Self-Supervised Graph Transformer on Large Molecular Data

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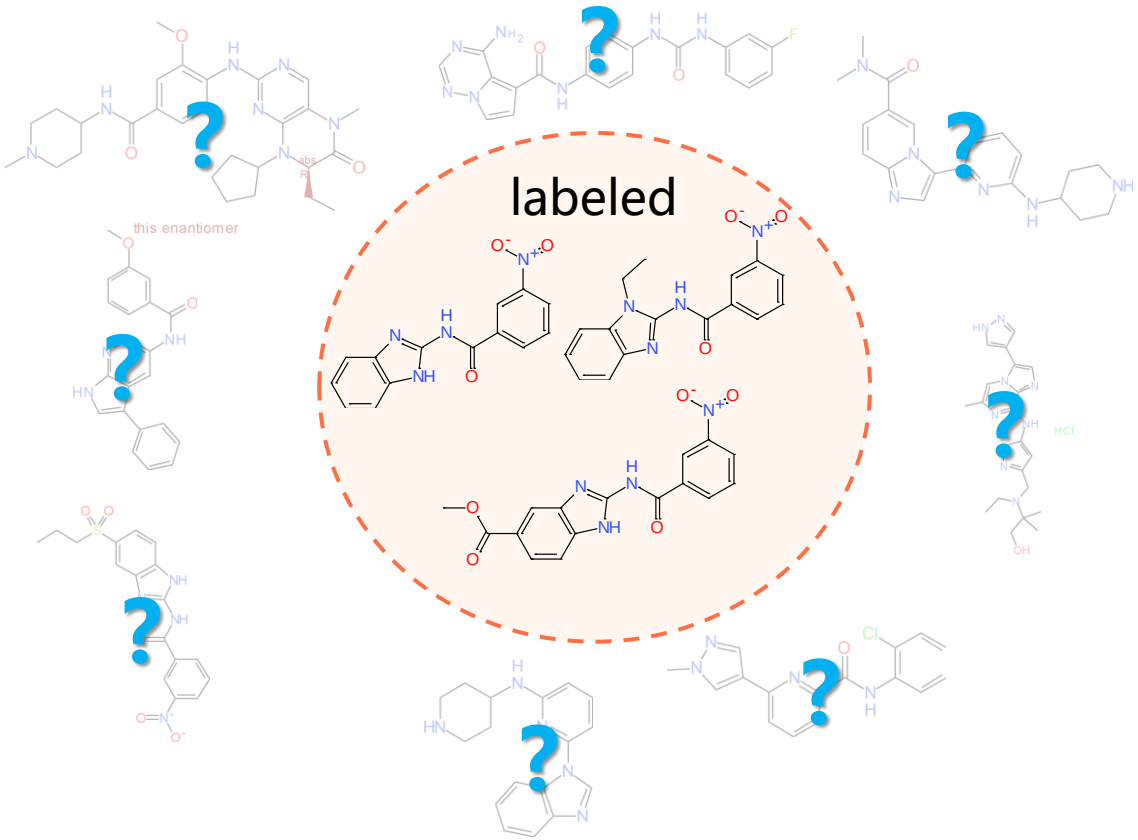
Background

- GNNs are widely adopted for molecular tasks.

- Challenges
  - Insufficient labeled molecules for supervised training
  - Poor generalization capabilities to newly-synthesized molecules



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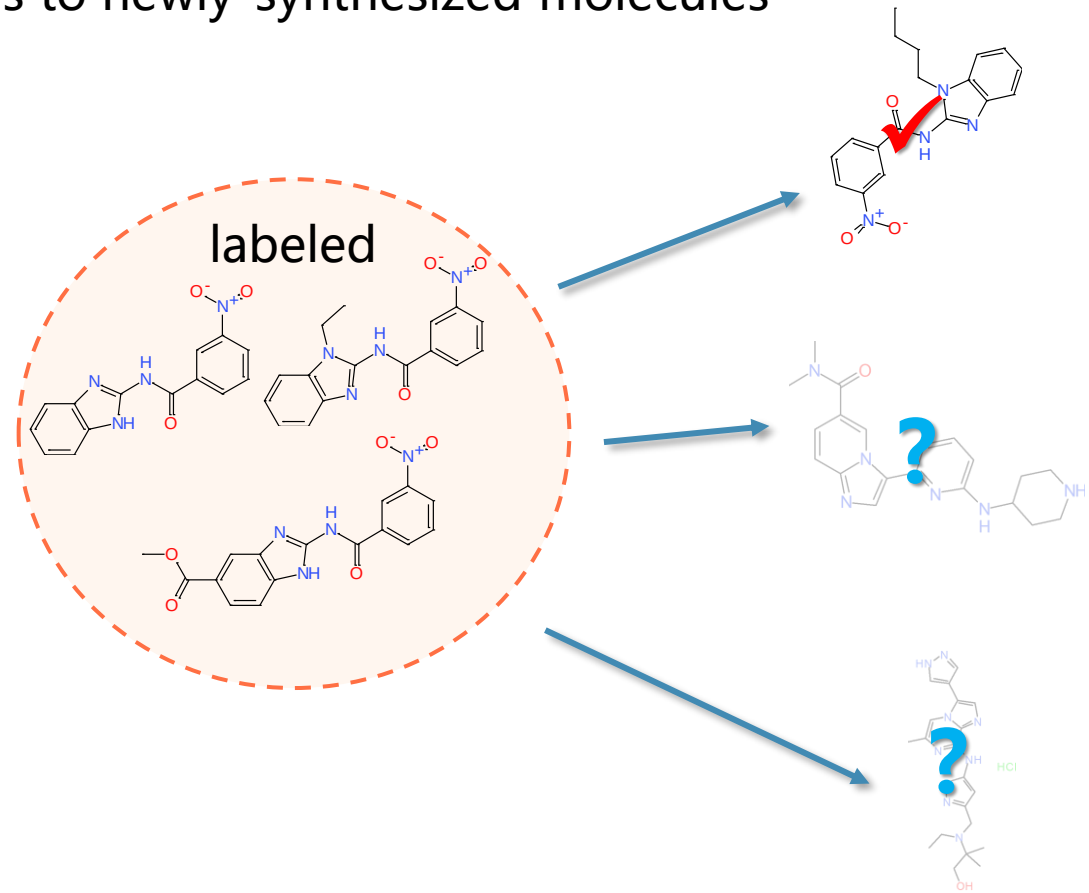


Contributions

- GROVER: **G**raph **R**epresentation fr**O**m self-super**V**ised m**E**ssage passing t**R**ansformer
- Overview of this molecular representation learning framework

GROVER

Integrating message passing networks with the Transformer-style architecture → delivers → More expressive encoders of molecules

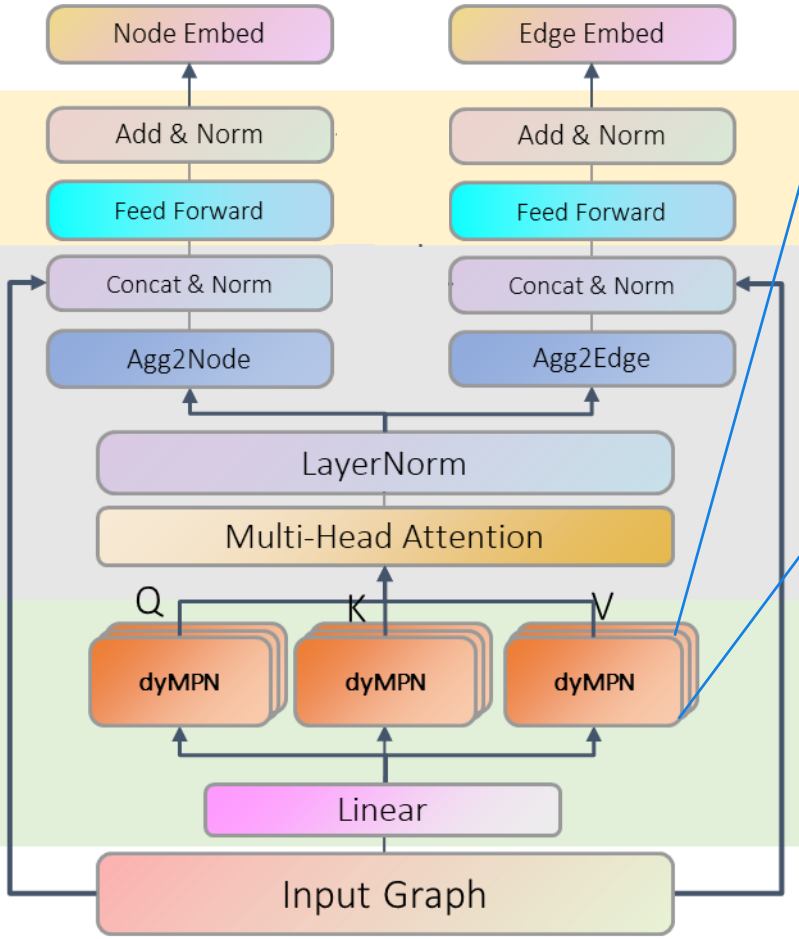
Carefully designed self-supervised tasks in node, edge & graph levels → enables → Rich structural and semantic information of molecules from enormous unlabeled data

GTransformer Architecture

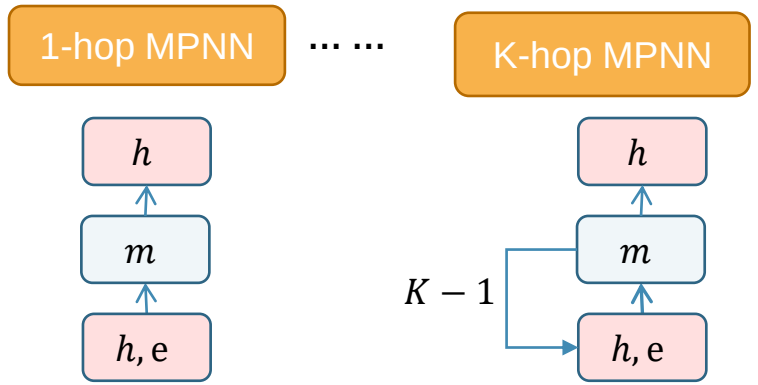
- Output for both node embedding and edge embeddings.

- **Multi-Head Attention**: model global interaction between nodes/edges.
- **Long-range Residual Connection**: alleviating the vanishing gradient and over-smoothing.

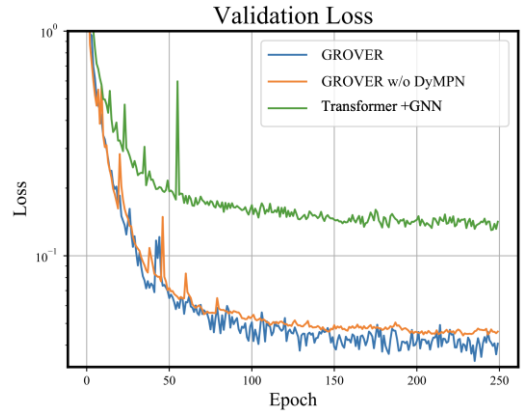
- **MPNN**: Extract local structural information of graphs.
- **dyMPN**: Randomize the message passing hops for the dynamic receptive field modeling.



Sample a random-hop MPNN at each iteration



Better generalization



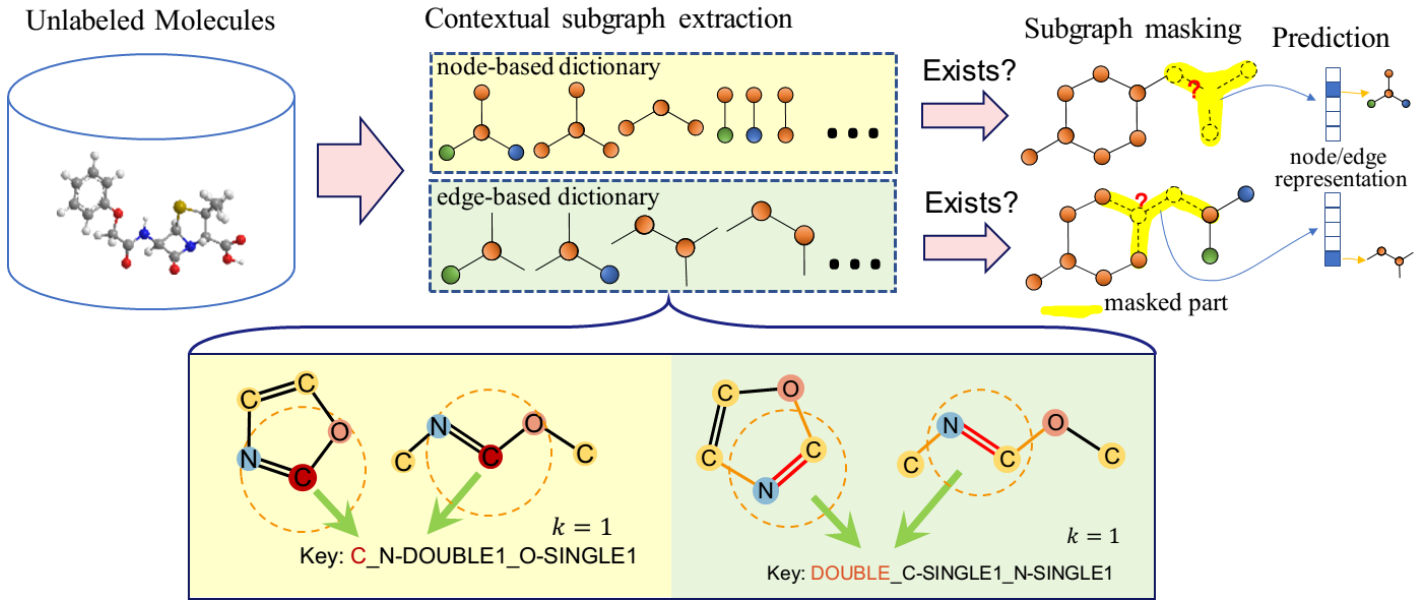
Self-supervised Tasks Construction

Good self-supervision task shall have *reliable* and *cheap* prediction target

Node/edge level task:
contextual property prediction

target reflects contextual property: recurrent statistical properties of local subgraph

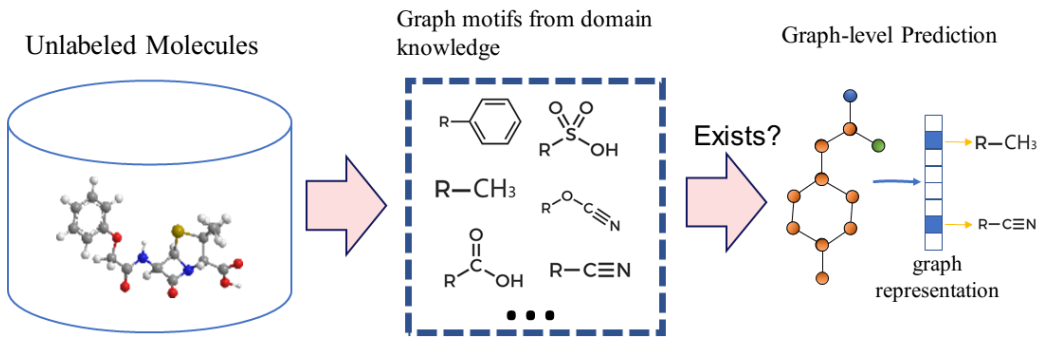
A multi-class classification problem



Graph level task:
motif prediction

Motifs: recurrent sub-graphs, such as functional groups.

A multi-label classification problem



Experimental Results

Pre-training GROVER with 100M params on 10M unlabelled molecules → Verifying on down-stream tasks with fine-tuning → Significant improvement (more than 6% on average) over SOTA models on 11 challenging benchmarks

Classification (Higher is better)						
Dataset # Molecules	BBBP 2039	SIDER 1427	ClinTox 1478	BACE 1513	Tox21 7831	ToxCast 8575
TF_Robust [40]	$0.860_{(0.087)}$	$0.607_{(0.033)}$	$0.765_{(0.085)}$	$0.824_{(0.022)}$	$0.698_{(0.012)}$	$0.585_{(0.031)}$
GraphConv [24]	$0.877_{(0.036)}$	$0.593_{(0.035)}$	$0.845_{(0.051)}$	$0.854_{(0.011)}$	$0.772_{(0.041)}$	$0.650_{(0.025)}$
Weave [23]	$0.837_{(0.065)}$	$0.543_{(0.034)}$	$0.823_{(0.023)}$	$0.791_{(0.008)}$	$0.741_{(0.044)}$	$0.678_{(0.024)}$
SchNet [45]	$0.847_{(0.024)}$	$0.545_{(0.038)}$	$0.717_{(0.042)}$	$0.750_{(0.033)}$	$0.767_{(0.025)}$	$0.679_{(0.021)}$
MPNN [13]	$0.913_{(0.041)}$	$0.595_{(0.030)}$	$0.879_{(0.054)}$	$0.815_{(0.044)}$	$0.808_{(0.024)}$	$0.691_{(0.013)}$
DMPNN [63]	$0.919_{(0.030)}$	$0.632_{(0.023)}$	$0.897_{(0.040)}$	$0.852_{(0.053)}$	$0.826_{(0.023)}$	$0.718_{(0.011)}$
MGCN [30]	$0.850_{(0.064)}$	$0.552_{(0.018)}$	$0.634_{(0.042)}$	$0.734_{(0.030)}$	$0.707_{(0.016)}$	$0.663_{(0.009)}$
AttentiveFP [61]	$0.908_{(0.050)}$	$0.605_{(0.060)}$	$0.933_{(0.020)}$	$0.863_{(0.015)}$	$0.807_{(0.020)}$	$0.579_{(0.001)}$
N-GRAM [29]	$0.912_{(0.013)}$	$0.632_{(0.005)}$	$0.855_{(0.037)}$	$0.876_{(0.035)}$	$0.769_{(0.027)}$	-[4]
HU. et.al[18]	$0.915_{(0.040)}$	$0.614_{(0.006)}$	$0.762_{(0.058)}$	$0.851_{(0.027)}$	$0.811_{(0.015)}$	$0.714_{(0.019)}$
$\text{GROVER}_{\text{base}}$	$0.936_{(0.008)}$	$0.656_{(0.006)}$	$0.925_{(0.013)}$	$0.878_{(0.016)}$	$0.819_{(0.020)}$	$0.723_{(0.010)}$
$\text{GROVER}_{\text{large}}$	$\mathbf{0.940}_{(0.019)}$	$\mathbf{0.658}_{(0.023)}$	$\mathbf{0.944}_{(0.021)}$	$\mathbf{0.894}_{(0.028)}$	$\mathbf{0.831}_{(0.025)}$	$\mathbf{0.737}_{(0.010)}$

★ Code and models will be released soon.