The quest for the GRAph Level autoEncoder.

NeurIPS 2025

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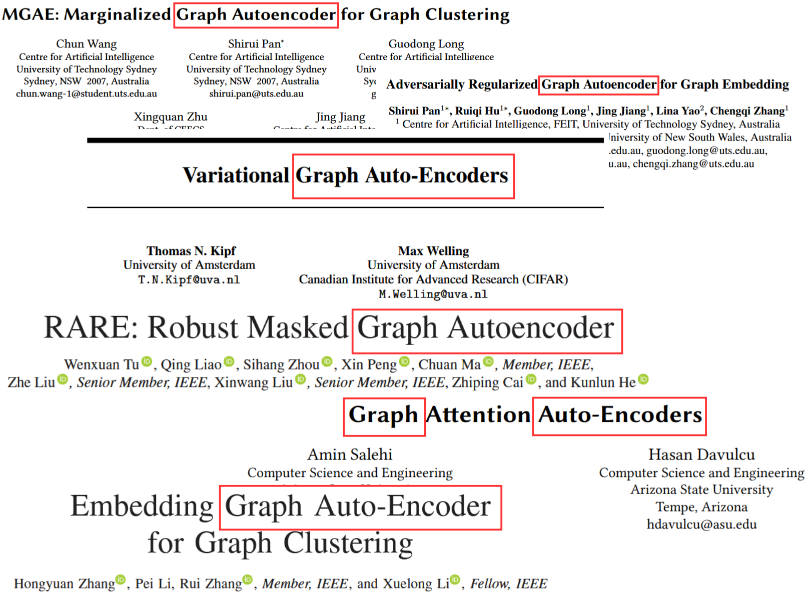
MGAE: Marginalized Graph Autoencoder for Graph Clustering
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Adversarially Regularized Graph Autoencoder for Graph Embedding
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Variational Graph Auto-Encoders
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RARE: Robust Masked Graph Autoencoder
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Zhe Liu, Senior Member, IEEE, Xinwang Liu, Senior Member, IEEE, Zhiping Cai, and Kunlun He
Graph Attention Auto-Encoders
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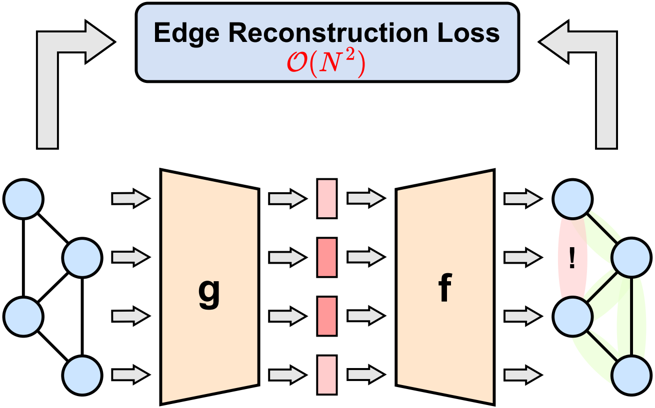
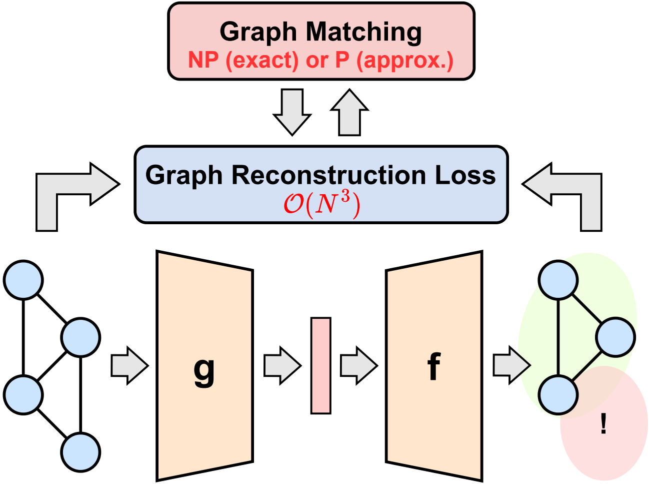
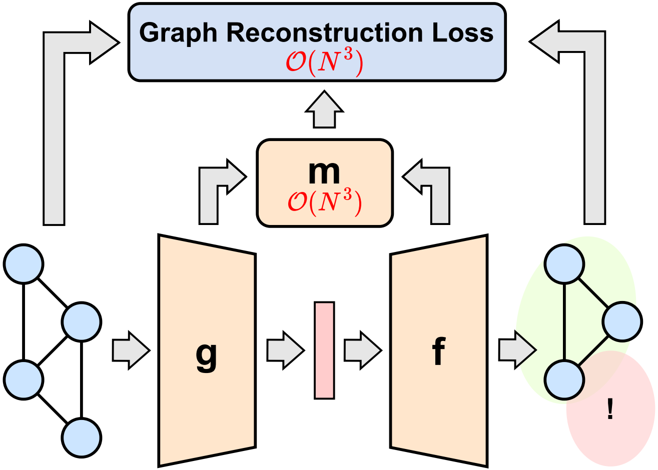
Embedding Graph Auto-Encoder
for Graph Clustering
Hongyuan Zhang, Pei Li, Rui Zhang, Member, IEEE, and Xuelong Li, Fellow, IEEE


Edge Reconstruction Loss
$\mathcal{O}(N^2)$
g
f
!

Graph-Level Autoencoders (Naive)



Graph-Level Autoencoders (GRALE)



Is it reasonable?

$\rightarrow$ Matching **two arbitrary graphs** is **NP-hard**

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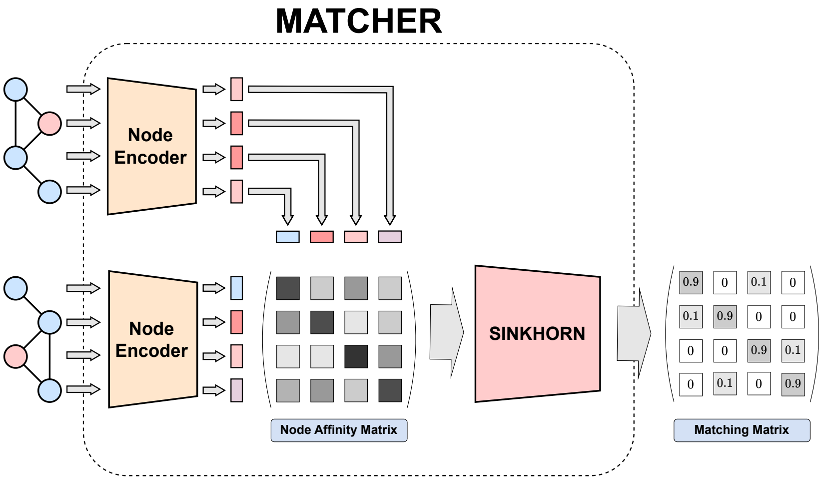
$\rightarrow$ For a given **dataset** a solver might exist!

$\rightarrow$ Let's **learn** it!

Challenges: trainable matching module



Challenges: loss choice

For $P \in \sigma_n$ permutation matrix,

$$||A - PA'P^T||_F^2 = ||AP - PA'||_F^2 = \sum_{i,j,k,l} P_{i,k} P_{j,l} d(A_{i,j}, A'_{k,l})$$

For $T \in \pi_n$ matching matrix:

$$||A - TA'T^T||_F^2 \neq ||AT - TA'||_F^2 \neq \underbrace{\sum_{i,j,k,l} T_{i,k} T_{j,l} d(A_{i,j}, A'_{k,l})}_{\mathcal{L}_{GW}(A,A',T)}$$

We need to choose a relaxation of the graph matching loss.

Theorem

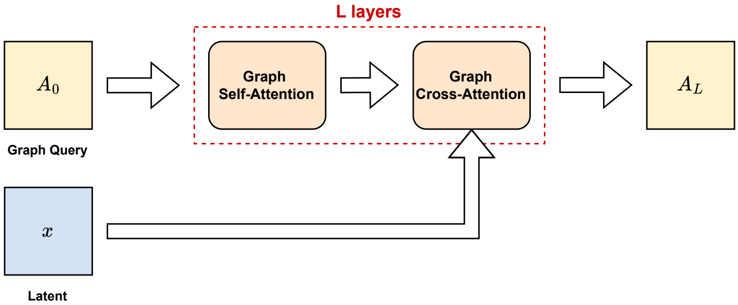
$\mathcal{L}_{GW}$ is the only relaxation such that

$$\mathcal{L}_{GW}(A, A', T) = 0 \iff \exists P \in \sigma_n, A = PA'P^T$$

Challenges: expressive decoder

- Many works on graph encoding models $x = f_\theta(A)$
- Few works on graph decoding models $A = f_\theta(x)$

High level idea: augment **Evoformer** (AlphaFold) with **cross-attention**.

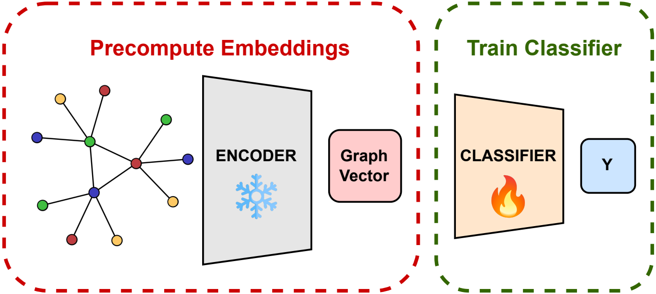


Applications:

Once GRALE is trained...

Any graph-level task can be performed in the **latent space** !

From **graph classification** ...

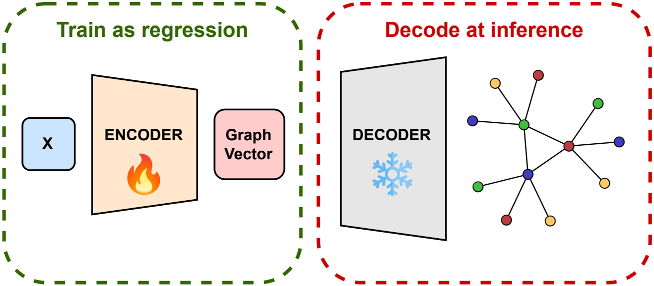


Applications:

Once GRALE is trained...

Any graph-level task can be performed in the **latent space** !

To **graph generation** ...



Applications:

Once GRALE is trained...

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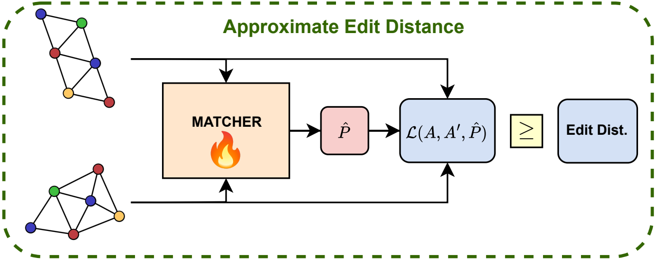
To **graph matching** ...



Applications:

Once GRALE is trained...

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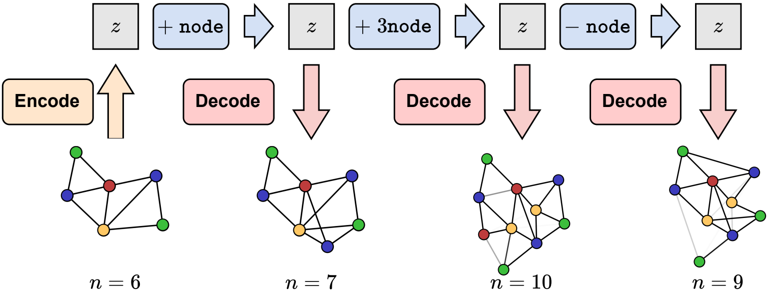
To **graph edition** ...



Applications:

Once GRALE is trained...

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To **graph interpolation** ...