Graph Neural Networks and Optimal Transport for Distance Learning between Graphs

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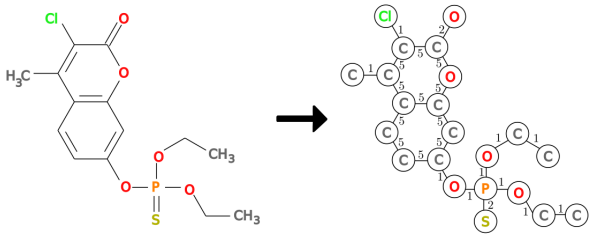
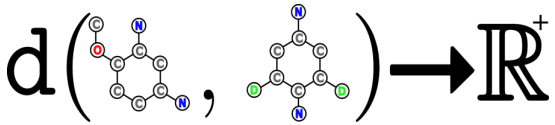
Graph representation



Challenge: graphs are non-euclidean objects and scalar products are not defined for graphs.
How to define the distance between two graphs?

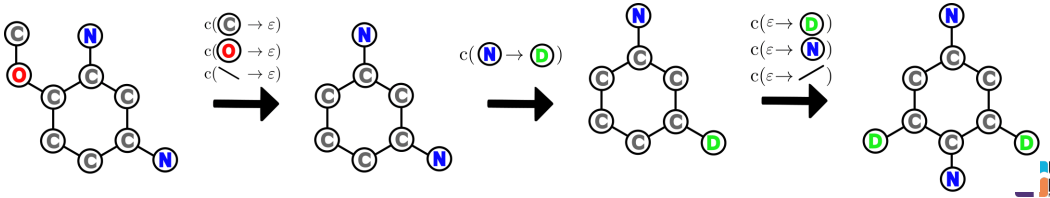


Graph Edit Distance (GED)

$$GED(G_1, G_2) = \min_{e_1,\ldots,e_k \in P(G_1,G_2)} \sum_{i=1}^{k} c(e_i)$$

with (e_i) edit operations of the path from G_1 to G_2.

Set of edit operations
- **node insertion**
- **node deletion**
- **node substitution**
- **edge insertion**
- **edge deletion**
- **edge substitution**



Traditional approaches

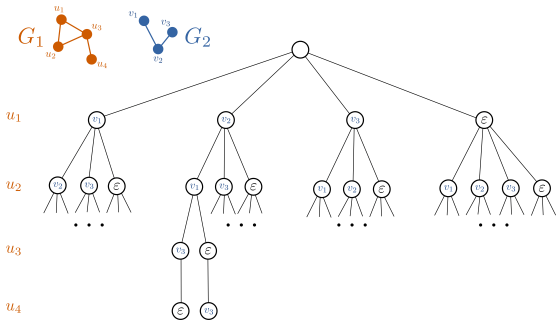
Exact computation :

- $\mathbf{A}^*$ algorithm with heuristic
- Depth-first search algorithm
- QAP solve with a constrained ILP solver (F1, F2)

NP-Hard problem

Approximation methods:
node-based methods

- LSAP relaxation of QAP
- Bipartite matching (BPGED)
- Hausdorff matching



Can we learn it?

Why?

- To by-pass the complexity
- To have a better approximation

How?

- Siamese architecture for graph pairs
- Through Graph Neural Network(GNN) for nodes embedding
- Optimal transport/LSAP to match sets of nodes embedding and infer distance cost

Already existing Deep Learning methods:

- SimGNN/GotSim/Greed...

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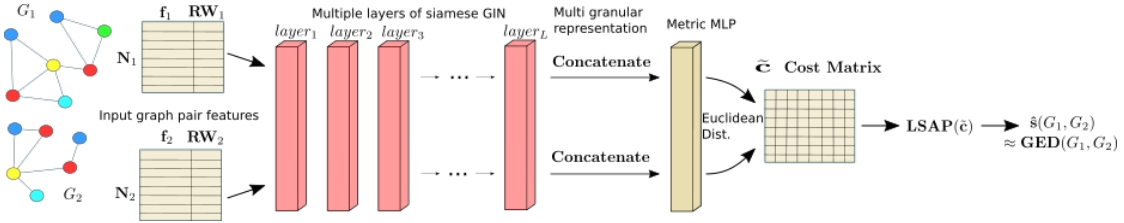
Our architecture Presentation



Nodes embedding with GNN

We use Graph Isomorphism Network (GIN) to learn an embedding of the nodes of the graph by aggregating each node's neighborhood at each layer:

$$\mathbf{h}_v^{(l)} = MLP^{(l)}\left(\left(1+\epsilon^{(l)}\right).\mathbf{h}_v^{(l-1)} + \sum_{u\in\mathcal{N}(v)} \mathbf{h}_u^{(l-1)}\right) \tag{1}$$

Where l is the l-th layer of GIN, $\mathcal{N}(v)$ the one-hop neighborhood of node v, $\epsilon^{(l)}$ a learnable parameter and MLP a multi-layer perceptron with two layers.
We then obtain, for L layers of GIN, the final nodes embedding :

$$\mathbf{H}_v = MLP^{(metric)}\left(\mathbf{h}_v^{(1)}|\mathbf{h}_v^{(2)}|...|\mathbf{h}_v^{(L-1)}|\mathbf{h}_v^{(L)}\right) \tag{2}$$

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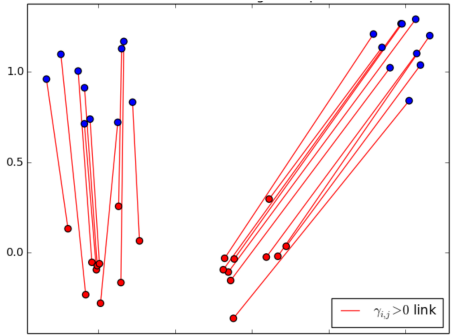
Discrete Optimal Transport

We will formulate this problem as an instance of Monge's Problem equivalent to the Linear Sum Assignment Problem (LSAP).
By introducing permutation matrix $\mathbf{X} = (x_{i,j})$ we can define LSAP as follow :

$$\textbf{LSAP}(\tilde{\mathbf{C}}) = \min_{\mathbf{X}} \sum_{i=1}^{N} \sum_{j=1}^{N} \tilde{c}_{i,j} x_{i,j}$$

$$\tilde{\mathbf{C}} = \left(\begin{array}{ccc|ccc} \mathbf{c}_{1,1} & \cdots & \mathbf{c}_{1,N_2} & \mathbf{d}_1 & \cdots & \infty \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{c}_{N_1,1} & \cdots & \mathbf{c}_{N_1,N_2} & \infty & \cdots & \mathbf{d}_{N_1} \\ \hline \mathbf{a}_1 & \cdots & \infty & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ \infty & \cdots & \mathbf{a}_{N_2} & 0 & \cdots & 0 \end{array}\right)$$



Substitution costs

Let be a graph pair (G, G') of size (N_1, N_2). We obtain as defined in (2), two sets of embedded nodes $\mathbf{H}, \mathbf{H}'$.
We can now compute a cost matrix by using the Euclidean distance between nodes representation.

$$\mathbf{C}_{i,j} = \left\| \mathbf{H}_i - \mathbf{H}'_j \right\|_2 \qquad \mathbf{C} = \begin{pmatrix} \mathbf{c}_{1,1} & \cdots & \mathbf{c}_{1,N_2} \\ \vdots & \ddots & \vdots \\ \mathbf{c}_{N_1,1} & \cdots & \mathbf{c}_{N_1,N_2} \end{pmatrix}$$

Costs of $\mathbf{C}$ correspond to GED's substitutions cost of nodes of G with those of G'.

Insertion and deletion costs

We can also use the Euclidean distance to define insertion and deletion costs. In this case, we use the norm of the embedding vector, it represents the distance to 0.

$$\text{for deletion : } \mathbf{D}_{i,j} = \begin{cases} \|\mathbf{H}_i\|_2 \text{ if } i = j, \text{ with } i, j \in [\![1, ..., N_1]\!] \\ \infty \text{ otherwise} \end{cases}$$

$$\text{and for insertion : } \mathbf{A}_{i,j} = \begin{cases} \|\mathbf{H}'_i\|_2 \text{ if } i = j, \text{ with } i, j \in [\![1, ..., N_2]\!] \\ \infty \text{ otherwise} \end{cases}$$

Final costs matrix

We then obtain a costs matrix $\tilde{\mathbf{C}}$ similar to those used in Bipartite matching.

$$\tilde{\mathbf{C}} = \begin{pmatrix} \mathbf{C} & \mathbf{D} \\ \mathbf{A} & 0 \end{pmatrix} \tag{3}$$

$$\tilde{\mathbf{C}} = \left(\begin{array}{ccc|ccc} \mathbf{c}_{1,1} & \cdots & \mathbf{c}_{1,N_2} & \mathbf{d}_1 & \cdots & \infty \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{c}_{N_1,1} & \cdots & \mathbf{c}_{N_1,N_2} & \infty & \cdots & \mathbf{d}_{N_1} \\ \hline \mathbf{a}_1 & \cdots & \infty & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ \infty & \cdots & \mathbf{a}_{N_2} & 0 & \cdots & 0 \end{array}\right)$$

Output and Loss

we can then obtain a GED approximation value $\hat{\mathbf{s}}$ through discrete Optimal Transport by using **LSAP** on the $\tilde{\mathbf{C}}$ matrix :

$$\hat{\mathbf{s}}(G, G') = \mathbf{LSAP}(\tilde{\mathbf{C}}) \tag{4}$$

The Loss function used to train the architecture is a mean squared error :

$$\mathcal{MSE}_{Loss} = \frac{1}{|\mathcal{T}|} \sum_{(G,G') \in \mathcal{T}} \left\| \hat{\mathbf{s}}(G, G') - GED(G, G') \right\|_2^2 \tag{5}$$

With $\mathcal{T}$ the set of training pairs of graphs.

Metric properties conservation

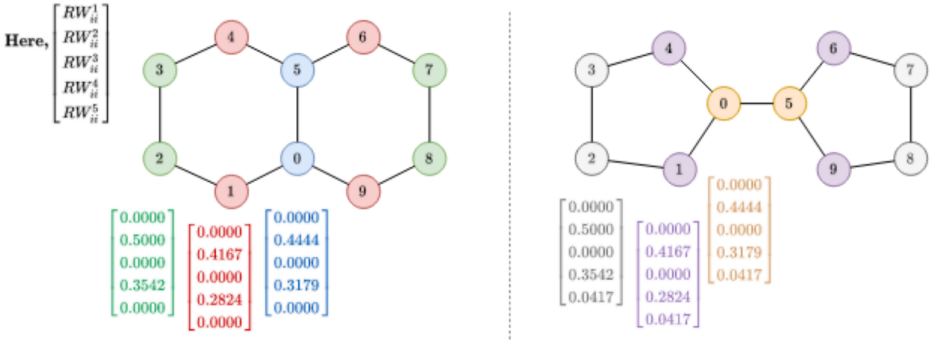
We want $\hat{\mathbf{s}}$ to respect the metric properties of GED. $\hat{\mathbf{s}} : \mathcal{G} \times \mathcal{G} \to \mathbb{R}^+$ satisfying the following axioms for all graphs $x, y, z \in \mathcal{G}$:

1)The distance from a graph to itself is zero: $\hat{\mathbf{s}}(x, x) = 0$. Holds.
2)Positivity: If $x \neq y$, then $\hat{\mathbf{s}}(x, y) > 0$. Not respected.
3)Symmetry: $\hat{\mathbf{s}}(x, y) = \hat{\mathbf{s}}(y, x)$. Holds.
4)The triangle inequality: $\hat{\mathbf{s}}(x, z) \leq \hat{\mathbf{s}}(x, y) + \hat{\mathbf{s}}(y, z)$. Holds.

All those properties are respected during learning except for the Positivity due to the Graph isomorphism problem which is NP-Hard. It came from the expressivity bound of GIN (first-order Weisfeiler-Lehman test).
Therefore $\hat{\mathbf{s}}(G, G')$ is a pseudo-metric. Indeed it exists $G \neq G'$ for which $\hat{\mathbf{s}}(G, G') = 0$.

Positional encoding

Discriminative power of Random Walk for graphs not differentiated by 1-WL.



$$\mathbf{RW}_i^{(k)} = [(\mathbf{D}^{-1}\mathbf{A})_{(i,i)}, (\mathbf{D}^{-1}\mathbf{A})^2_{(i,i)}, ..., (\mathbf{D}^{-1}\mathbf{A})^{k-1}_{(i,i)}, (\mathbf{D}^{-1}\mathbf{A})^k_{(i,i)}] \quad (6)$$

Where $\mathbf{D}^{-1}\mathbf{A}$ is the random walk Laplacian.

Experiments and results

- AIDS: 490 000 graph pairs, max 10 nodes, 29 features.
- LINUX: 1 Million graph pairs, max 10 nodes, no features.
- IMDB: 2.25 Million graph pairs, max 100 nodes, no features.

Results are expressed with Root Mean Squared Error (RMSE) metric.

Methods	AIDS'	LINUX	IMDB
Branch	3.322	2.474	**6.875**
MIP-F2	2.929	1.245	82.124
GREED	0.796	0.415	49.81
H^2MN	0.994	0.734	86.077
GENN-A*	0.907	**0.267**	NA
GotSIM	0.996	0.574	37.831
SimGNN	1.037	0.666	66.250
Ours	0.799	0.474	31.354
Ours-RW	**0.698**	0.328	27.147

Conclusion?

- The supervised learning of the GED works
- Representations of the graphs and nodes are very important
- Two main blocks in the architecture, GNN for embedding node distributions, Euclidean distance and discrete Optimal transport for metric matching.
- LSAP brings explainability through the matching performed.
- Good Problem definition? Do not scale to larger graphs.
- Unsupervised learning? Other metric labels?

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Thank you for your attention!