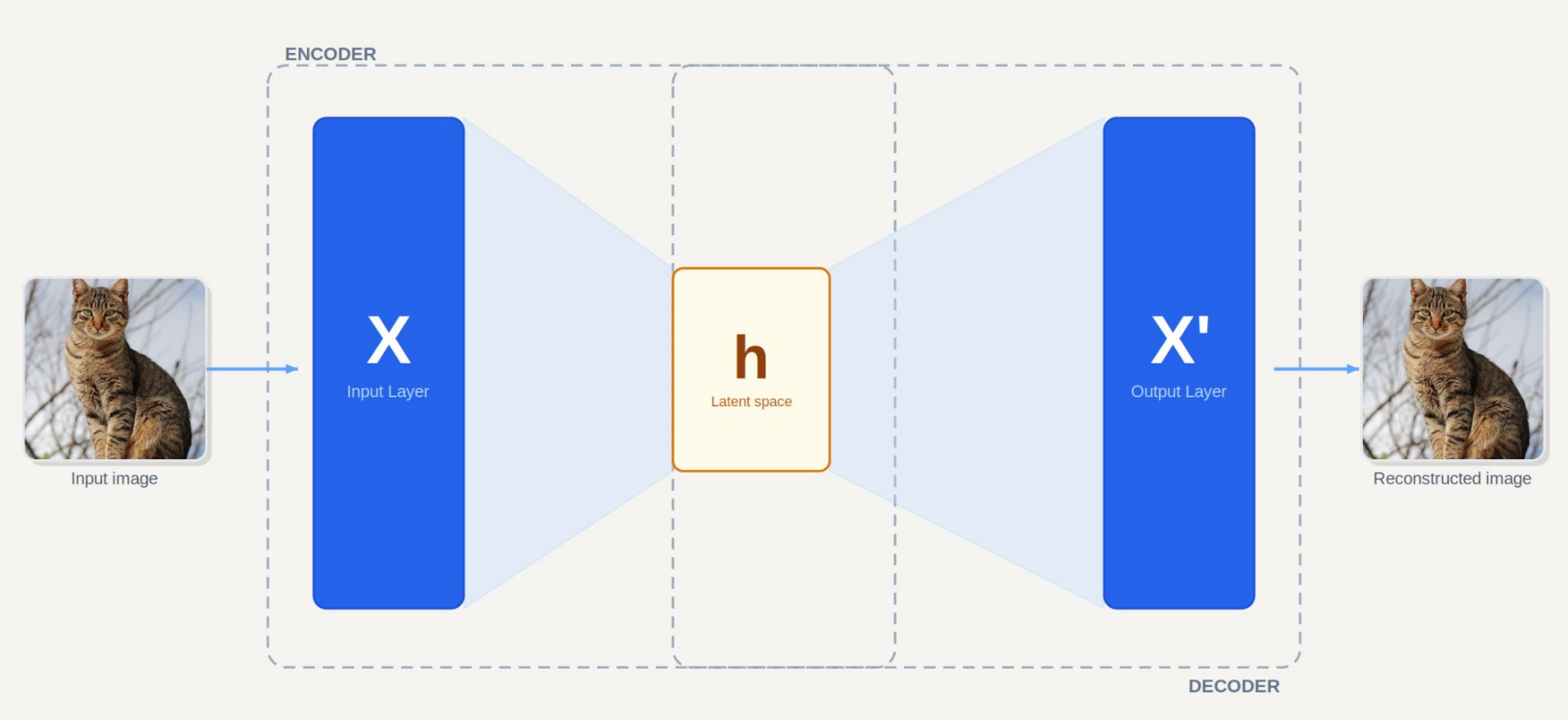
ETH zürich

The quest for the GRAph Level autoEncoder (GRALE)

stud. Ioana Gabor
MSc. Computer Science
31 March 2026

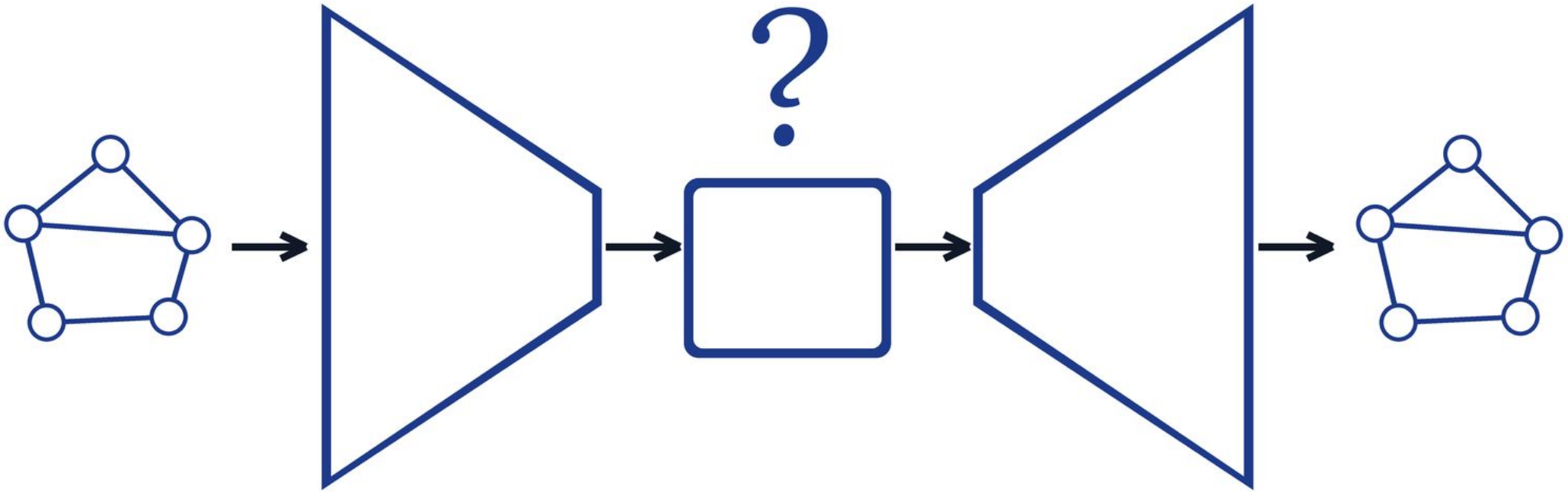
Motivation

Autoencoders



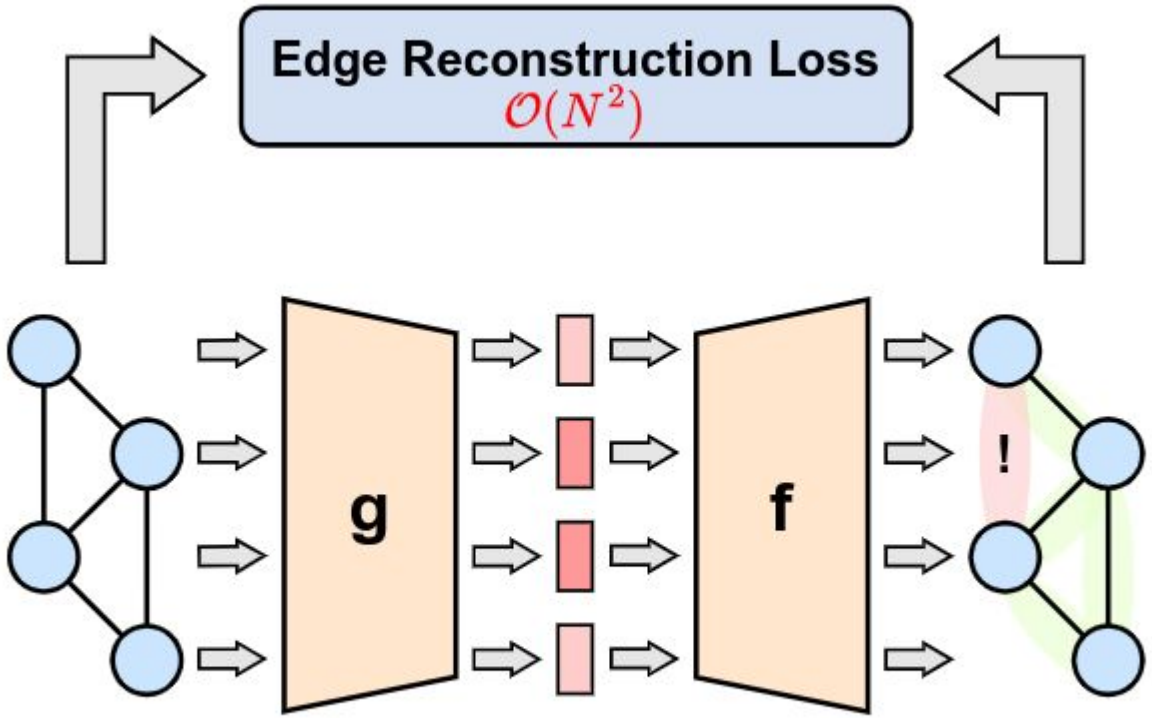
Motivation

Can we find something similar for graphs?



Related work

Node Level Autoencoders



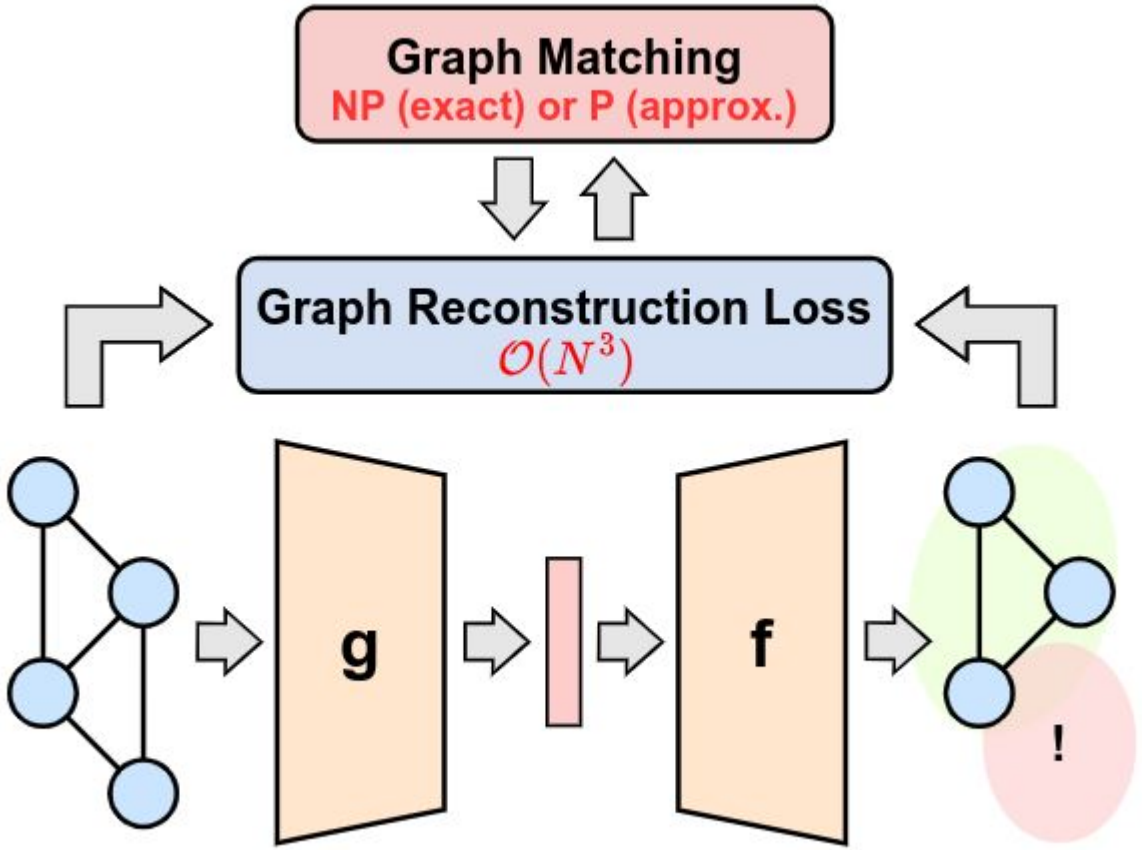
Examples:

- GVAE
- GraphGAN

Krzakala et al., "The Quest for the GRAph Level AutoEncoder (GRALE)", NeurIPS 2025

Related work

Graph Level Autoencoders



Examples:

- GraphVAE
- PIGVAE

Krzakala et al., "The Quest for the GRAph Level AutoEncoder (GRALE)", NeurIPS 2025

Related work

Graph Level Autoencoders - comparison

Graph VAE	PIGVAE
✓ True graph-level embedding ✓ Decodes full graph including size ✗ Needs external graph matching solver ✗ $O(N^4)$, not differentiable end-to-end	✓ Replaces solver with a learned matching module ✓ Differentiable, $O(N^3)$ ✗ Decoder needs ground truth graph size ✗ Loss can be zero for non-isomorphic graphs

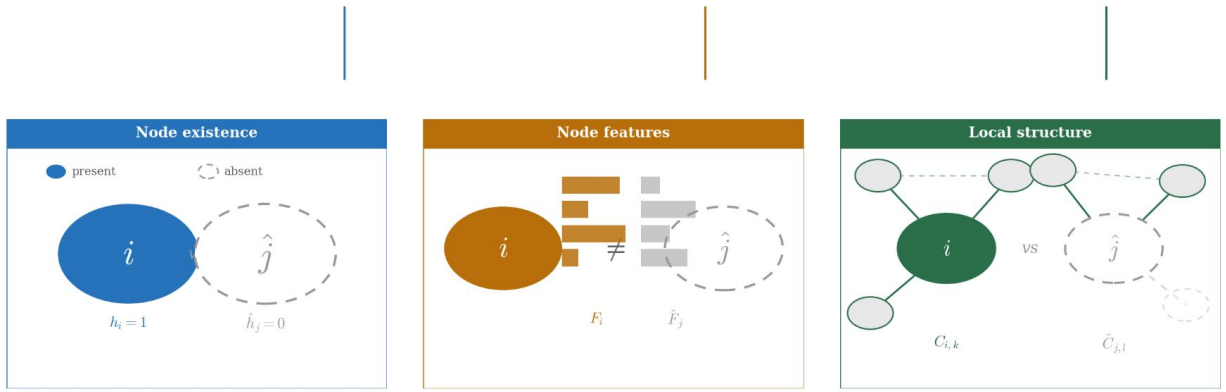
Related work

The loss computation

$$\mathcal{L}_{\mathrm{PI}}(G, \hat{G}) = \min_{P \in \sigma_N} \mathcal{L}_{\mathrm{ALIGN}}(G, P[\hat{G}])$$ -> NP-complete

Any2Graph:

$$\mathcal{L}_{\mathrm{OT}}(G, \hat{G}, T) = \sum_{i,j} \ell_h(h_i, \hat{h}_j)\, T_{i,j} + \sum_{i,j} h_i\, \ell_F(F_i, \hat{F}_j)\, T_{i,j} + \sum_{i,j,k,l} h_i h_k\, \ell_C(C_{i,k}, \hat{C}_{j,l})\, T_{i,j} T_{k,l}$$



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Related work

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$$\mathcal{L}_{\text{PI}}(G, \hat{G}) = \min_{P \in \sigma_N} \mathcal{L}_{\text{ALIGN}}(G, P[\hat{G}])$$ -> NP-complete

PIGVAE:

✓ predict T, instead of optimizing

✓ permute, then compare $\mathcal{L}_{\text{PIGVAE}}(G, \hat{G}, \hat{T}) = \mathcal{L}_{\text{ALIGN}}(G, \hat{T}[\hat{G}])$

✗ the loss can be 0 even if the graphs are not isomorphic

GRALE

The quest for the GRAph Level autoEncoder (GRALE)

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Gabriel Melo
LTCI, Télécom Paris, IP Paris

Charlotte Laclau
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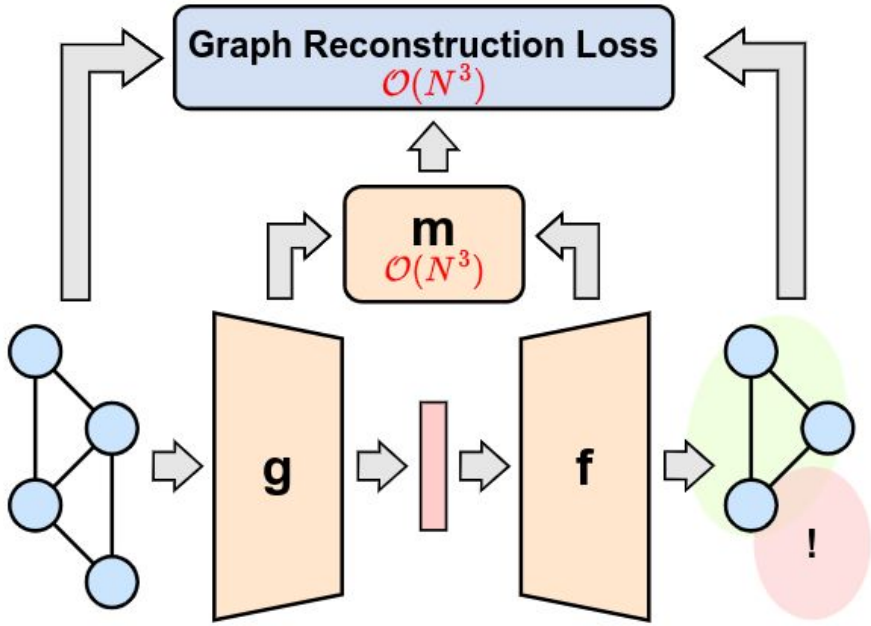
Florence d'Alché-Buc
LTCI, Télécom Paris, IP Paris

Rémi Flamary
CMAP, Ecole Polytechnique, IP Paris

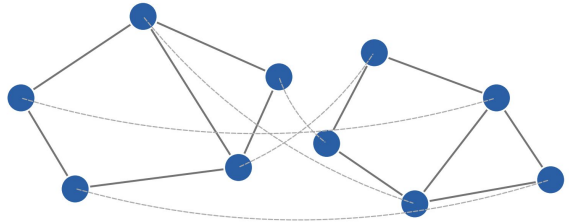


Krzakala et al., "The Quest for the GRAph Level AutoEncoder (GRALE)", NeurIPS 2025

Challenges

The problem statement

1. **Encoder** $g : \mathcal{G} \to \mathbb{Z}$ must be permutation invariant



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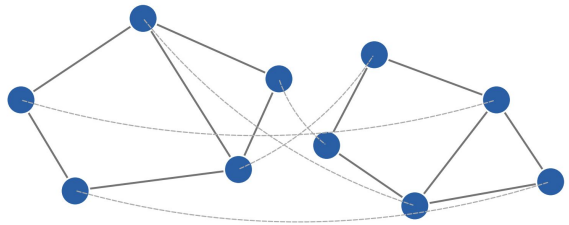
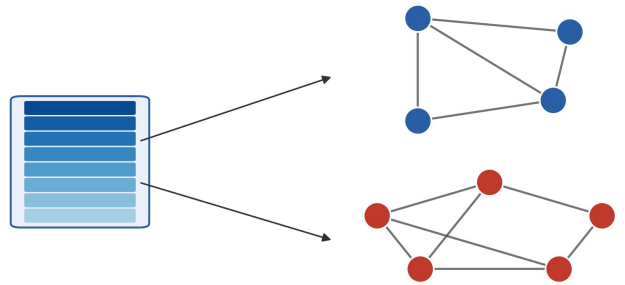


2. **Decoder** $f : \mathbb{Z} \to \mathcal{G}$ must handle variable output size



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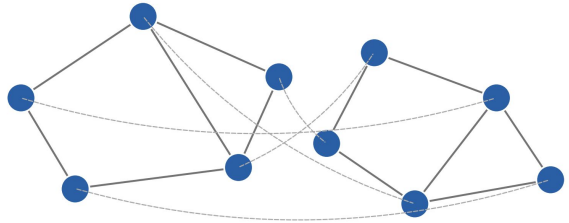
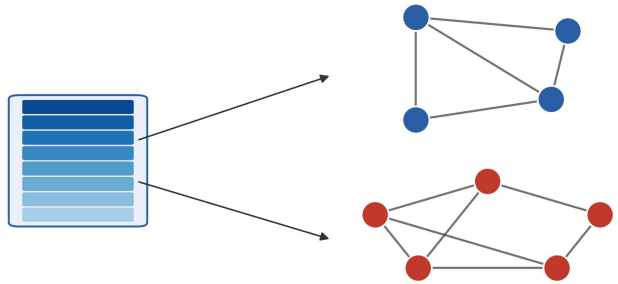


2. **Decoder** f : $\mathbb{Z} \to \mathcal{G}$ must handle variable output size

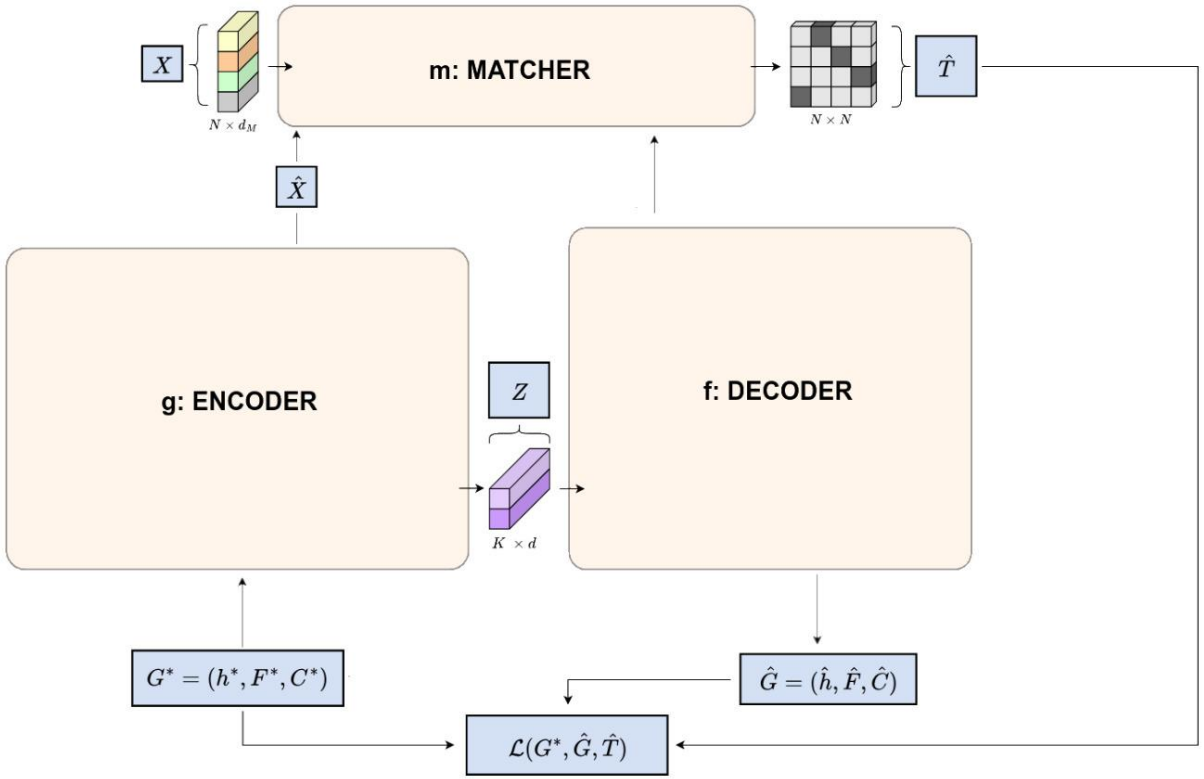


3. **Loss** L(f ◦ g(x), x) must be permutation invariant and differentiable

$$\mathcal{L}_{\text{GRALE}}(G, \phi, \psi, \theta) = \mathcal{L}_{\text{OT}}\left(G, \underbrace{f^{\phi}_{\text{graph}} \circ g^{\psi}_{\text{graph}}(G)}_{\hat{G}}, \underbrace{m^{\theta}\left(g^{\psi}_{\text{nodes}}(G), f^{\phi}_{\text{nodes}} \circ g^{\psi}_{\text{graph}}(G)\right)}_{\hat{T}}\right).$$

Architecture

General Structure



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Architecture

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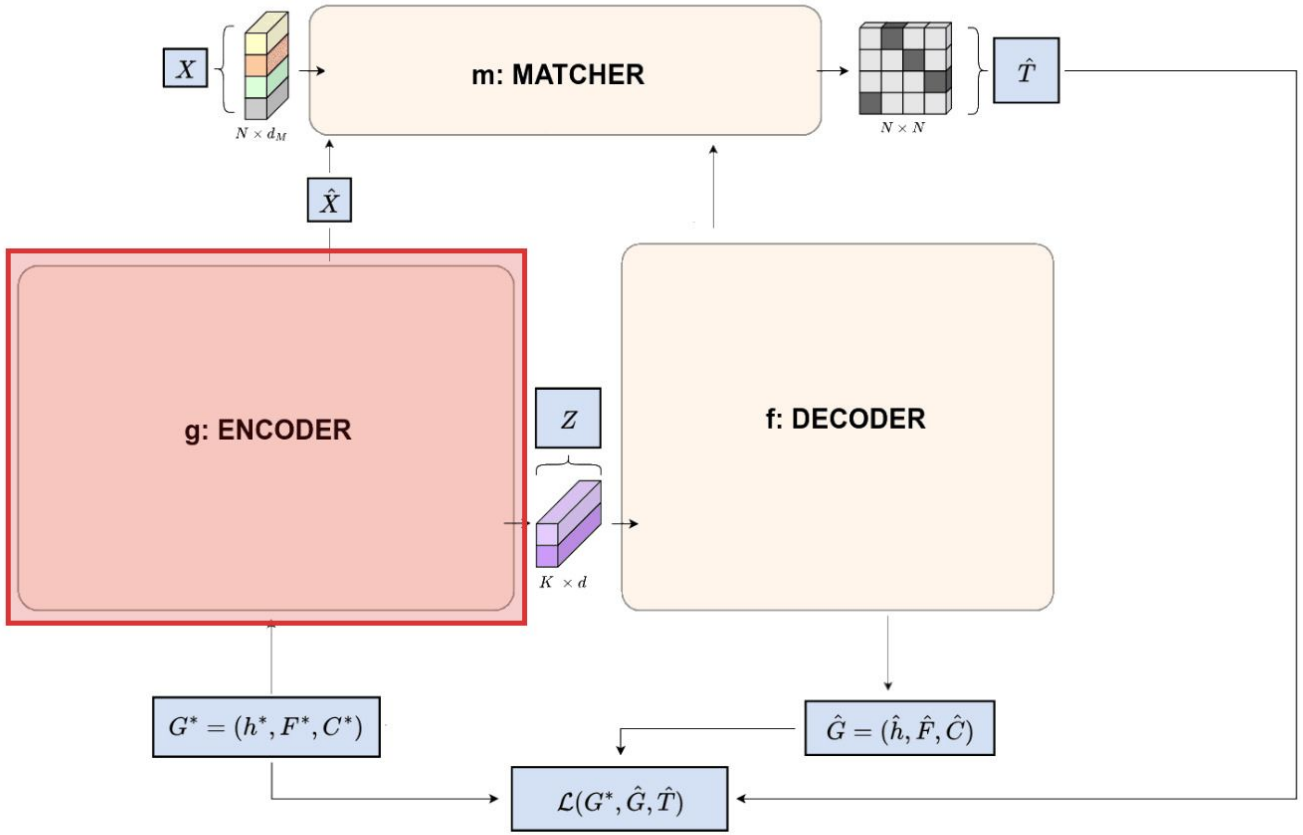
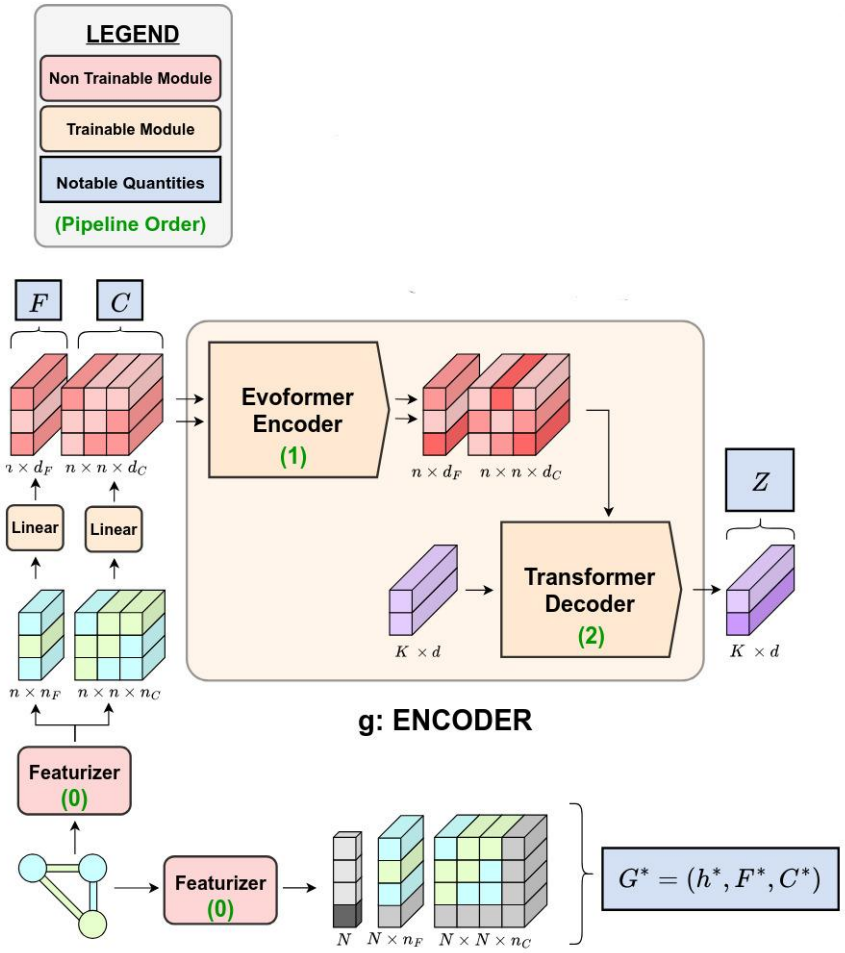


Step 1 — Encode
Z, X = g(G)

g: ENCODER

Architecture

Encoder



Article

Highly accurate protein structure prediction with AlphaFold

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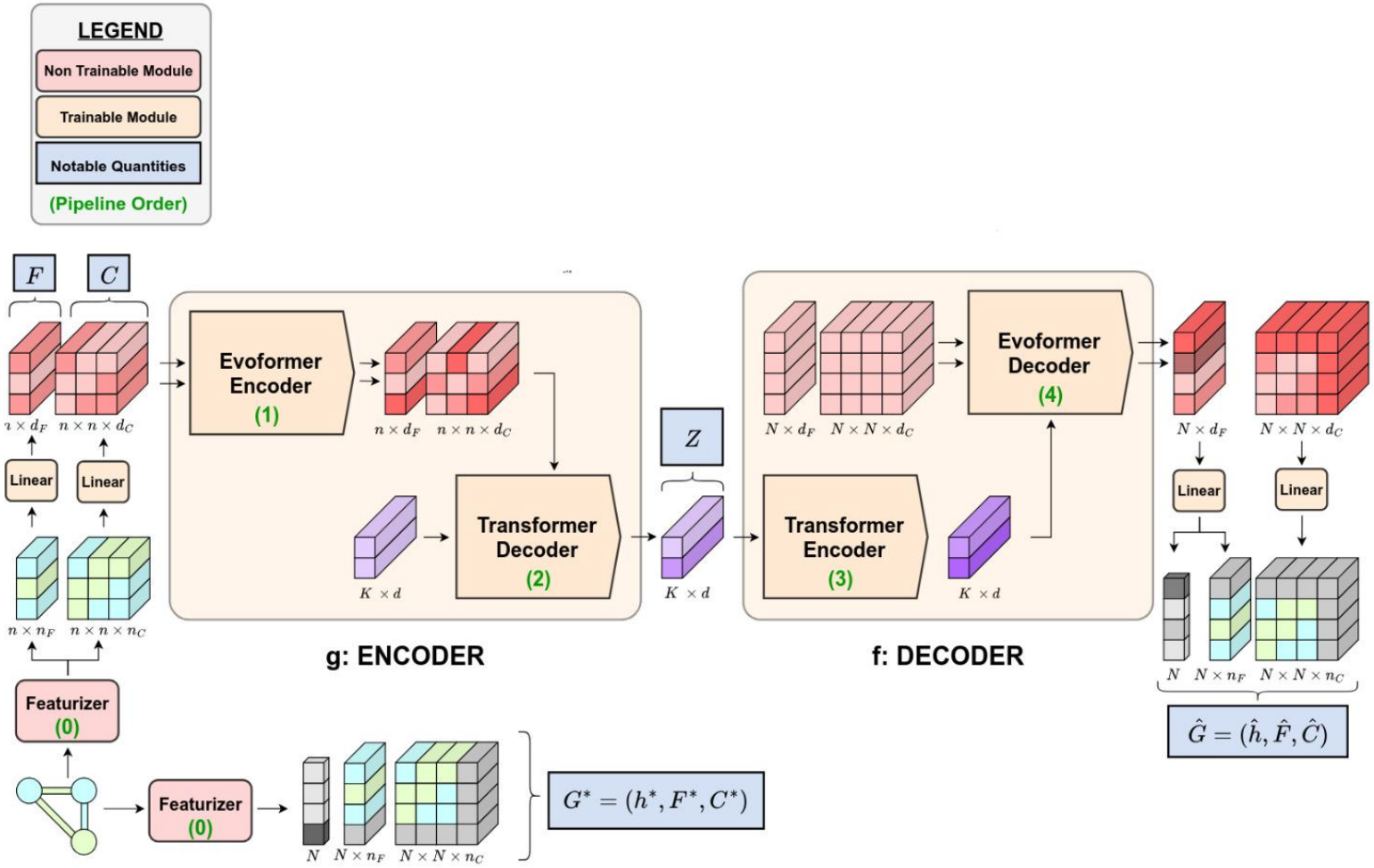
Check for updates

John Jumper[1,4], Richard Evans[1,4], Alexander Pritzel[1,4], Tim Green[1,4], Michael Figurnov[1,4], Olaf Ronneberger[1,4], Kathryn Tunyasuvunakool[1,4], Russ Bates[1,4], Augustin Žídek[1,4], Anna Potapenko[1,4], Alex Bridgland[1,4], Clemens Meyer[1,4], Simon A. A. Kohl[1,4], Andrew J. Ballard[1,4], Andrew Cowie[1,4], Bernardino Romera-Paredes[1,4], Stanislav Nikolov[1,4], Rishub Jain[1,4], Jonas Adler[1], Trevor Back[1], Stig Petersen[1], David Reiman[1], Ellen Clancy[1], Michal Zielinski[1], Martin Steinegger[2,3], Michalina Pacholska[1], Tamas Berghammer[1], Sebastian Bodenstein[1], David Silver[1], Oriol Vinyals[1], Andrew W. Senior[1], Koray Kavukcuoglu[1], Pushmeet Kohli[1] & Demis Hassabis[1,4]

Architecture

Decoder



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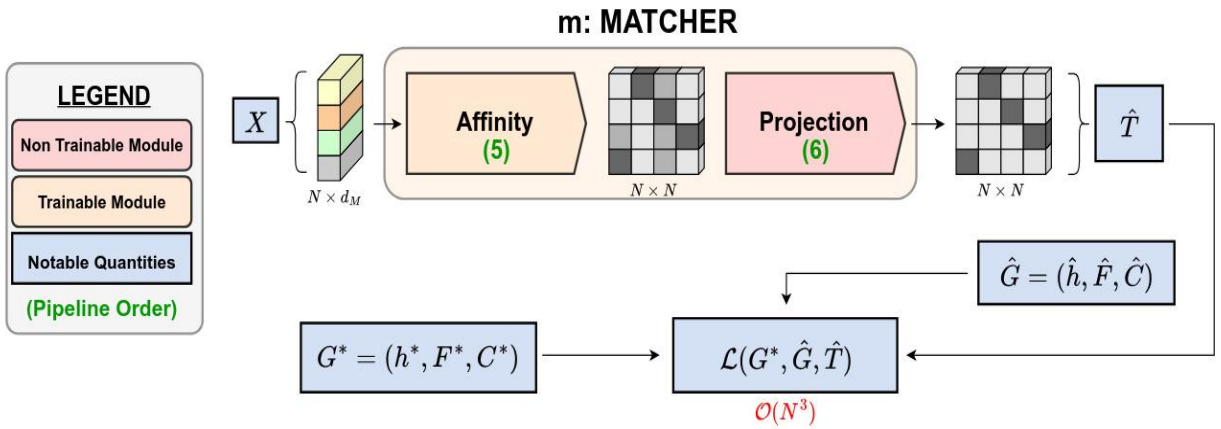
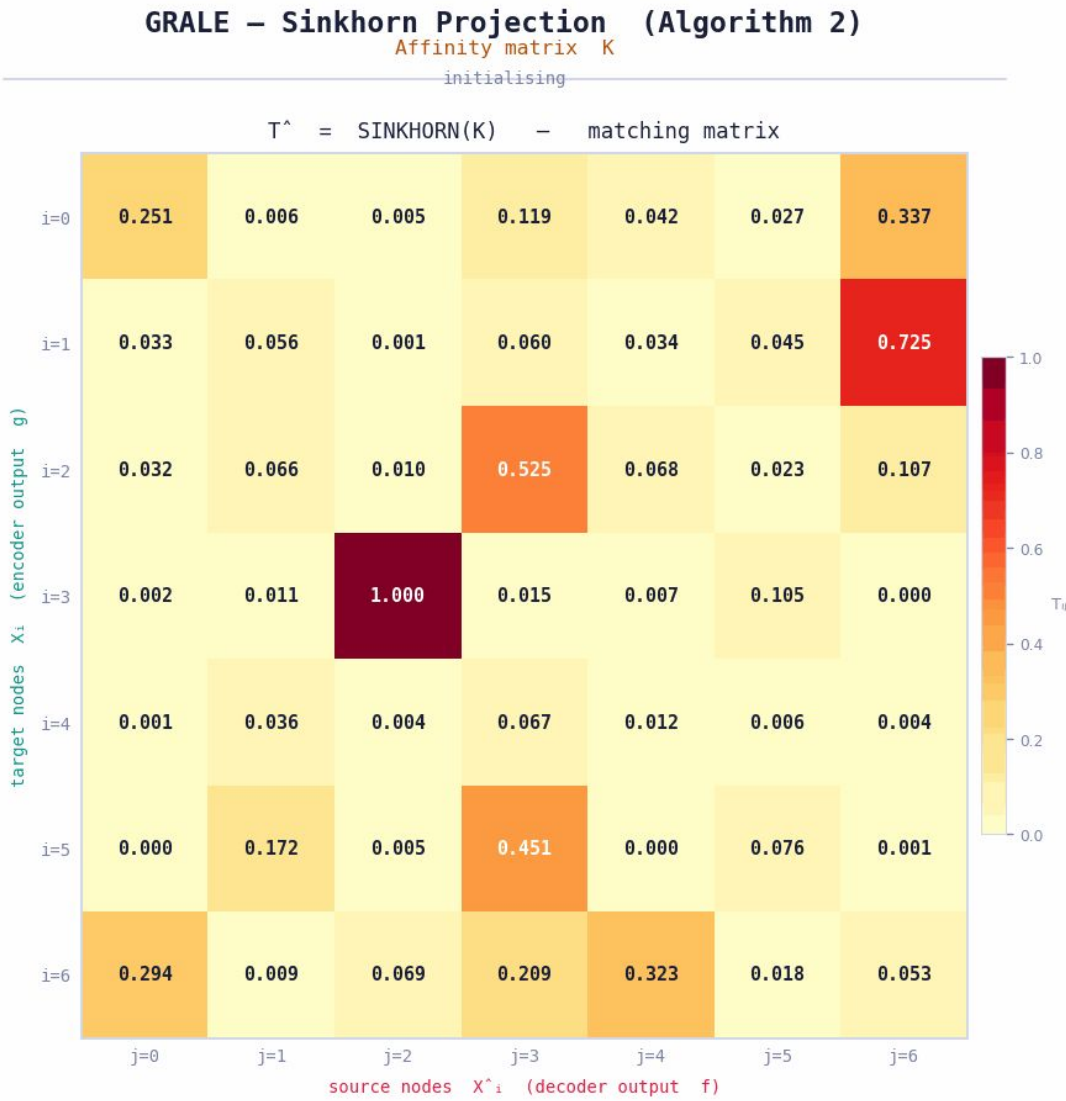
Architecture

Matcher Module





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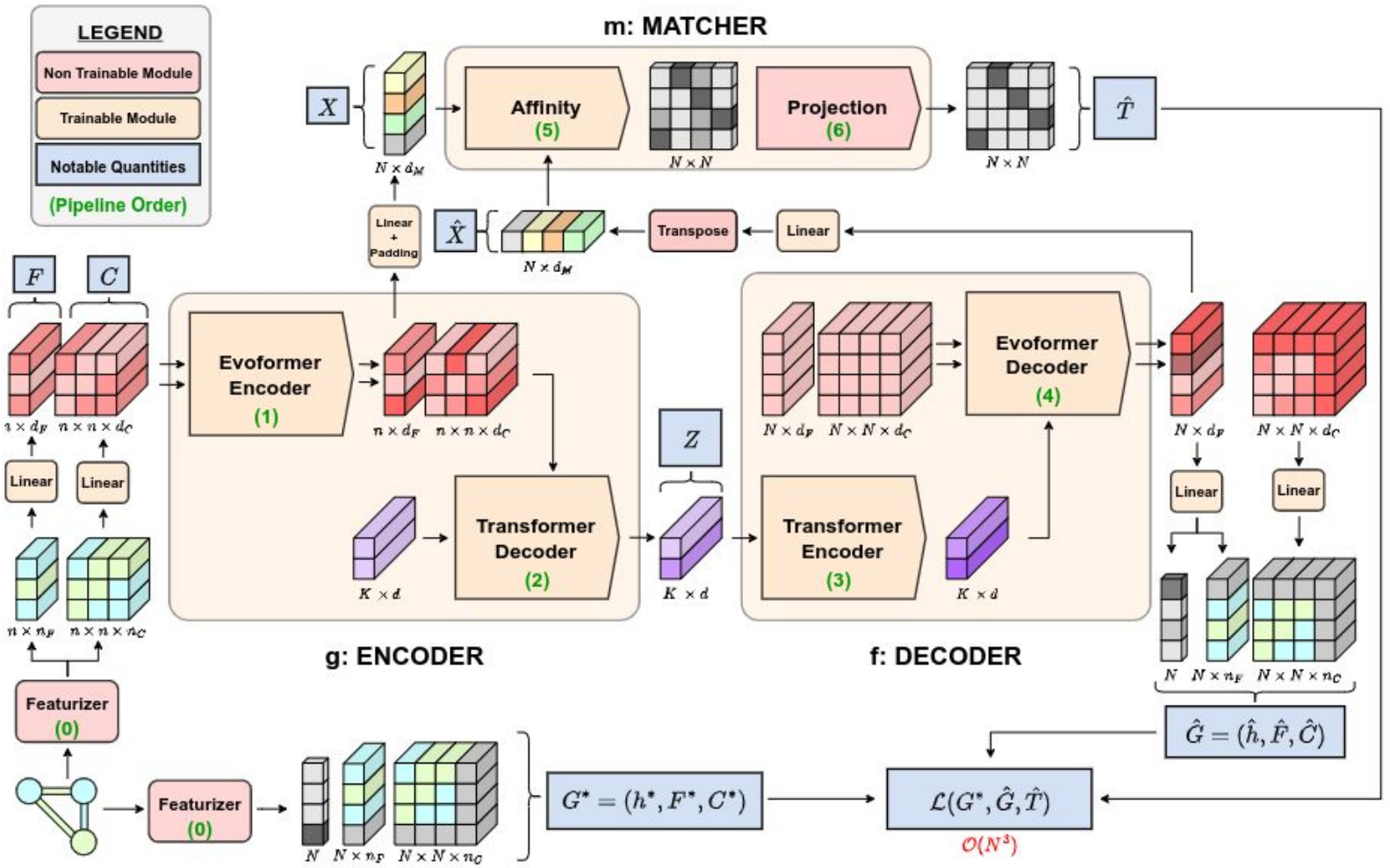
Architecture

Full picture



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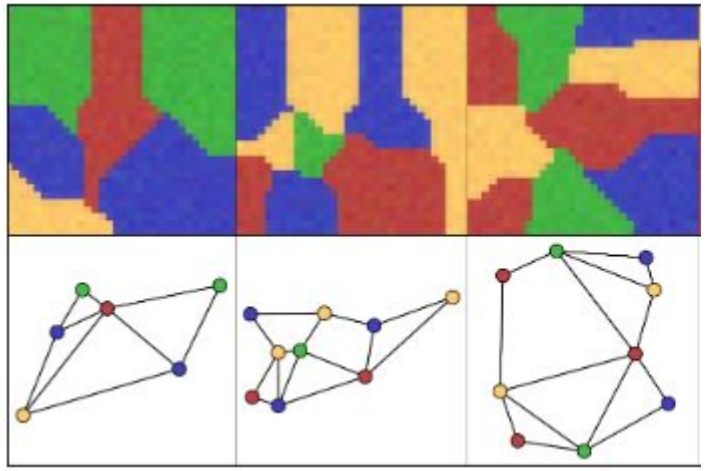
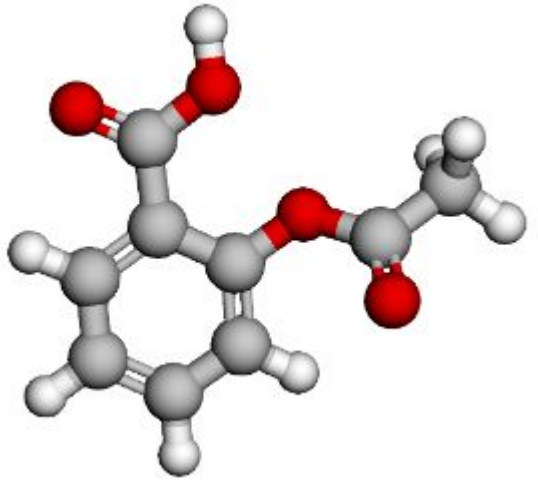
Experiments

Datasets



COLORING



PUBCHEM

Experiments

Reconstruction quality across the three datasets

Model	COLORING		PUBCHEM 16		PUBCHEM 32	
	Edit. Dist. (↓)	GI Acc. (↑)	Edit. Dist. (↓)	GI Acc. (↑)	Edit. Dist. (↓)	GI Acc. (↑)
GraphVAE	2.13	35.90	3.72	07.8	N.A.	N.A.
PIGVAE*	0.09	85.30	1.69	41.0	2.53	24.91
GRALE	**0.02**	**99.20**	**0.11**	**93.0**	**0.78**	**66.80**

Experiments

Component-by-component ablation performance impact

Model component	Proposed	Remplaced by	Edit Dist.	GI Acc.
Loss	$\mathcal{L}_{\text{OT}}$	$\mathcal{L}_{\text{PIGVAE}}$ + Regularization [69]	0.13 ± 0.16	91.8 ± 5.01
Featurizer ϕ	Second Order	First Order	0.24 ± 0.17	90.3 ± 6.46
Encoder f	Evoformer	GNN	1.32 ± 0.16	53.2 ± 2.69
Decoder g	Evoformer	Transformer Decoder [39]	0.71 ± 0.09	66.6 ± 2.78
Matcher m	Sinkhorn	Softsort [69]	1.47 ± 0.36	49.7 ± 9.15
Disambiguation Noise	With	Without	1.16 ± 0.03	64.4 ± 1.64
GRALE (no remplacement)			$\mathbf{0.11} \pm 0.04$	$\mathbf{93.0} \pm 0.18$

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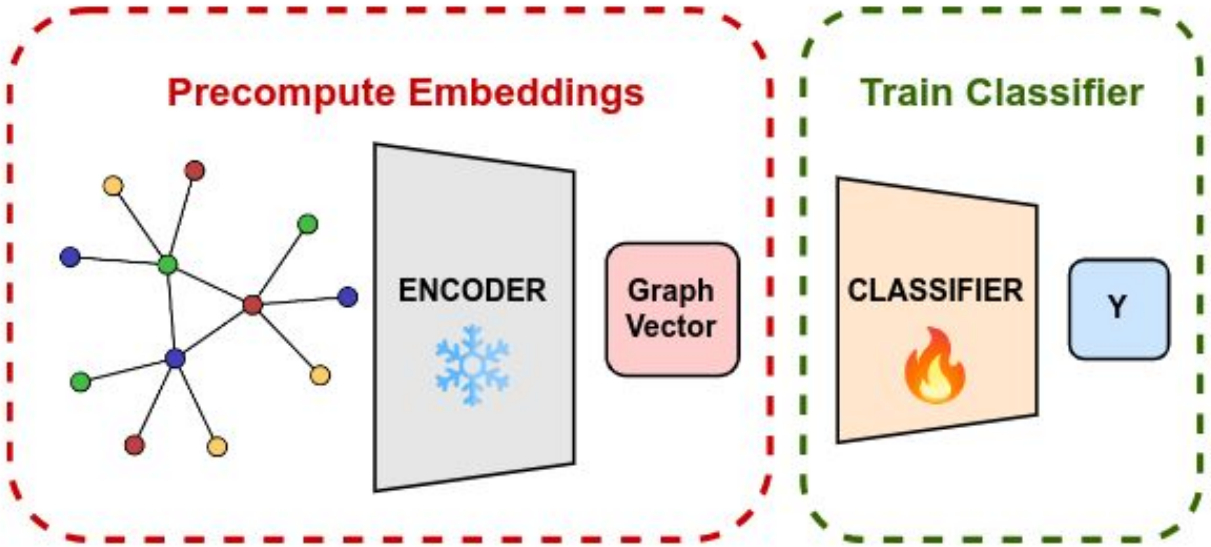
Applications

Graph classification / regression



Model	MLP Regression (MAE ↓) QM9	QM40	SVR Regression (MAE ↓) ESOL	LIPO	FreeSolv	SVC Classif. (ROC-AUC ↑) BBBP	BACE
SimGRACE	0.110 ± 0.003	0.025 ± 0.005	0.293 ± 0.020	0.534 ± 0.023	0.374 ± 0.008	0.745 ± 0.072	**0.866** ± 0.050
InfoGraph	0.122 ± 0.001	0.020 ± 0.001	**0.255** ± 0.016	**0.495** ± 0.013	0.297 ± 0.010	0.729 ± 0.053	0.845 ± 0.046
GraphMAE	0.222 ± 0.016	0.247 ± 0.036	0.291 ± 0.012	0.527 ± 0.029	0.378 ± 0.028	**0.773** ± 0.036	0.857 ± 0.039
GVAE	0.765 ± 0.005	0.328 ± 0.005	0.306 ± 0.027	0.668 ± 0.014	0.344 ± 0.022	0.705 ± 0.060	0.771 ± 0.049
PIGVAE	0.031 ± 0.001	0.019 ± 0.001	0.279 ± 0.020	0.523 ± 0.019	0.283 ± 0.013	0.675 ± 0.079	0.816 ± 0.049
GRALE	**0.015** ± 0.001	**0.018** ± 0.003	0.274 ± 0.014	0.511 ± 0.022	**0.272** ± 0.017	0.731 ± 0.025	0.821 ± 0.051

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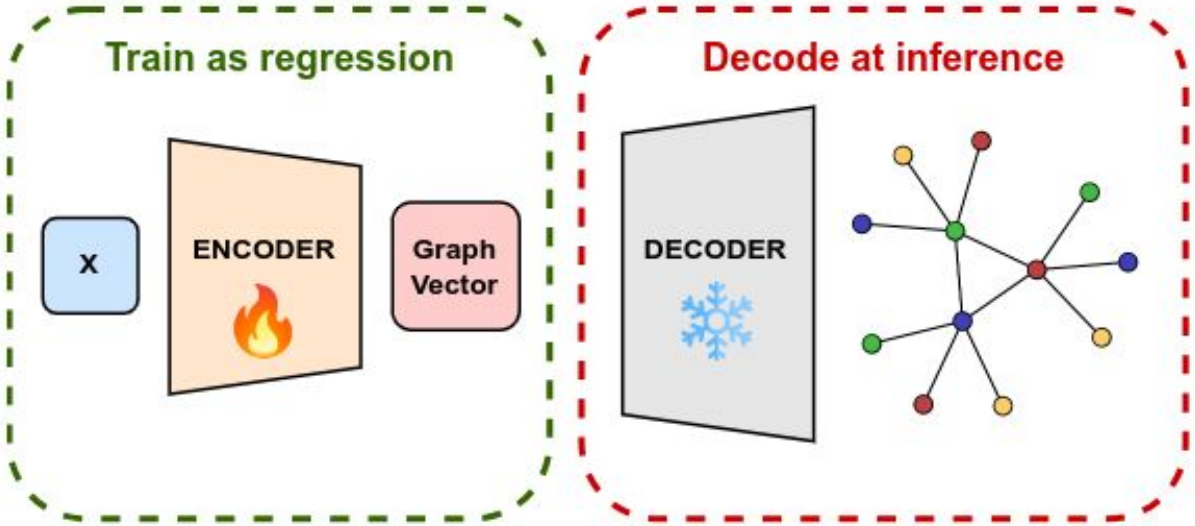
Applications

Graph generation



Model	Edit Dist. (↓) COLORING 10	COLORING 15	QM9	GDB13	GI Acc. (↑) COLORING 10	COLORING 15	QM9	GDB13
FGWBARY	6.73	N.A.	2.84	N.A.	01.00	N.A.	28.95	N.A.
RELATIONFORMER	5.47	2.64	3.80	7.45	18.14	21.99	09.95	00.05
ANY2GRAPH	**0.19**	1.22	2.61	3.63	84.44	43.77	29.85	16.25
GRALE	0.39	0.67	3.62	4.43	89.66	86.02	30.77	32.02
GRALE + FINETUNING	0.27	**0.45**	**2.13**	**2.25**	**90.04**	**88.87**	**35.27**	**53.22**

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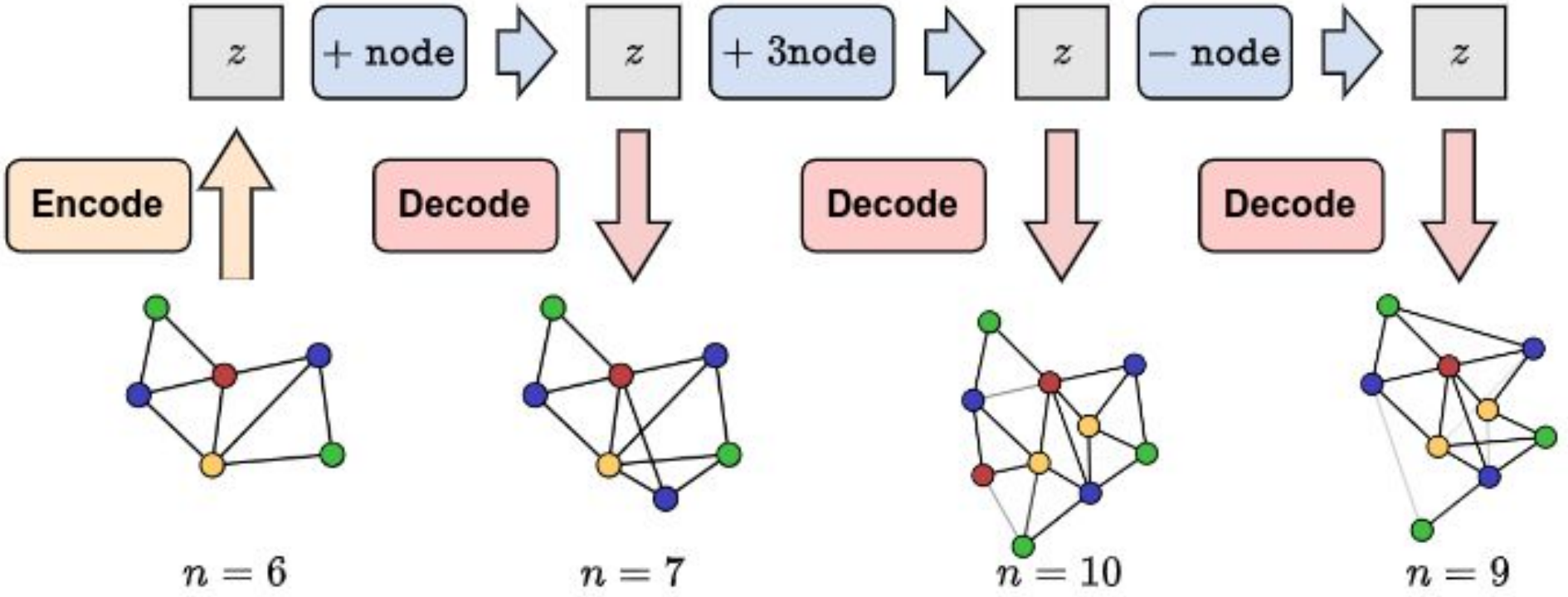
Applications

Graph edition



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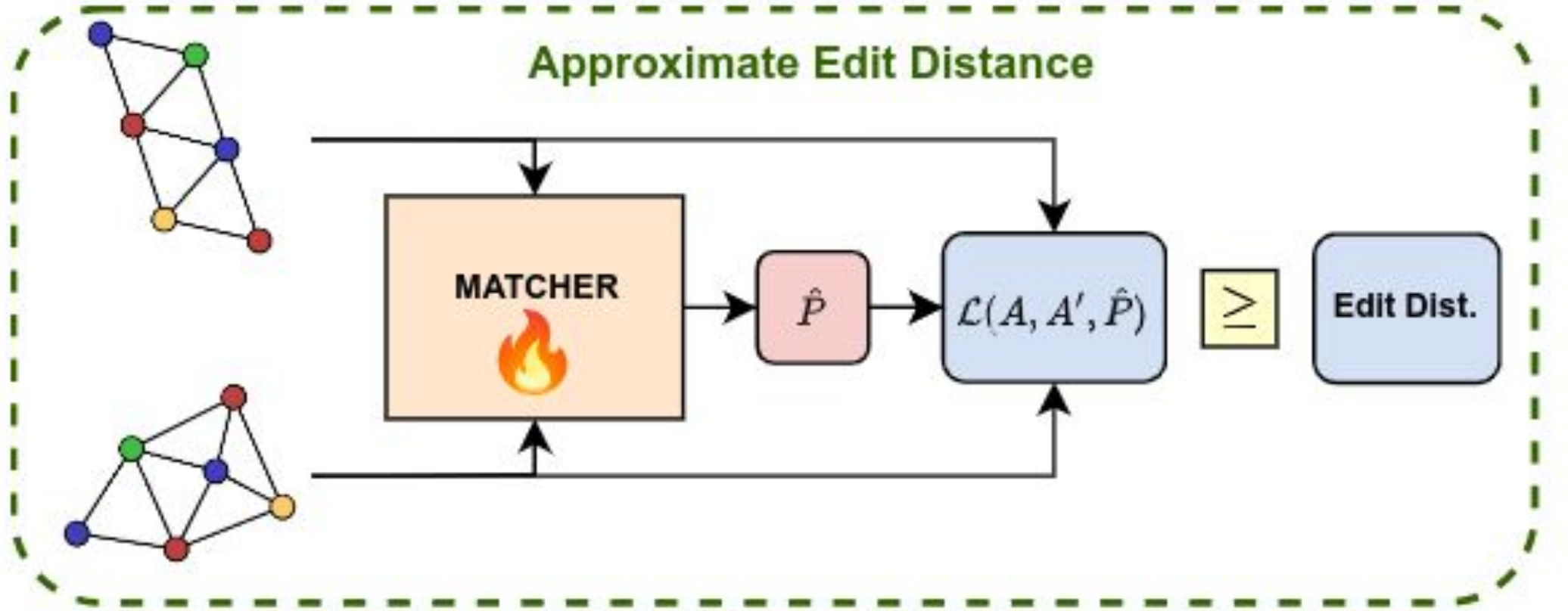
Applications

Graph matching



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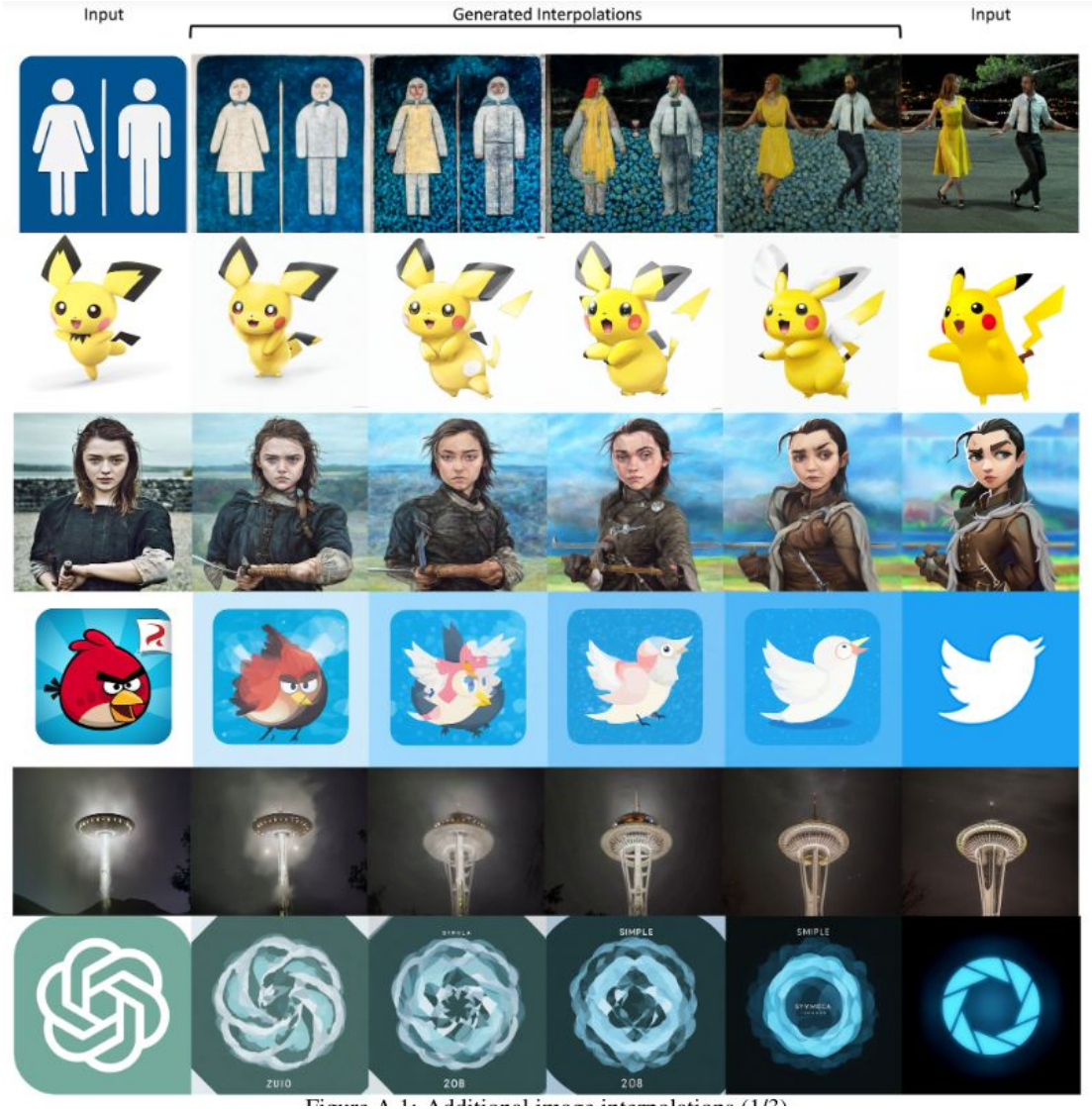
Applications

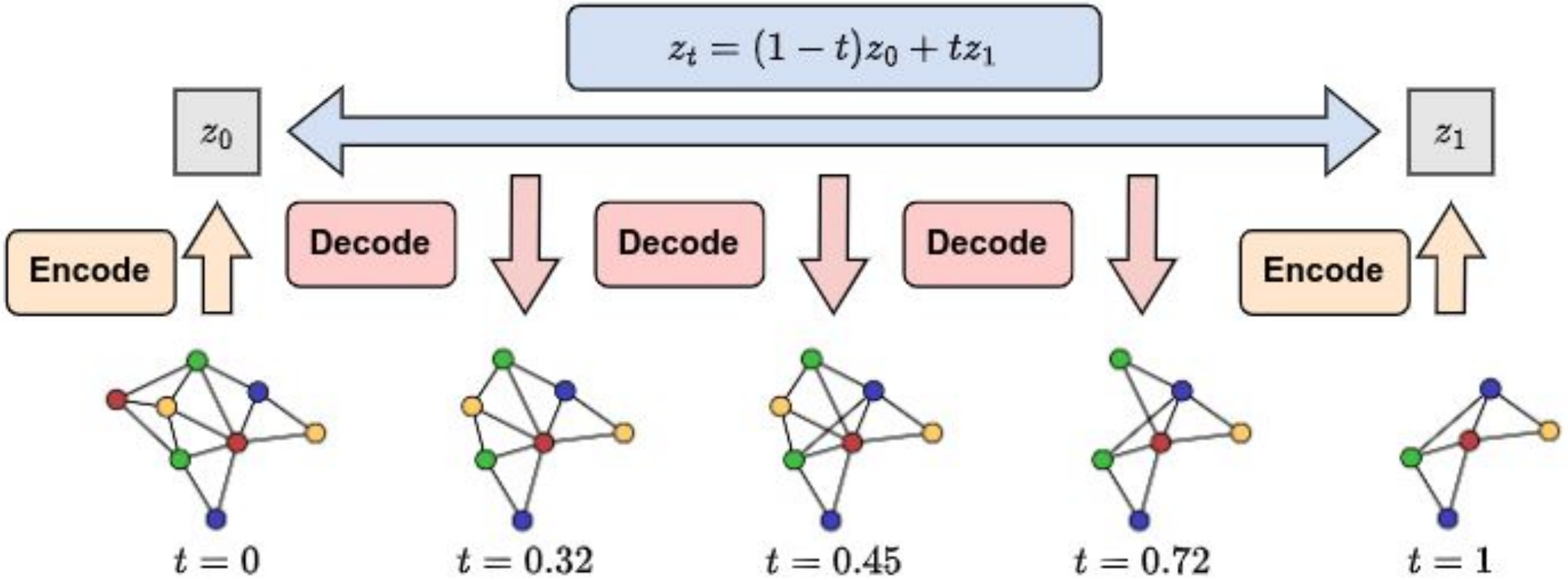
Motivation: Image interpolation



Wang, C. J., & Golland, P. (2025). *Interpolating between Images with Diffusion Models*.

Applications

Graph interpolation



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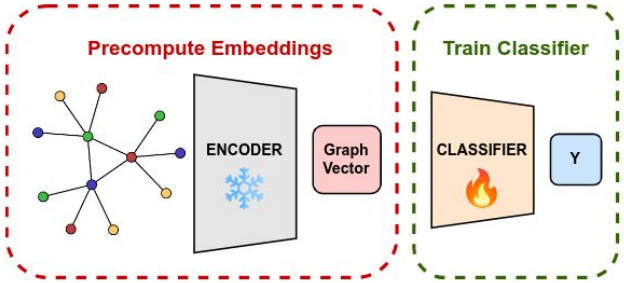
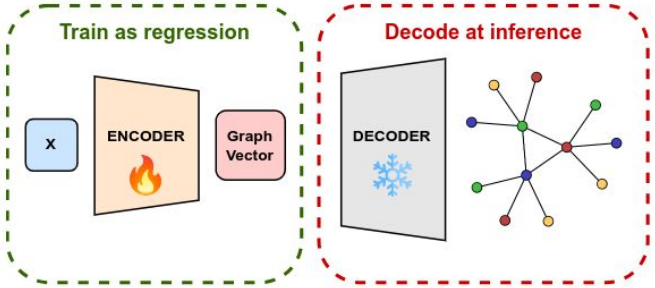
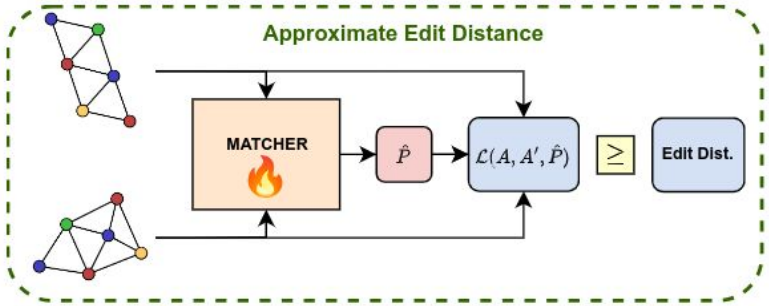
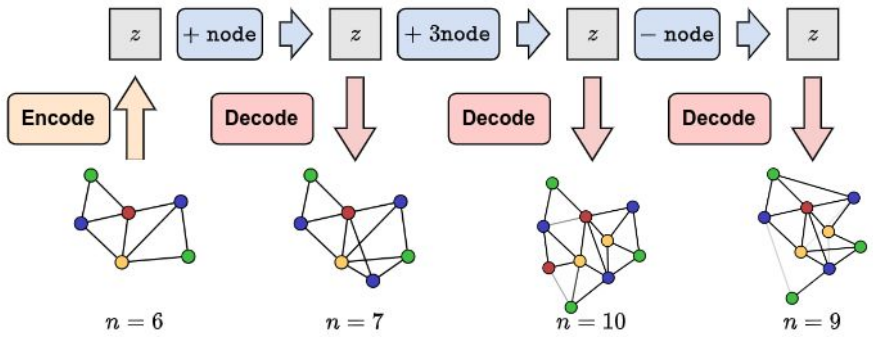
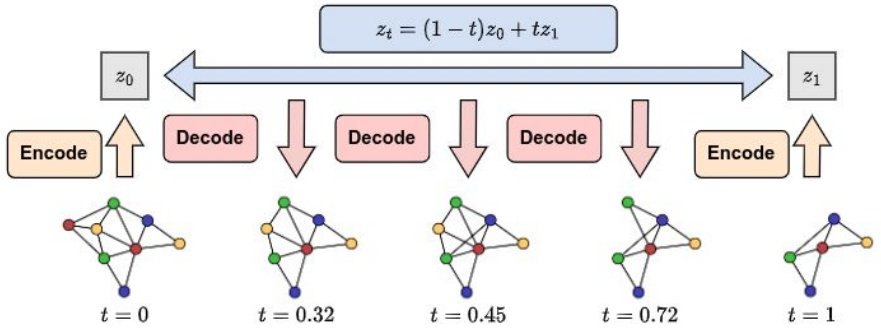
Applications











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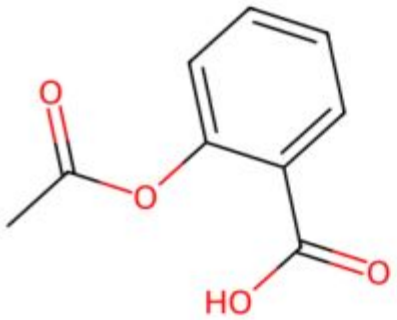
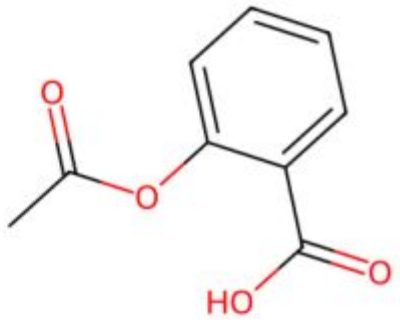
Demo

Reconstruction notebook

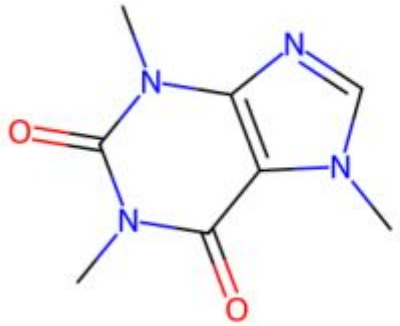
Input Molecule



Reconstructed Molecule



Input Molecule



Reconstructed Molecule

Krzakala et al., "The Quest for the GRAph Level AutoEncoder (GRALE)", NeurIPS 2025

Conclusions & My opinion

✓ SOTA reconstruction, matching, prediction

✓ Latent space enables interpolation, editing, denoising

✗ $O(N^3)$ limits to $N \leq 32$

Next improvements:

- Scale up
- Graph VAE
- Molecular elucidation

Thank you!
Q & A

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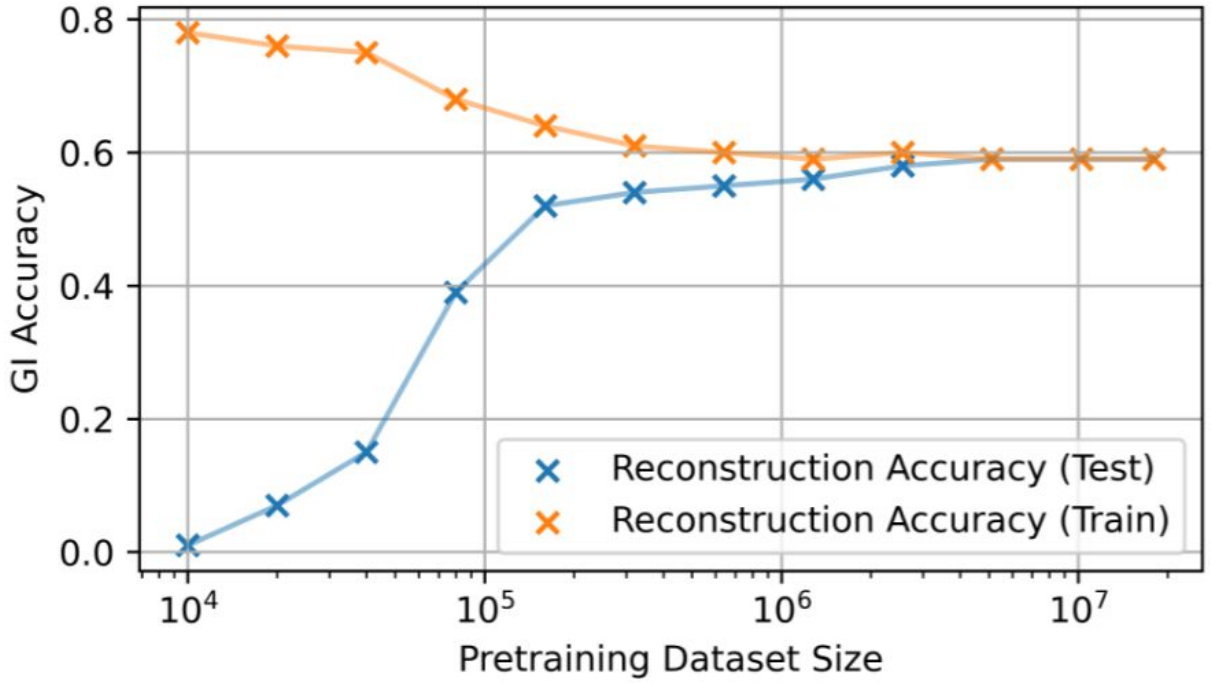
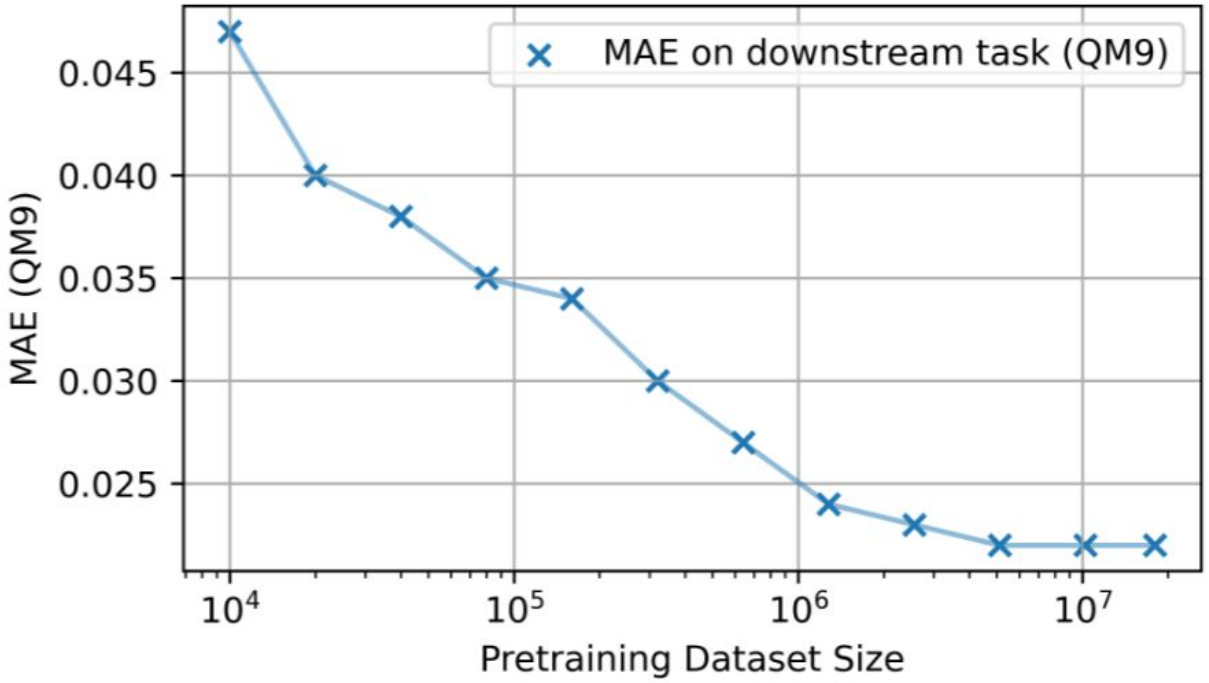
Extra Slides

Experiment results

Additional training details



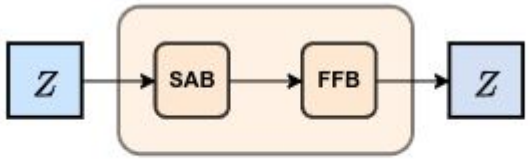


Krzakala et al., "The Quest for the GRAph Level AutoEncoder (GRALE)", NeurIPS 2025

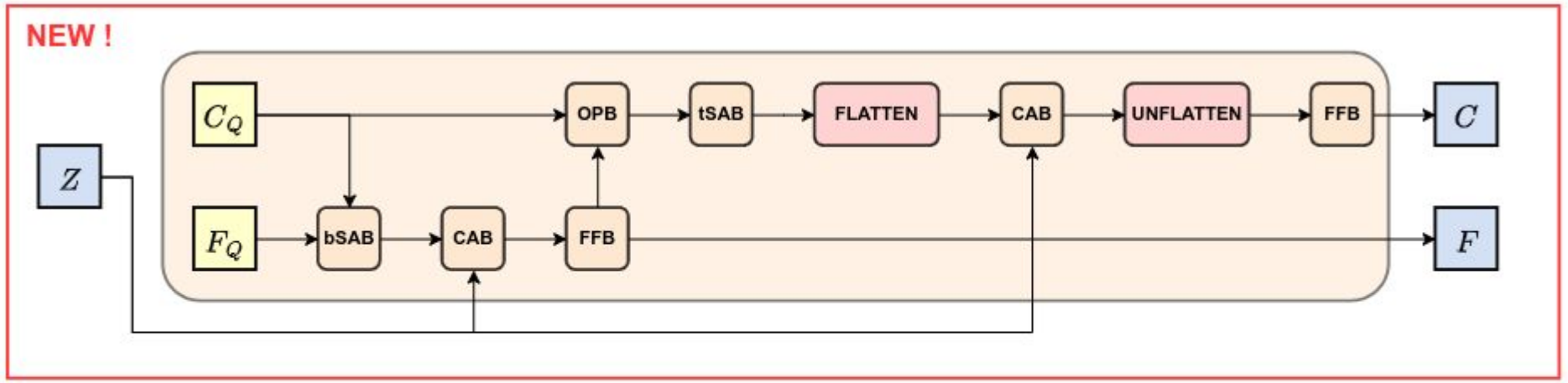
Architecture

Decoder

Transformer Encoder



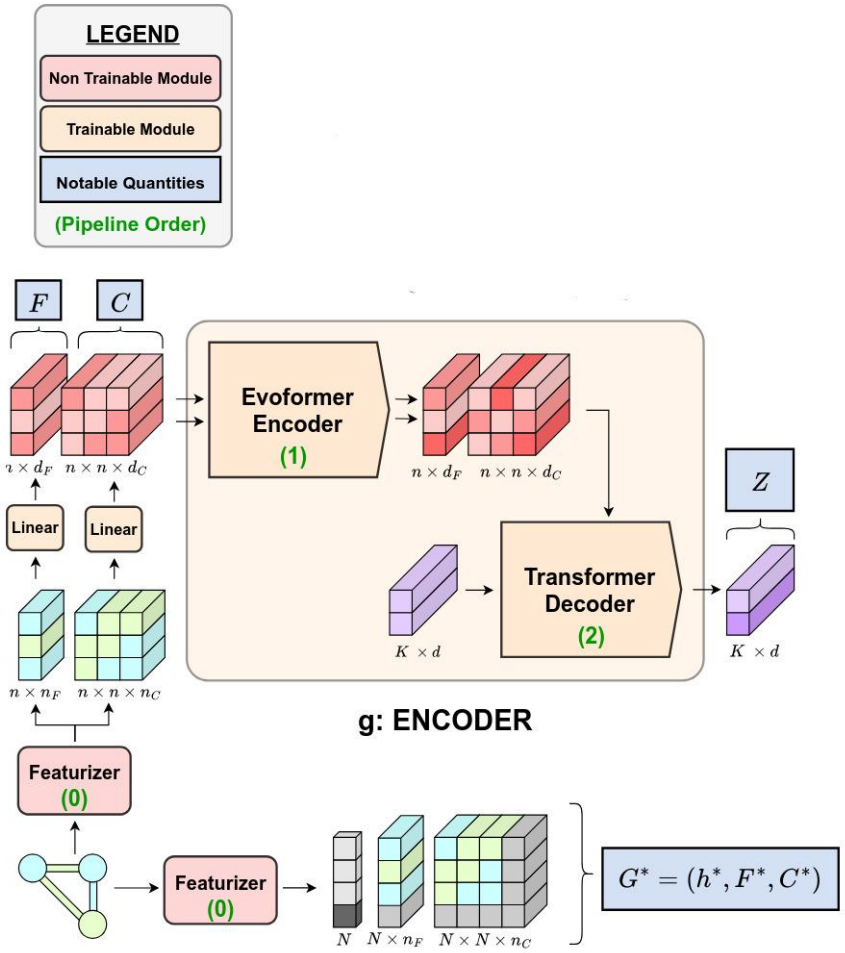
Evoformer Decoder (new)



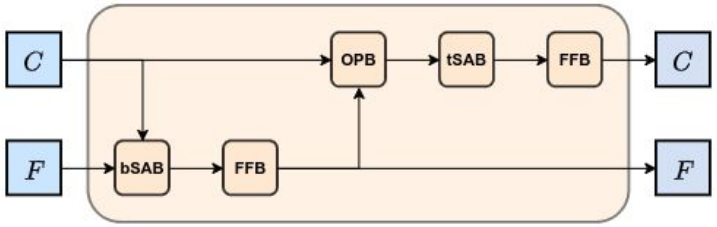
Krzakala et al., "The Quest for the GRAph Level AutoEncoder (GRALE)", NeurIPS 2025

Architecture

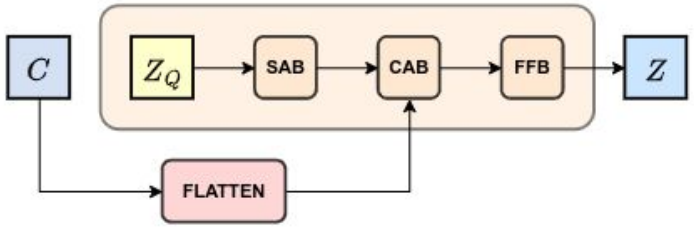
Encoder



Evoformer Encoder



Transformer Decoder



Krzakala et al., "The Quest for the GRAph Level AutoEncoder (GRALE)", NeurIPS 2025

Experiment results

Additional training details

MODEL	COLORING	PUBCHEM 16	PUBCHEM 32	COMPLEXITY
GRAPHVAE	40H	80H	N.A.	$O(N^4)$
PIGVAE	8H	18H	95H	$O(N^3)$
GRALE	8H	20H	100H	$O(N^3)$

Experiment results

Graph matching speed vs. accuracy tradeoff

Model	Edit Dist. (↓) COLORING	Edit Dist. (↓) PUBCHEM	Compute time in seconds (↓) COLORING	Compute time in seconds (↓) PUBCHEM
IPFP	21.10 ± 10.83	40.66 ± 12.16	0.006 ± 0.013	<u>0.073</u> ± 0.052
RRWM	20.66 ± 10.90	42.24 ± 12.71	0.540 ± 0.190	1.271 ± 0.244
SM	20.90 ± 10.91	43.20 ± 12.86	**0.002** ± 0.001	0.076 ± 0.022
Greedy A*	20.41 ± 11.21	<u>32.53</u> ± 08.15	0.021 ± 0.016	0.110 ± 0.054
A*	19.66 ± 11.01	N.A.	3.487 ± 1.928	>100
GRALE	<u>08.92</u> ± 05.61	32.77 ± 11.67	<u>0.005</u> ± 0.001	**0.008** ± 0.002
GRALE + Finetuning	**07.64** ± 04.42	**19.33** ± 07.85		

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