau

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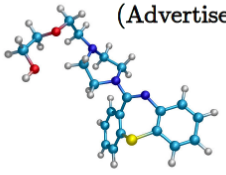
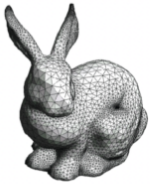
Supervised Graph Prediction

Graphs are everywhere

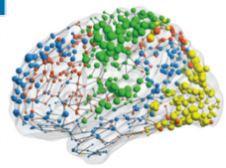
Social networks
(Advertisement)



Drug/Material
molecules
(Chemistry)

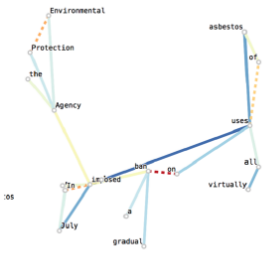


3D Meshes
(Computer Graphics)

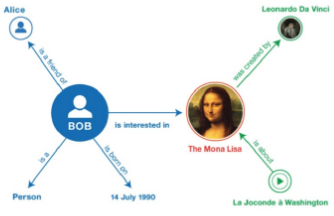


Brain
connectivity
(Neuroscience)

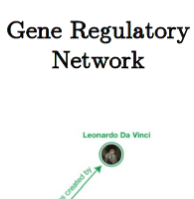
Transportation
networks



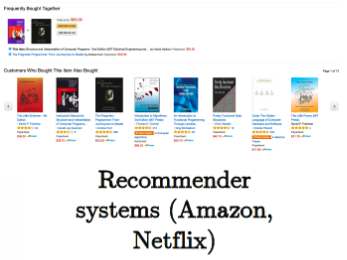
Words relationships
(NLP)



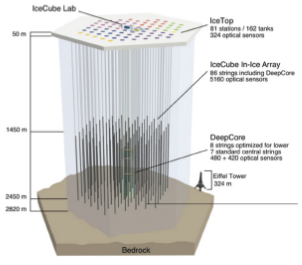
Knowledge graph
(Causality)



Gene Regulatory
Network



Recommender
systems (Amazon,
Netflix)



Neutrino
detection (High-
energy Physics)

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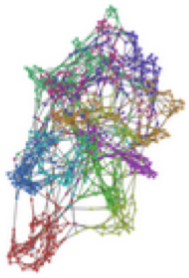
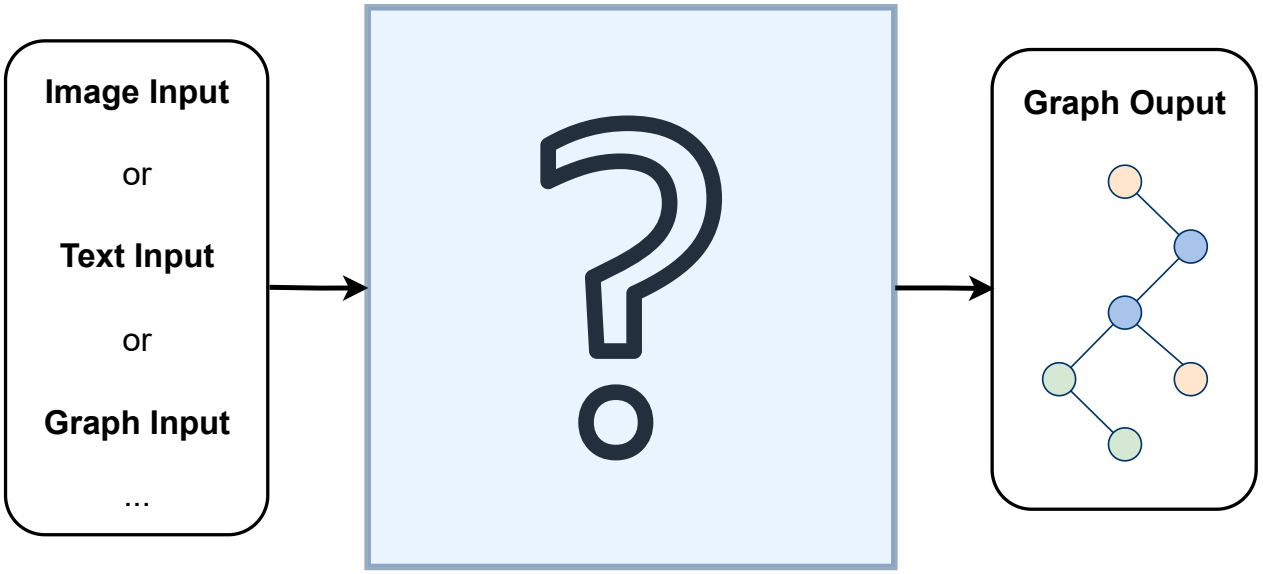


Graphs/
Networks

- Classical approaches : spectral and Fourier based analysis and processing.
- More recently : deep learning on graphs (GNN).
- This talk is about **supervised graph prediction**.

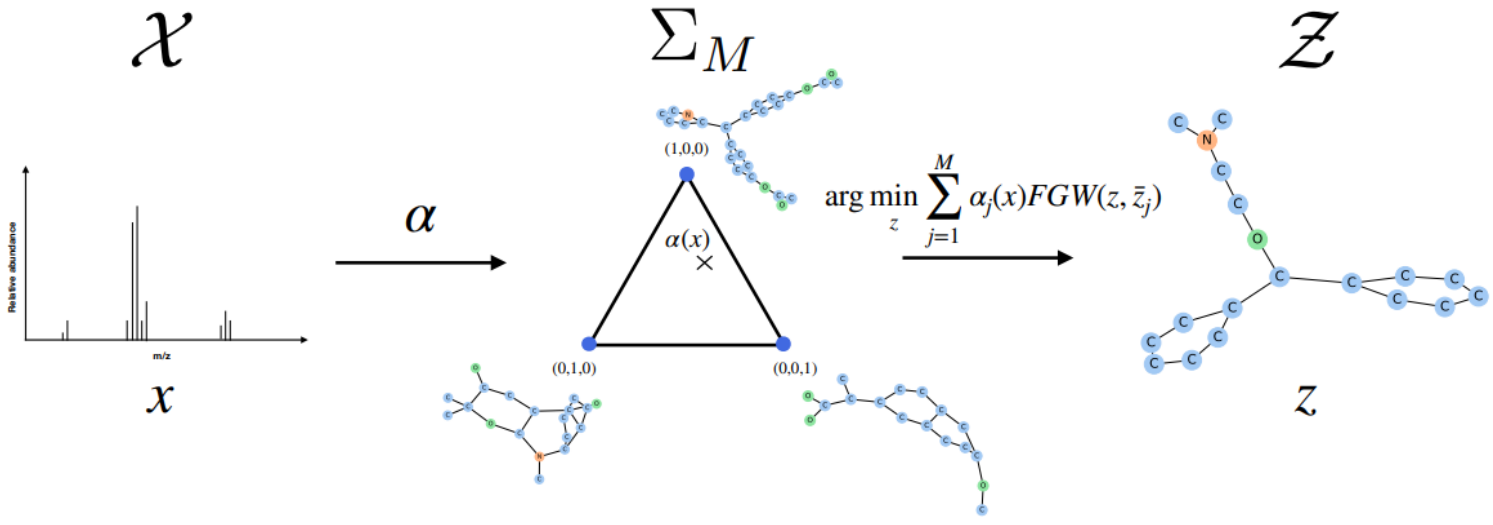
Supervised Graph prediction



Supervised graph prediction

- Special case of structured prediction.
- 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]
- Most methods are data specific and/or slow at inference.

How to predict a graph? (1)



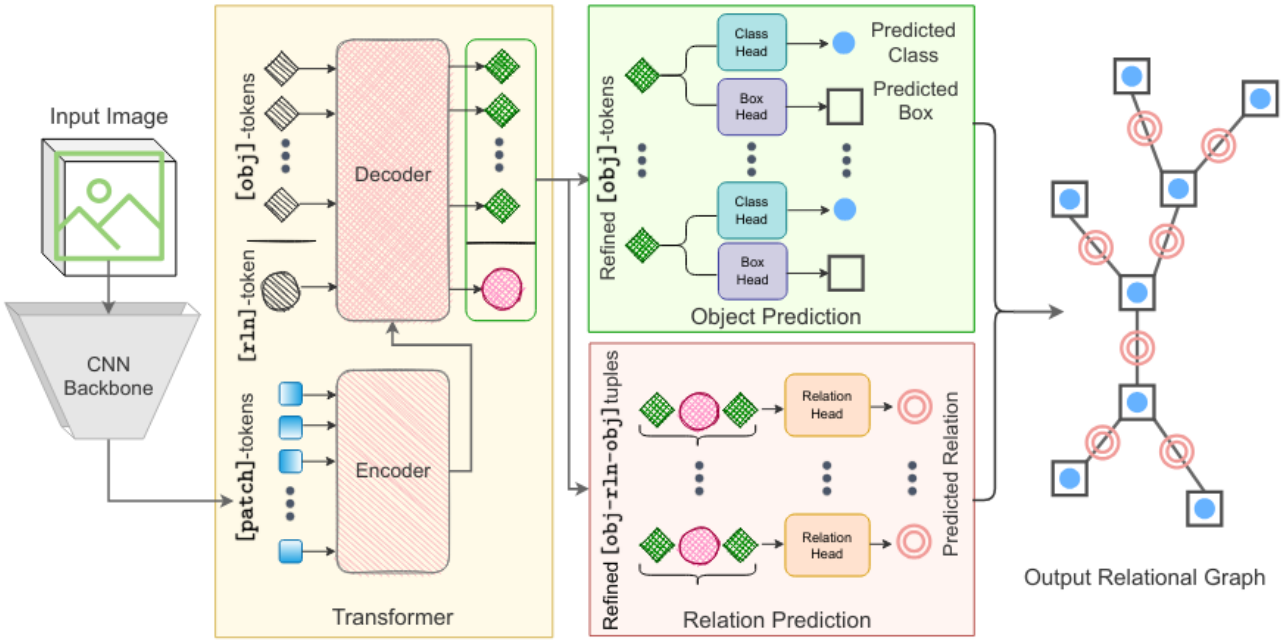
Surrogate based methods [Brouard et al., 2016, El Ahmad et al., 2024]

- 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).

Graph prediction with OT barycenters [Brogat-Motte et al., 2022]

- Decoding done with a conditional FGW.
- Can learn parametric (NN) and non-parametric (kernel) models.
- Slow at training and prediction due to barycenter computation.

How to predict a graph? (2)

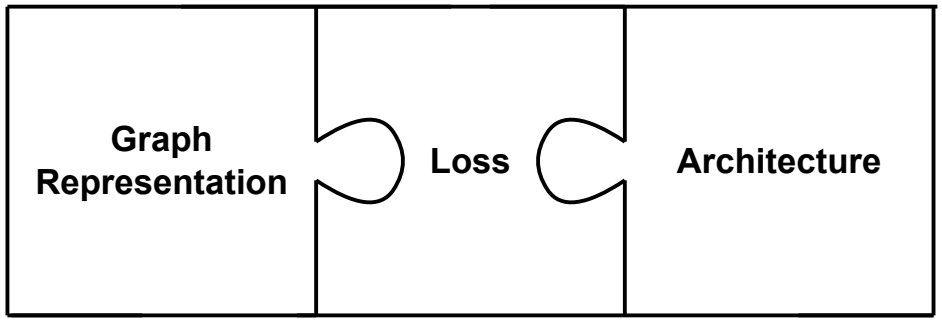


Relationformer [Shit et al., 2022]

- 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.

Deep end-to-end supervised graph prediction

Any2Graph framework



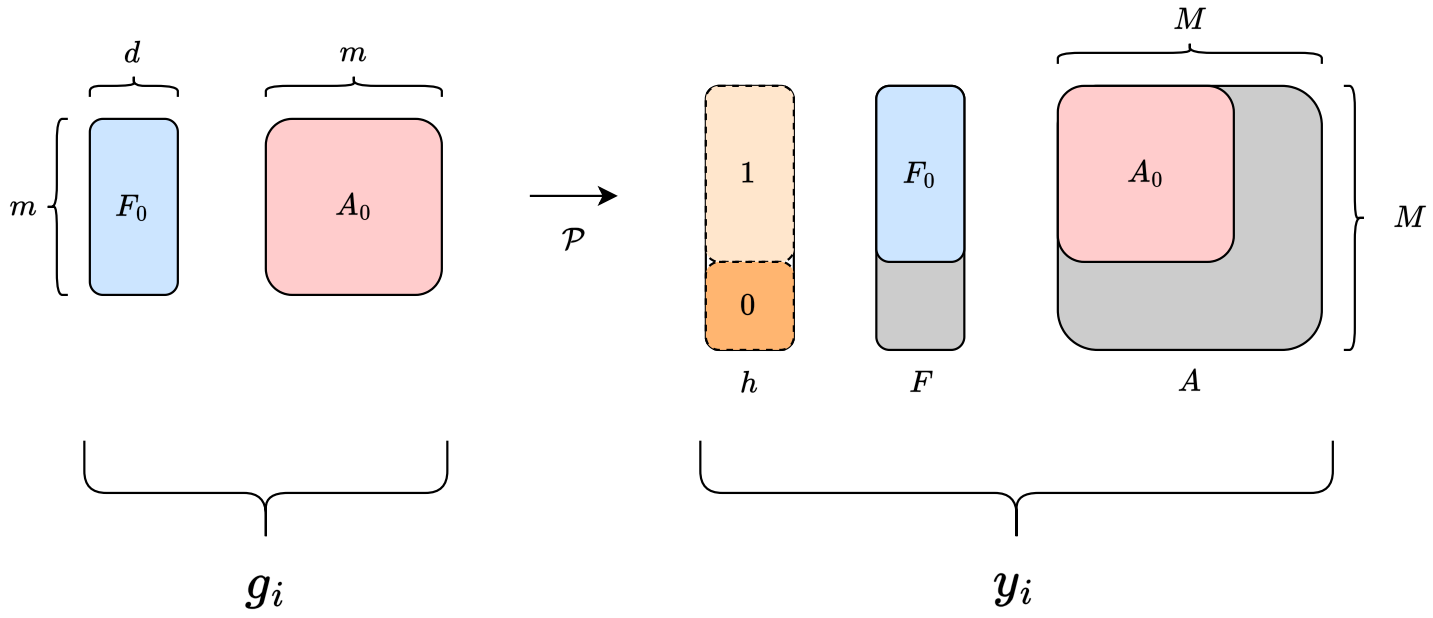
Principle [Krzakala et al., 2024]

- 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.

Forcing the target graph size with padding

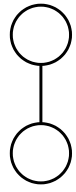


Padding Operator

$$\mathcal{P}(g) = \left(\begin{pmatrix} \mathbf{1}_m \\ \mathbf{0}_{M-m} \end{pmatrix}, \begin{pmatrix} \mathbf{F}_m \\ \mathbf{0}_{M-m} \end{pmatrix}, \begin{pmatrix} \mathbf{A}_m & \mathbf{0}_{M-m} \\ \mathbf{0}_{M-m}^T & \mathbf{0}_{M-m,M-m} \end{pmatrix} \right)$$

- $g = (\mathbf{F}_m, \mathbf{A}_m) \in \mathcal{G}_m$ is a labeled graph of size $m \leq M$.
- $\mathbf{A}_m$ is the adjacency matrix and $\mathbf{F}_m$ is the node feature matrix.
- $\mathcal{P}(g) = (\mathbf{h}, \mathbf{F}, \mathbf{A})$ where $\mathbf{h} \in 0, 1^M$ is a padding identification vector.
- Pad all graphs in training set to have the same size M.

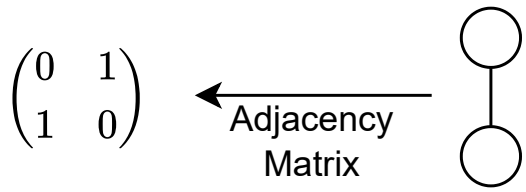
End-to-end SGP pipeline



Target Graph

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

End-to-end SGP pipeline



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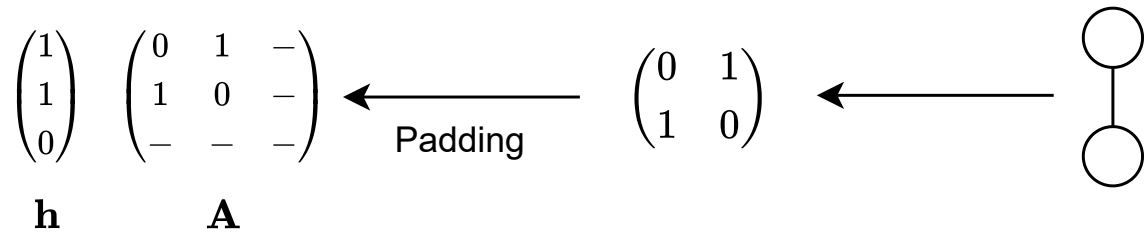

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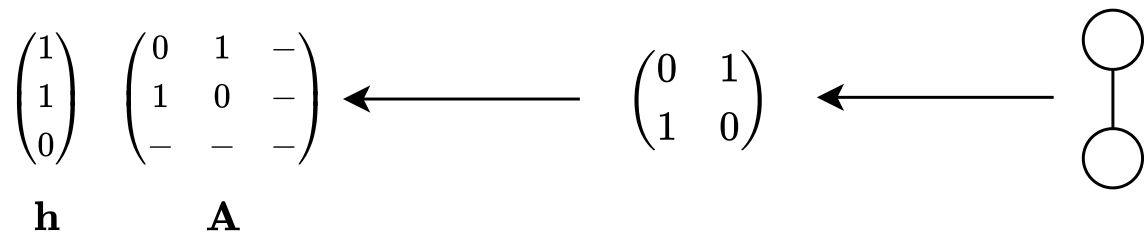
End-to-end SGP pipeline

Input

$\mathbf{x}$



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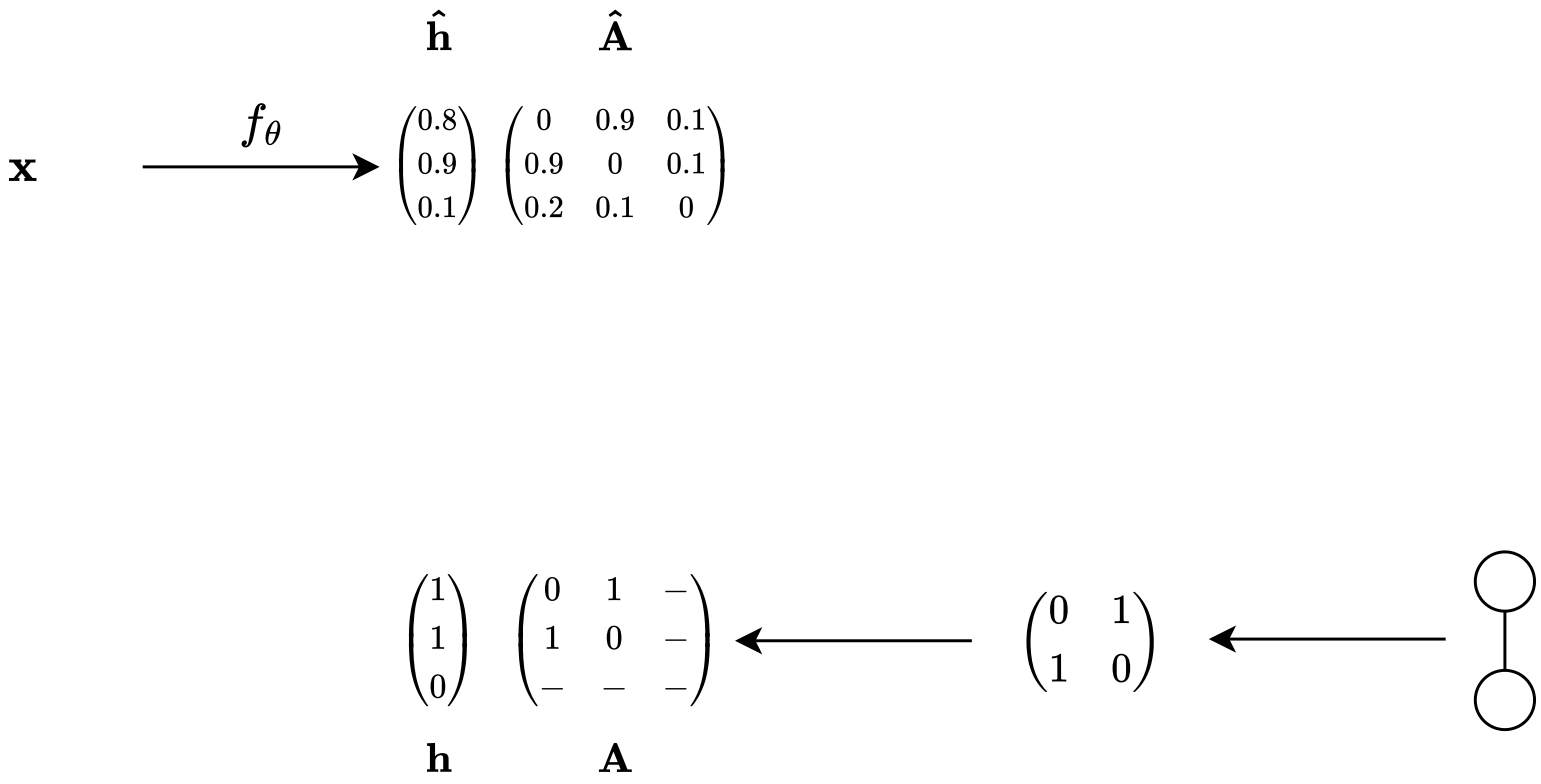

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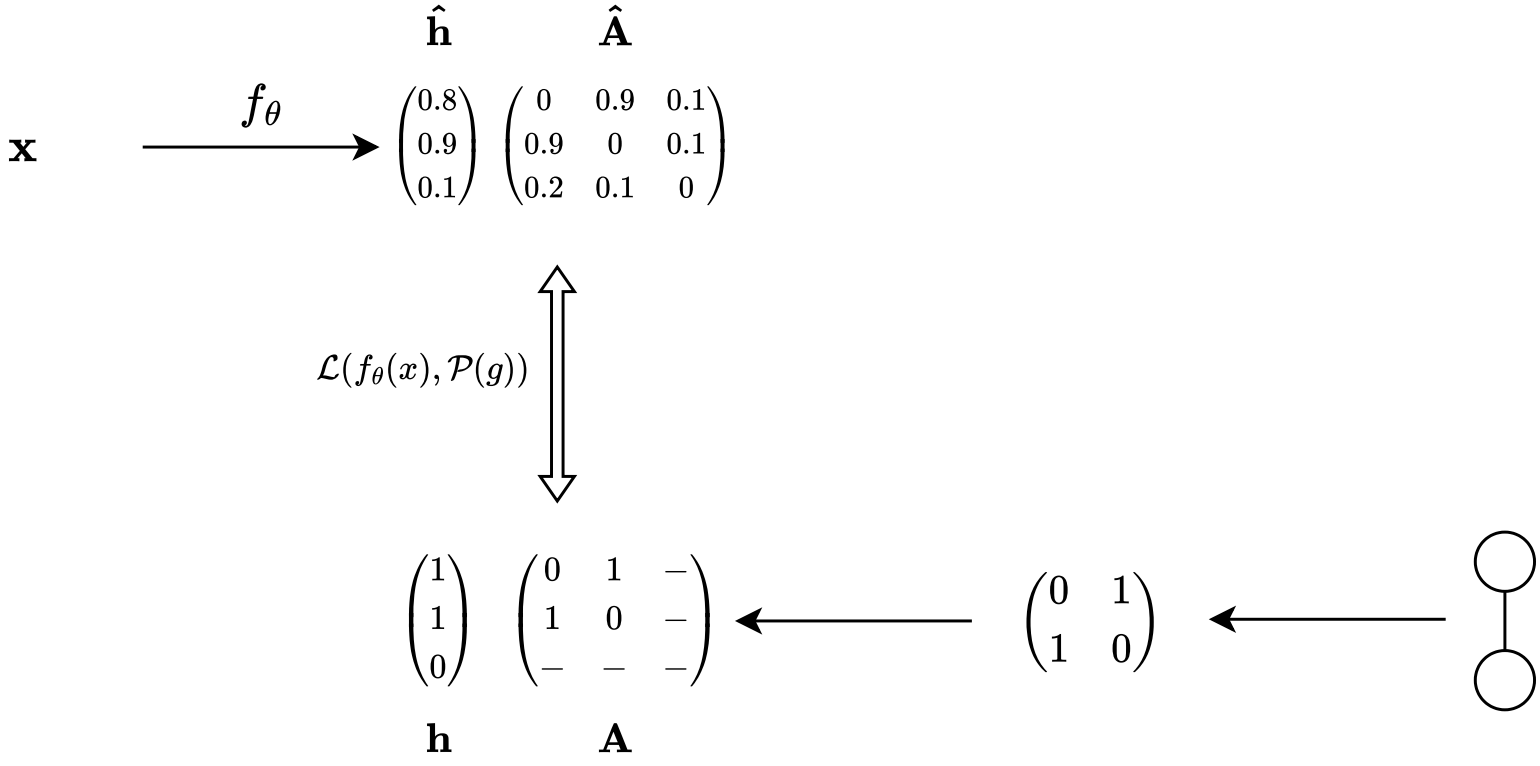

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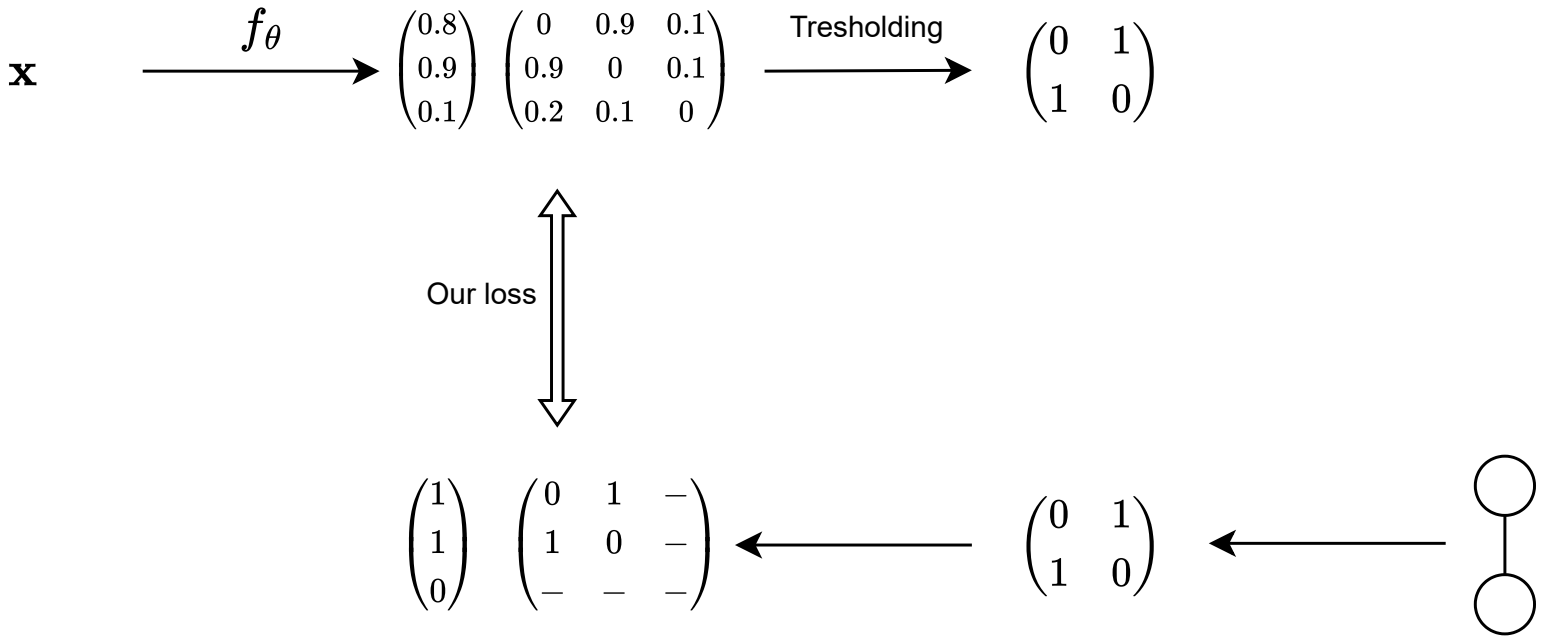

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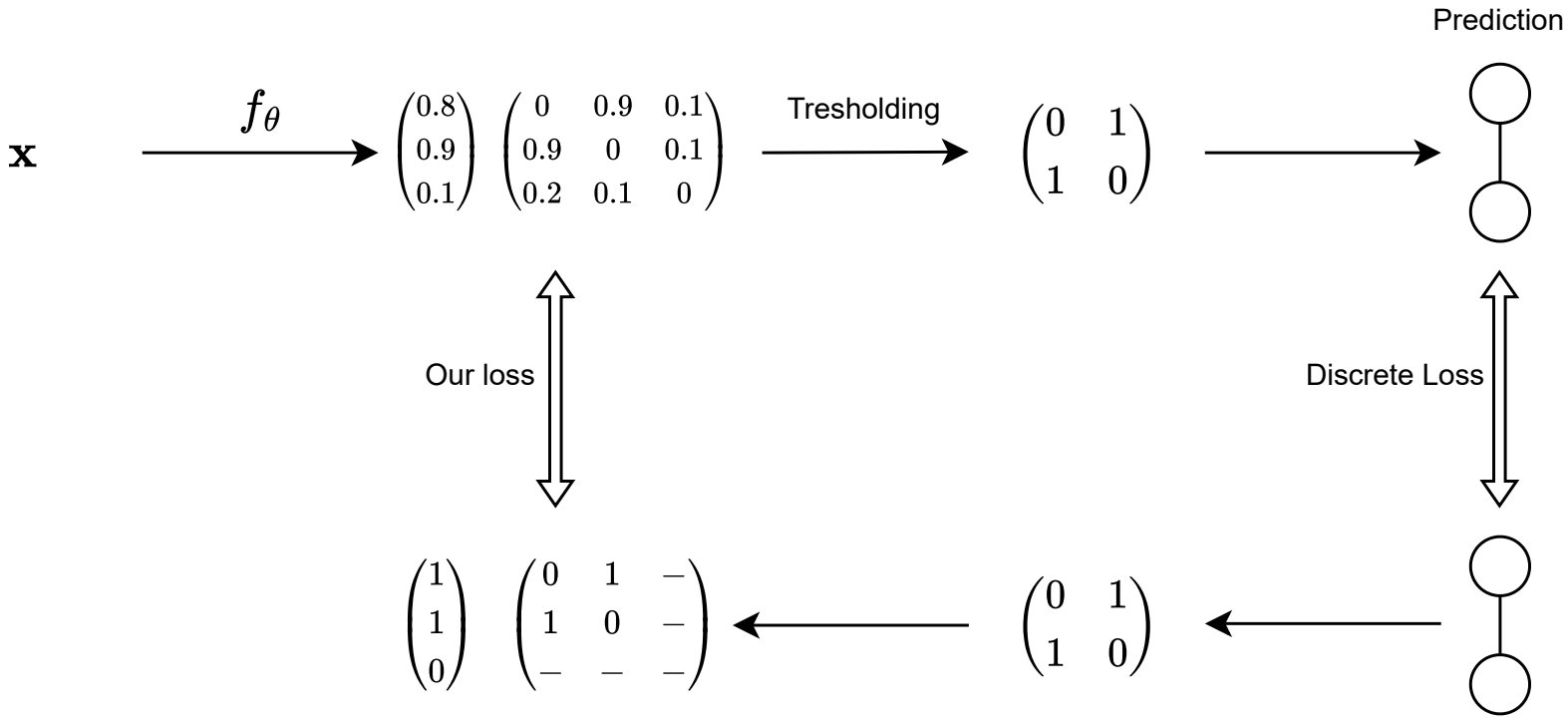

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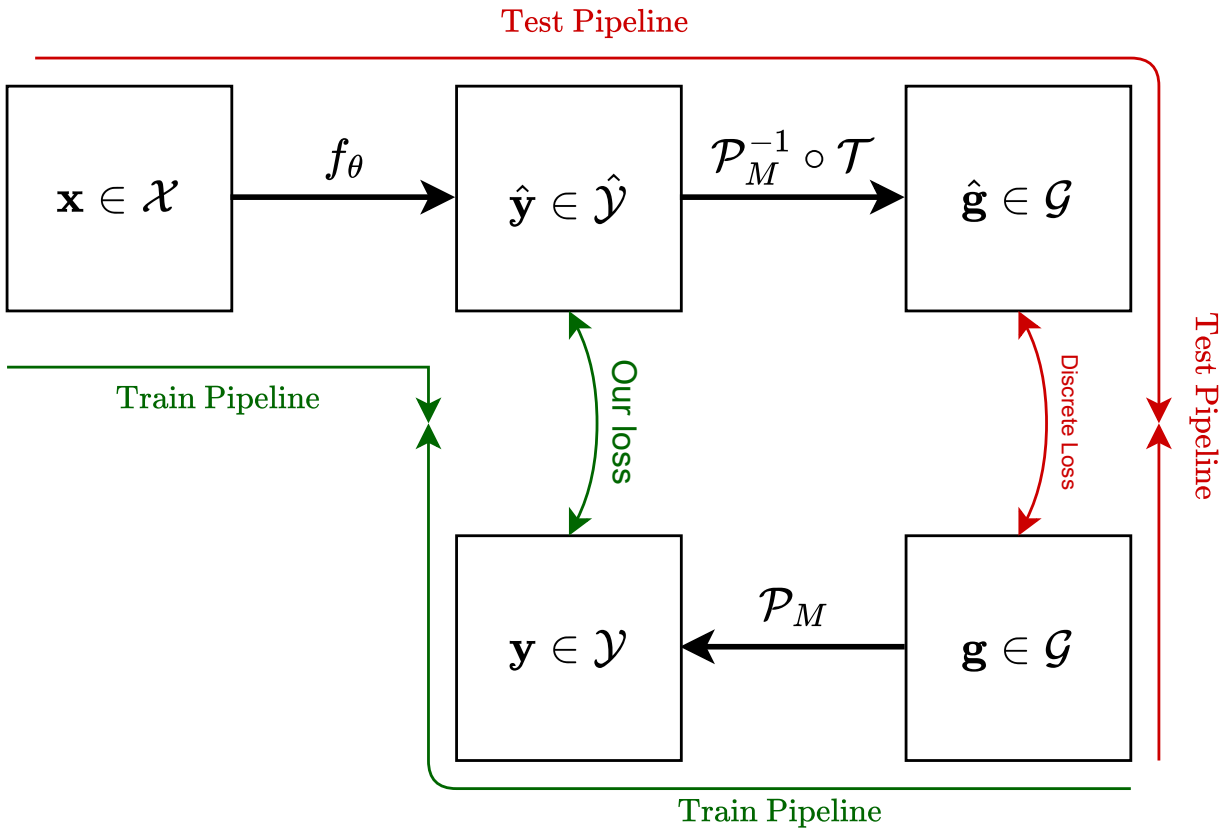

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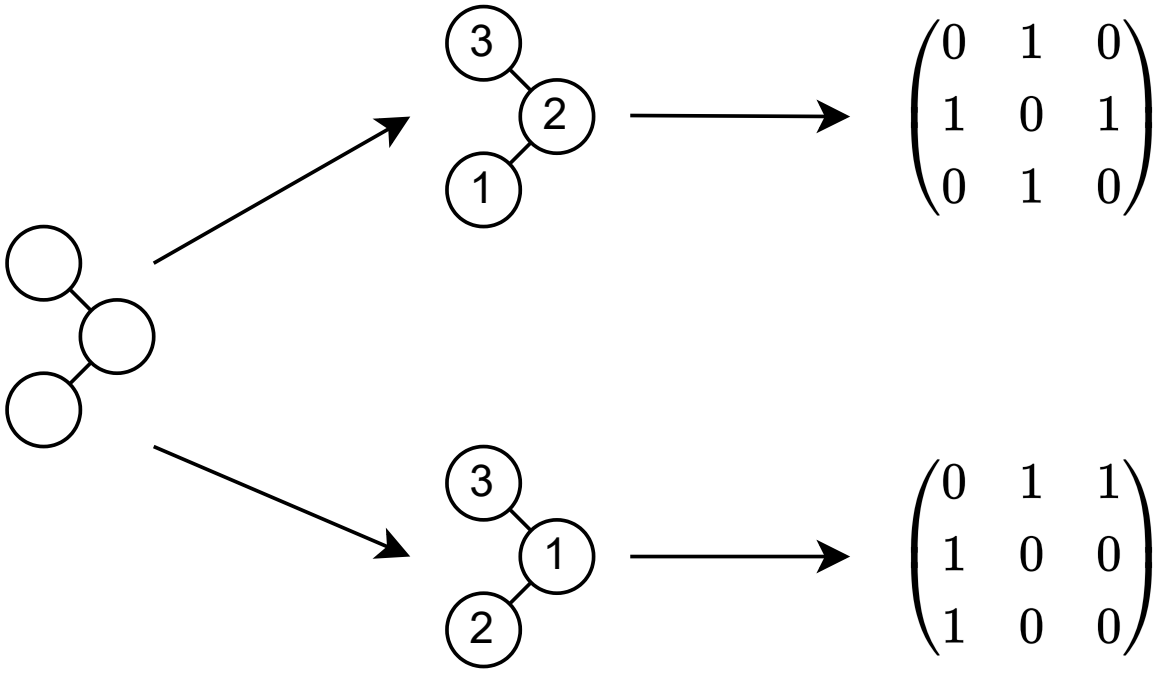
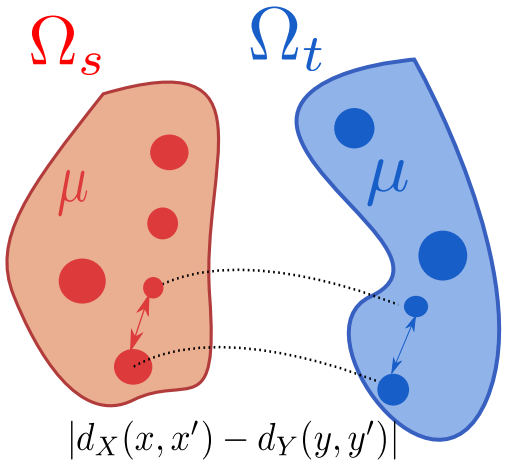
Data fitting loss for graph prediction

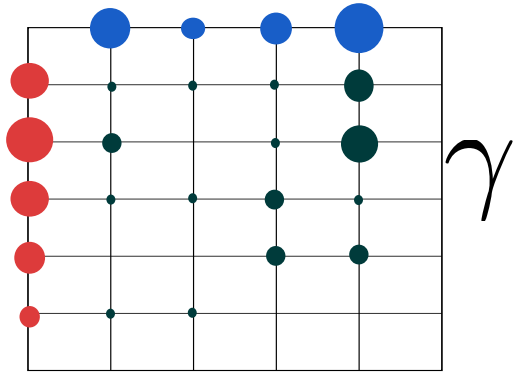


Requirements for loss $\mathcal{L}$

- Works between continuous predicted triplet $\hat{y} = (\hat{\mathbf{h}}, \hat{\mathbf{F}}, \hat{\mathbf{A}})$ and discrete target triplet $y = (\mathbf{h}, \mathbf{F}, \mathbf{A})$ with padding.
- Permutation (graph isomorphism) Invariant.
- Differentiable : for end-to-end training.
- Fused Gromov Wasserstein proposed in [Brogat-Motte et al., 2022].

Gromov-Wasserstein and Fused Gromov-Wasserstein





Inspired from Gabriel Peyré

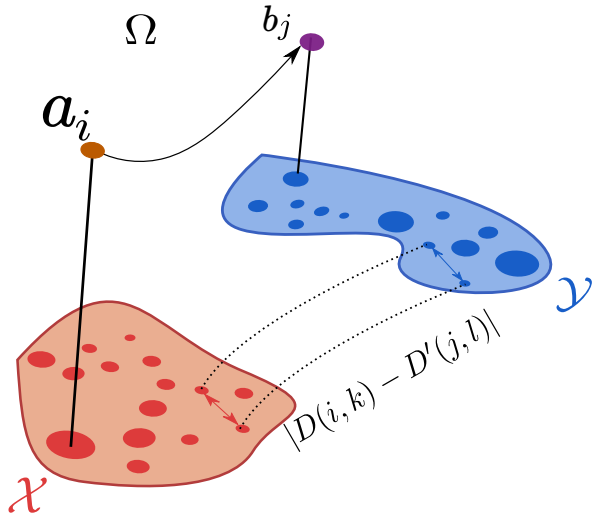
GW for discrete distributions [Memoli, 2011]

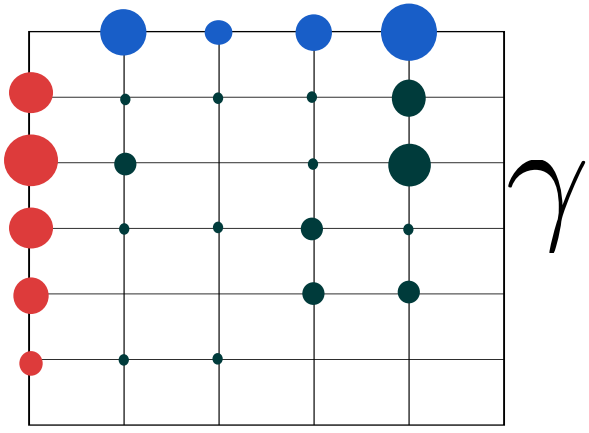
$$\mathcal{GW}_p^p(y_s, y_t)) = \min_{T \in \Pi} \sum_{i,j,k,l} |D_{i,k} - D'_{j,l}|^p T_{i,j}\, T_{k,l}$$

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

- $\mathbf{D}$ and $\mathbf{D}'$ encode relationships between nodes (adjacency, shortest path).
- $\mathbf{a}$ and $\mathbf{b}$ are node weights of same total mass.
- Entropy regularized GW proposed in [Peyré et al., 2016].
- Fused GW interpolates between Wass. and GW [Vayer et al., 2018] with $C_{i,j}$ the cost between labels across graphs.

Gromov-Wasserstein and Fused Gromov-Wasserstein





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

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

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

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

Definition of PM-FGW

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

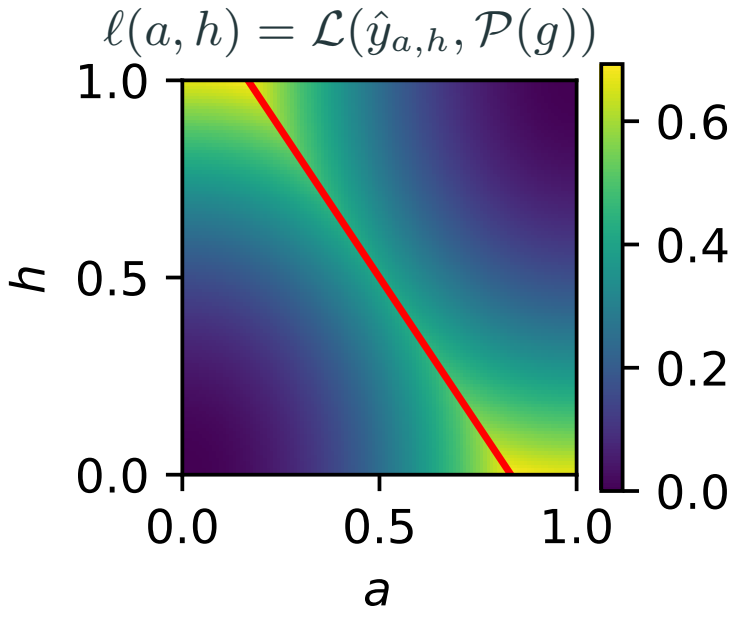
$$\text{with } \mathcal{L}_{\mathbf{P}}(\hat{y}, y) = \frac{\alpha_{\mathsf{h}}}{M} \sum_{i,j} T_{i,j} \ell_h(\hat{h}_i, h_j) \qquad \text{Padding loss}$$

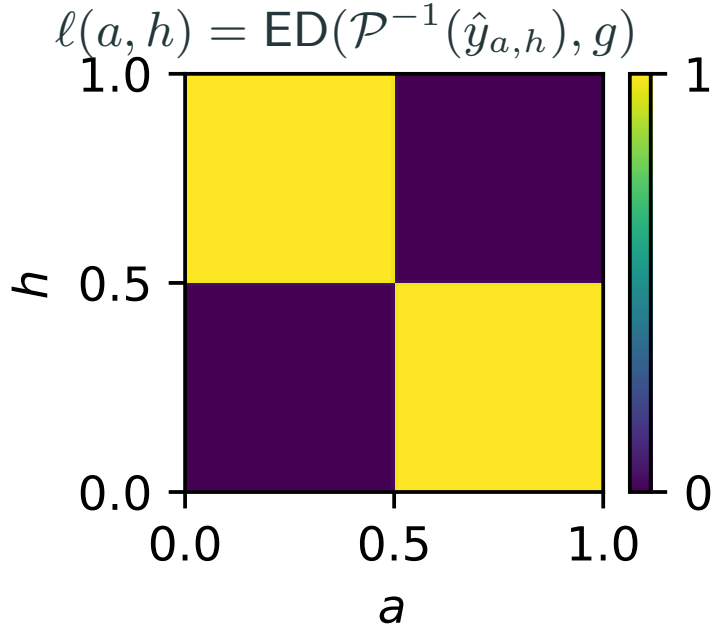
$$+ \frac{\alpha_{\mathsf{f}}}{m} \sum_{i,j} T_{i,j} \ell_f(\hat{\mathbf{f}}_i, \mathbf{f}_j) h_j \qquad \text{Feature loss}$$

$$+ \frac{\alpha_{\mathsf{A}}}{m^2} \sum_{i,j,k,l} T_{i,j} T_{k,l} \ell_A(\hat{A}_{i,k}, A_{j,l}) h_j h_l. \qquad \text{Structure loss}$$

- 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.

Illustration of PM-FGW loss





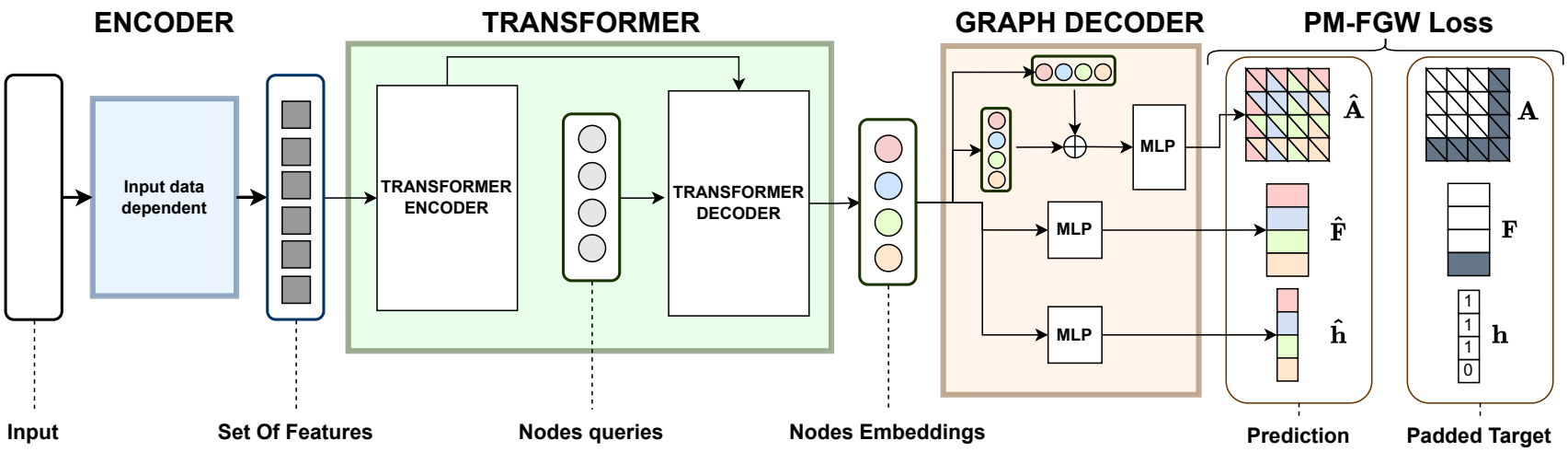
- The target graph is $g = (\mathbf{F}, \mathbf{A})$ with

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

- 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

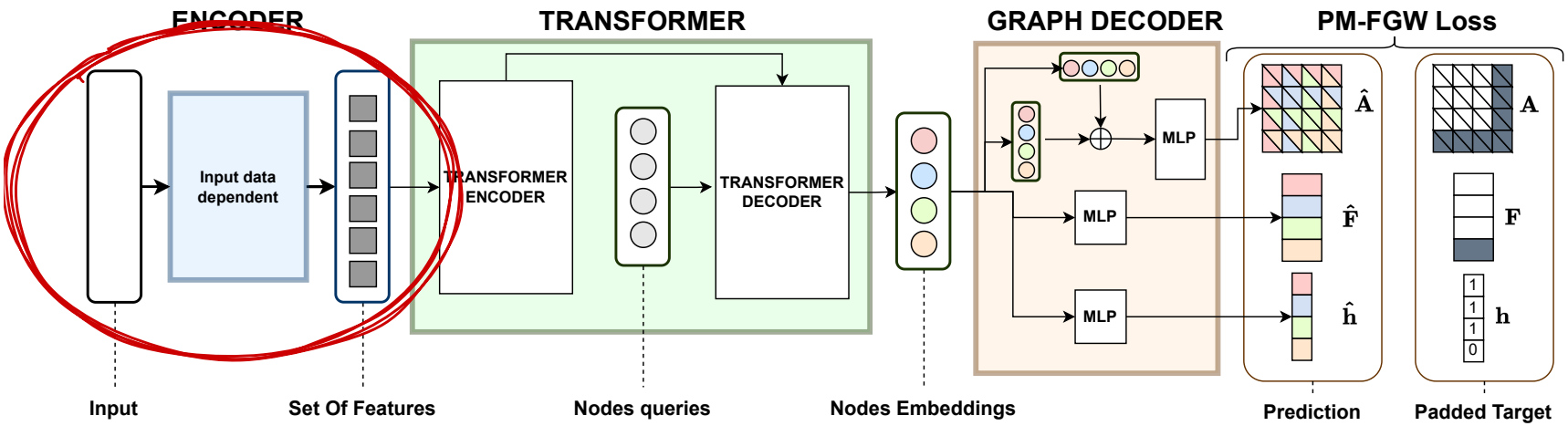
$$\hat{h}_i = \sigma(\mathrm{MLP}_m(\mathbf{z}_i)) \qquad \forall i \in \{1, \ldots, M\}$$

$$\hat{F}_i = \mathrm{MLP}_f(\mathbf{z}_i) \qquad \forall i \in \{1, \ldots, M\}$$

$$\hat{A}_{i,j} = \sigma(\mathrm{MLP}_s(\mathbf{z}_i + \mathbf{z}_j)) \qquad \forall i, j \in \{1, \ldots, M\}^2$$

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

Neural network architecture : the encoder

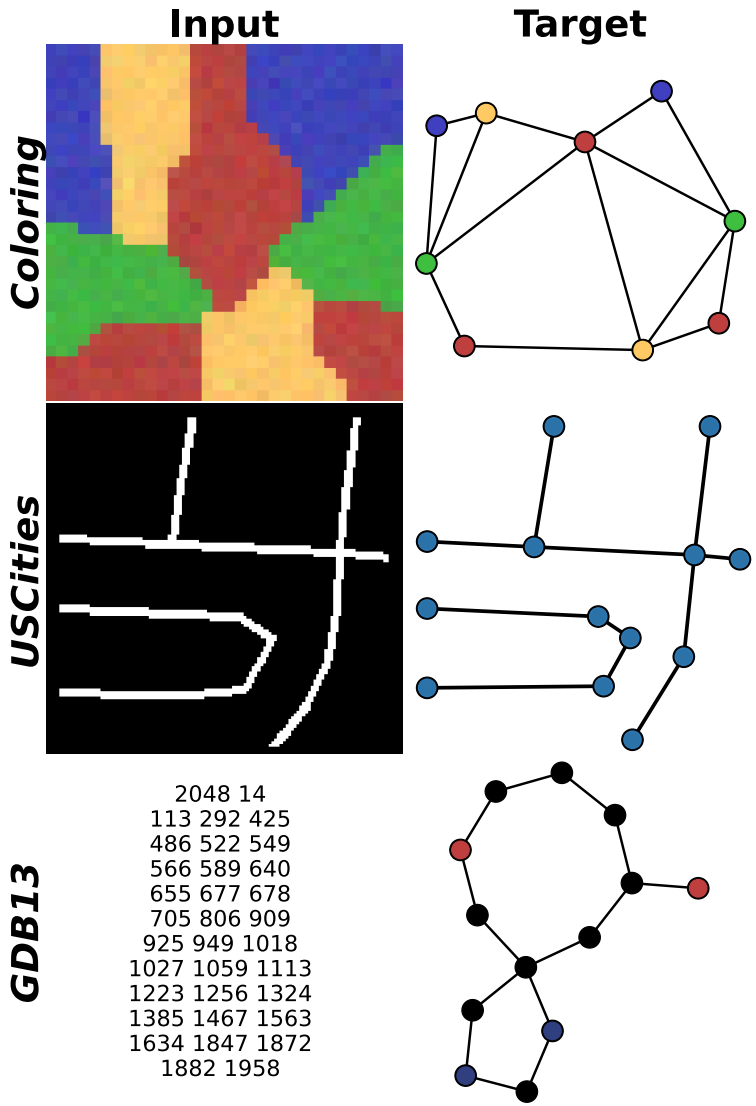


About the encoder

- Architecture adapts to input modality.
- Can leverage pretrained models.
- Must extract a **list of features** to avoid vector bottleneck.
- List of feature can be seen as a distribution [De Bie et al., 2019].
- Examples:
  - Text: token embeddings.
  - Image: CNN features (no global pooling).
  - Graph: GNN features (no global pooling).

Numerical experiments

Graph prediction experiments



Datasets

- Coloring
  - Input: 2D RGB images (100k train)
  - Output: 4-color graph (up to 20 nodes).
- Toulouse & USCities
  - Input: binary images (80k & 130k train)
  - Output: road network (up to 20 nodes).
- QM9 & GDB13
  - Input: Fingerprint (120k & 1300k train)
  - Output: molecule graph (up to 9 & 13 nodes).

Compared methods

- FGWBary (known size) [Brogat-Motte et al., 2022]
- Relationformer [Shit et al., 2022]
- Any2Graph (Ours)

FD : feature diffusion : $\mathbf{F} \mapsto [\mathbf{F}, \mathbf{AF}]$ [Barbe et al., 2020]

Prediction performances

Dataset	Model	Graph Level			Edge Level		Node Level Acc.	
		Edit Dist. ↓	GI Acc. ↑	PMFGW ↓	Prec. ↑	Rec. ↑	Node ↑	Size ↑
Coloring	FGWBary-NN*	6.73	1.00	0.91	75.19	84.99	77.58	n.a.
	FGWBary-ILE*	7.60	0.90	0.93	72.17	83.81	79.15	n.a.
	Relationformer	5.47	18.14	0.32	80.39	86.34	92.68	99.32
	Any2Graph	**0.20**	**85.20**	**0.03**	**99.15**	**99.37**	**99.95**	**99.50**
Toulouse	FGWBary-NN*	8.11	0.00	1.15	84.09	79.68	10.10	n.a.
	FGWBary-ILE*	9.00	0.00	1.21	72.52	56.30	1.62	n.a.
	Relationformer	**0.13**	93.28	**0.02**	99.25	99.24	99.25	98.30
	Any2Graph	**0.13**	**93.62**	**0.02**	**99.34**	**99.26**	**99.39**	**98.81**
USCities	Relationformer	2.09	55.00	0.13	**92.96**	87.98	95.18	**79.80**
	Any2Graph	**1.86**	**58.10**	**0.12**	92.91	**90.85**	**95.70**	78.95
QM9	FGWBary-NN*	5.55	1.00	0.96	87.81	70.78	78.62	n.a.
	FGWBary-ILE*	3.54	7.10	0.59	80.40	75.14	91.47	n.a.
	FGWBary-ILE* + FD	2.84	28.95	0.28	82.96	79.76	92.99	n.a.
	Relationformer	9.15	0.05	0.48	21.42	4.77	99.28	91.80
	Relationformer + FD	3.80	9.95	0.22	86.07	73.31	99.34	**96.0**
	Any2Graph	3.44	7.50	0.21	86.21	77.27	99.26	93.65
	Any2Graph + FD	**2.13**	**29.85**	**0.14**	**90.19**	**88.08**	**99.77**	95.45
GDB13	Relationformer	11.40	0.00	0.43	81.96	31.49	97.77	97.45
	Relationformer + FD	8.83	0.01	0.29	84.14	55.89	97.57	**98.65**
	Any2Graph	7.45	0.05	0.22	87.20	60.41	99.41	96.15
	Any2Graph + FD	**3.63**	**16.25**	**0.11**	**90.83**	**84.86**	**99.80**	98.15

- Any2Graph is SOTA for graph prediction on all datasets.
- Feature diffusion helps on molecules [Brogat-Motte et al., 2022].

Sensitivity analysis

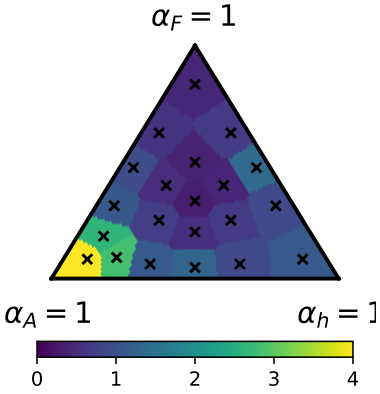


Figure 1: Edit dist.

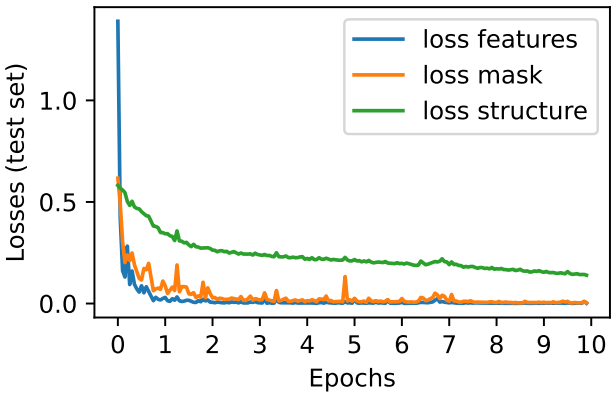


Figure 2: $\alpha = [1, 1, 1]$.

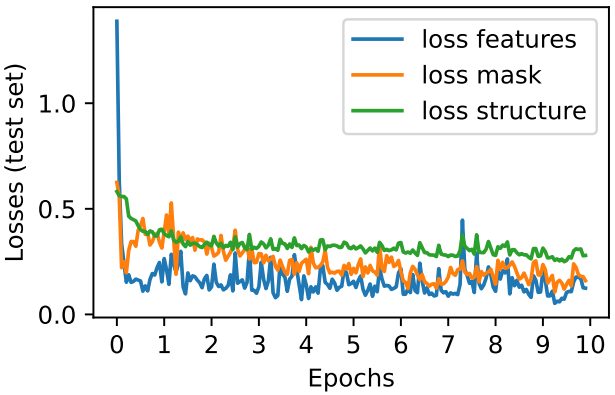


Figure 3: $\alpha = [10, 1, 1]$.

Results on Coloring dataset

- Robustness to α (Fig 1.).
- Mask and features learned first (Fig 2.).
- Failure for large α_A (Fig 1. and 3.).
- For increasing M edit distance is stable.
- Effective active nodes number do not increase with M (Fig 4.)

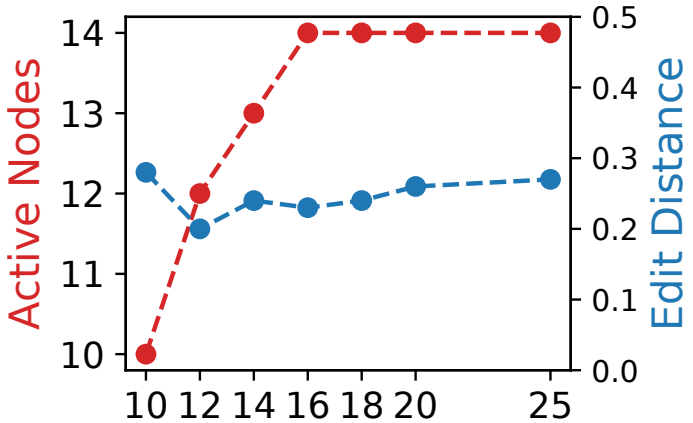


Figure 4: Effect of M.

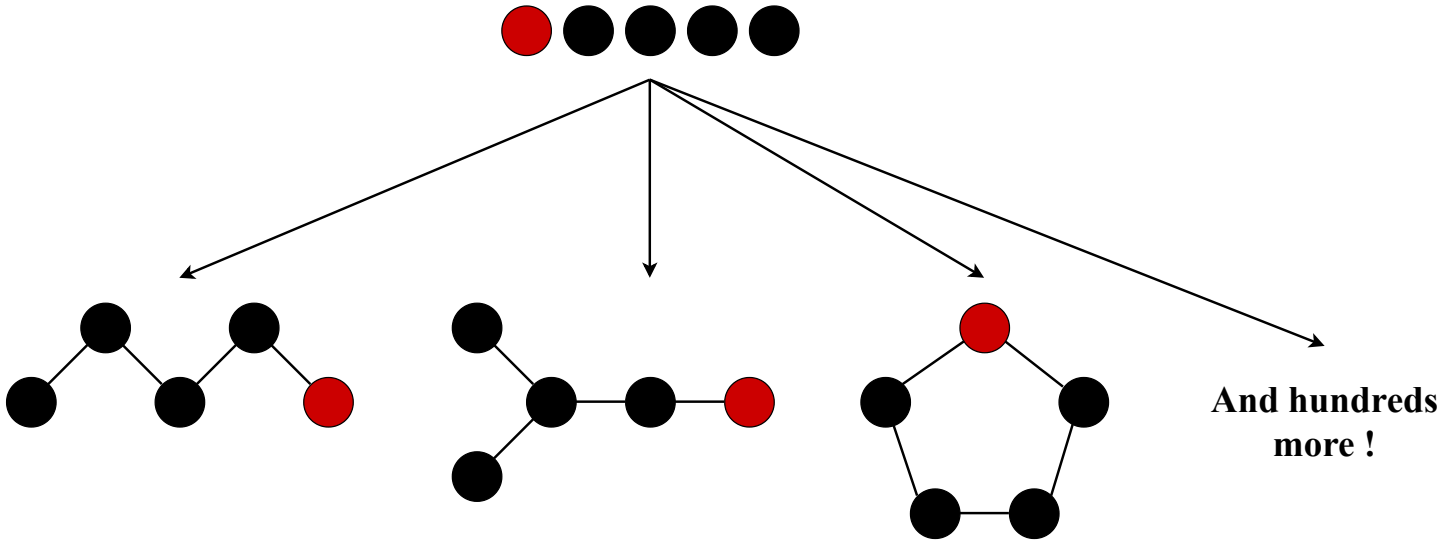
Computational Performances

Method	Training	Inference
FGWBary-ILE (K=25)	n.a.	1
FGWBary-NN (K=10)	10	10
Relationformer	9k	20k
PM-FGW (ours)	3k	20k

Table 1: Computational Performances (In graph per second)

- FGWBary-ILE uses thresholding of weights yet still slow.
- FGWBary-NN with learned dictionary is a little faster.
- Relationformer and Any2Graph are fastest at inference.
- Any2Graph is slightly slower that Relationforme during training.

Why diffusion of feature on molecules?

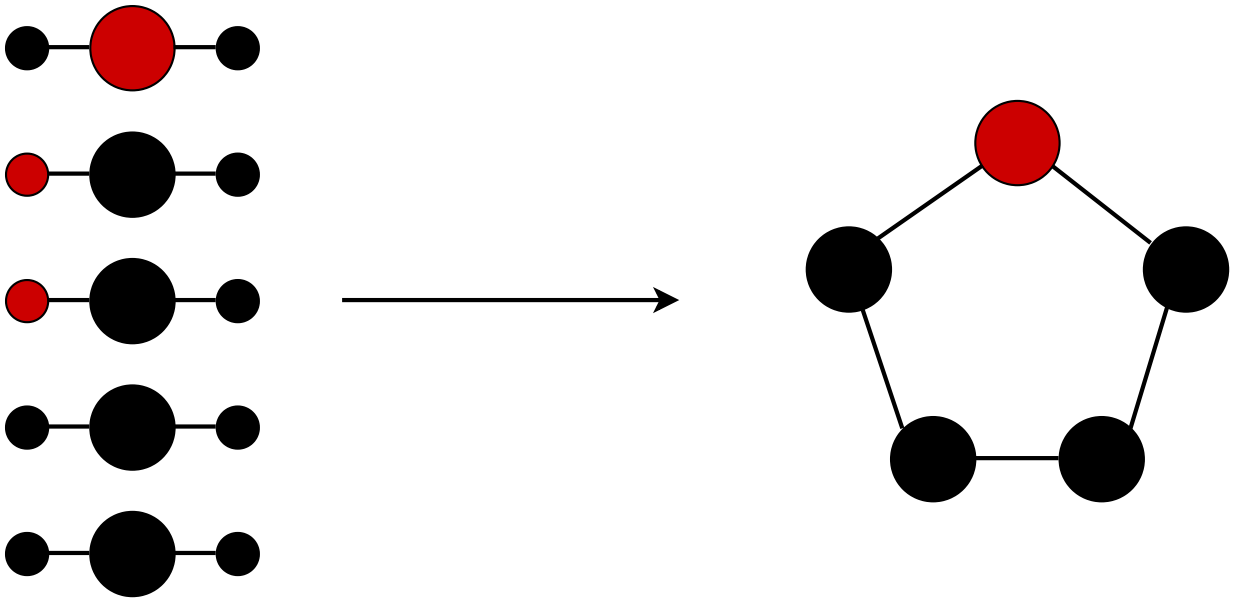


Diffusion of features [Barbe et al., 2020]

$$\mathbf{F} \mapsto [\mathbf{F}, \mathbf{AF}]$$

- On some graphs, nodes features are not enough to predict the structure.
- Diffusion of features encode labels + labels of neighbors.
- Helps the model for structure identification with more information in the linear term for molecule graphs.

Why diffusion of feature on molecules?



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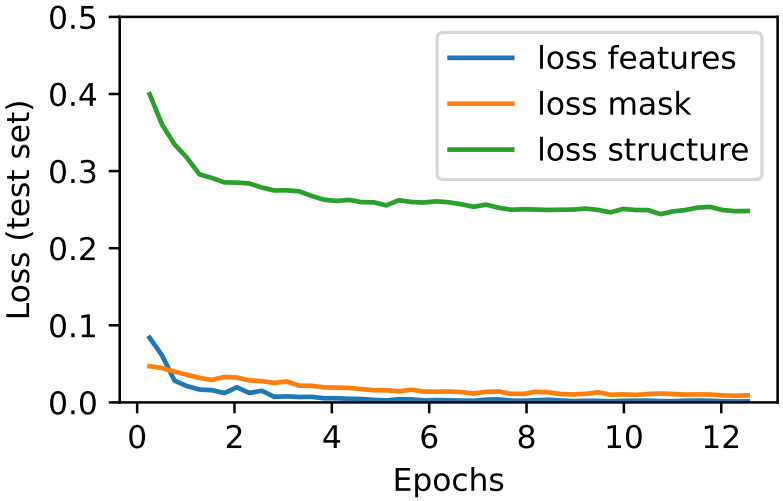


Figure 5: Without Feature Diffusion.

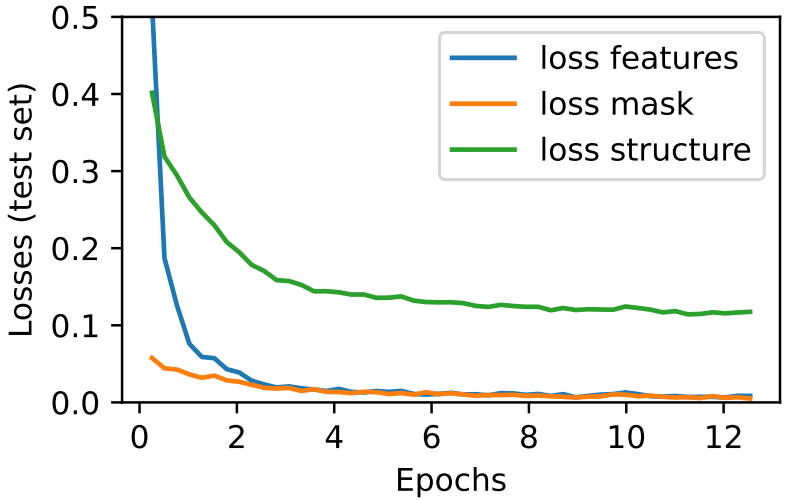


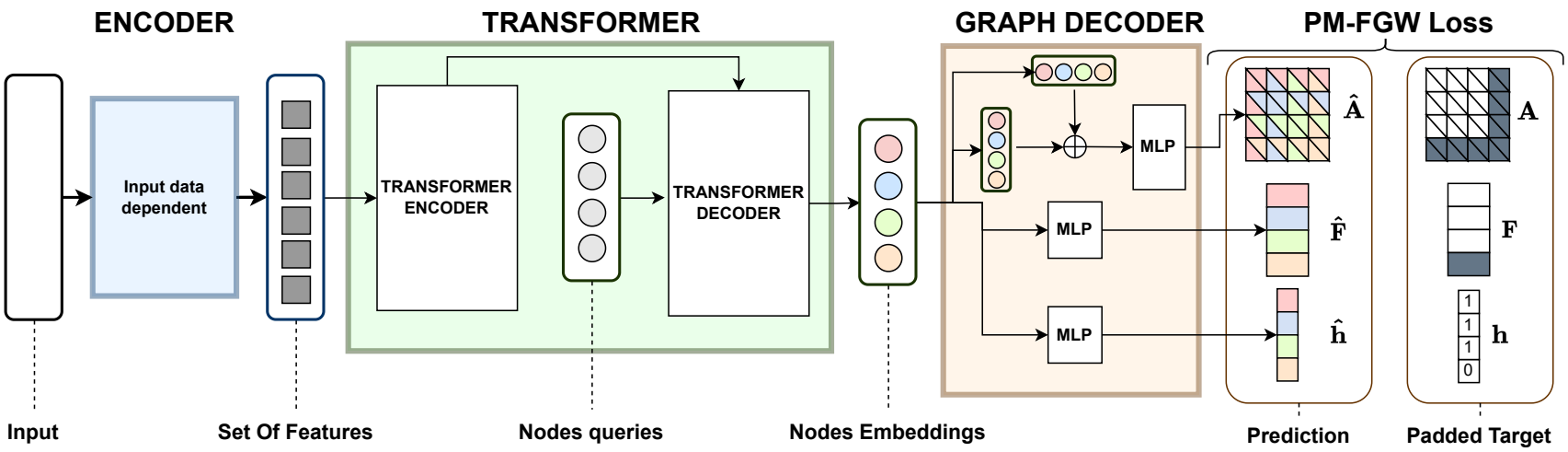
Figure 6: With Feature Diffusion.

Diffusion of features [Barbe et al., 2020]

$$\mathbf{F} \mapsto [\mathbf{F}, \mathbf{AF}]$$

- On some graphs, nodes features are not enough to predict the structure.
- Diffusion of features encode labels + labels of neighbors.
- Helps the model for structure identification with more information in the linear term for molecule graphs.

Conclusion



Any2Graph [Krzakala et al., 2024]

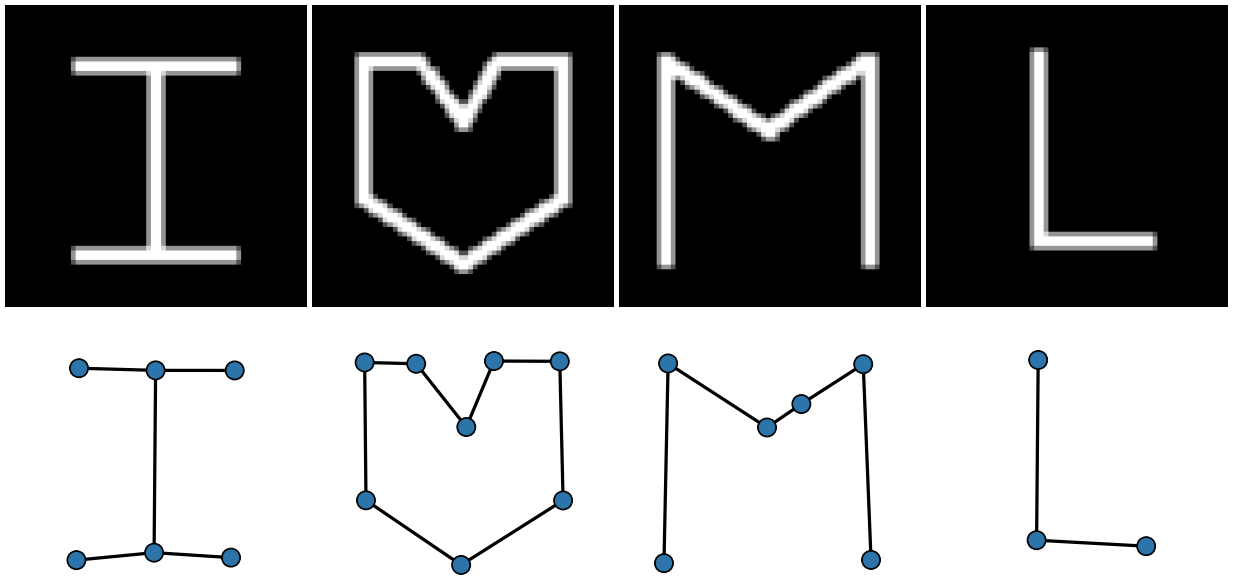
- Generic framework for supervised graph prediction from any input.
- End-to-end trainable with a neural network with OT loss.
- Good performance on variety of (input/output) datasets.

Limits and future works

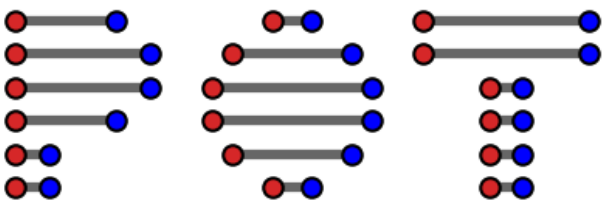
- Only tested on relatively small graphs ($M \leq 20$).
- Use higher order relationship matrices (Power of Laplacian L^k).
- Investigate graph auto-encoders.

Thank you for your $\texttt{softmax}(QK^T)V$!

Any2Graph model trained on Toulouse :



POT Python Optimal Transport library



- `https://pot.readthedocs.io/en/stable/`
- Solvers for OT problems.
- Backends in Numpy/Pytorch.

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Why not [X] OT loss?

Fused Gromov-Wasserstein [Vayer et al., 2020]

- $\mathbf{h}$ and $\hat{\mathbf{h}}$ can be normalized to sum to 1 and used as marginal weights.
- But : (Sub)-gradients on the masses are not very numerically stable.
- For multi-label learning use unbalanced OT [Frogner et al., 2015].

Unbalanced FGW [Thual et al., 2022]

- Works out of the bow with $\mathbf{h}$ and $\hat{\mathbf{h}}$ as marginal weights.
- But: many parameters to tune (did not manage to make it work).

Partial (F)GW [Chapel et al., 2020]

- Can force to move only the actual number of nodes.
- But: No weights on not active nodes so node classifier cannot be learned.

Solving for PM-FGW

Conditional Gradient solver

$$\min_{\mathbf{T} \in \pi_M} \langle \mathbf{T}, \mathbf{U} \rangle + \langle \mathbf{T}, \mathbf{L} \otimes \mathbf{T} \rangle$$

with $\mathbf{U}_{i,k} = \ell_h(\hat{h}_i, h_k) + \ell_F(\hat{f}_i, f_k) h_k$ and $(\mathbf{L} \otimes \mathbf{T})_{i,k} = \sum_{j,l} T_{j,l} \ell_A(\hat{A}_{i,j}, A_{k,l}) h_k h_l$

- Solve iteratively linearized version of the loss with $\mathbf{C}^{(k)} = \mathbf{U} + \mathbf{L} \otimes \mathbf{T}^{(k)}$.
- Each step requires :
  - Solving a standard OT problem $O(M^3 \log M)$.
  - Selecting a linesearch step.

Computational complexity

- $O(M^3)$ factorization for PM-FGW (similar to [Peyré et al., 2016]).
- Closed form for the linesearch at each iteration.
- Typical convergence is 5-10 iteration in experiments.