Triplet Interaction Improves Graph Transformers

Accurate Molecular Graph Learning with Triplet Graph Transformers

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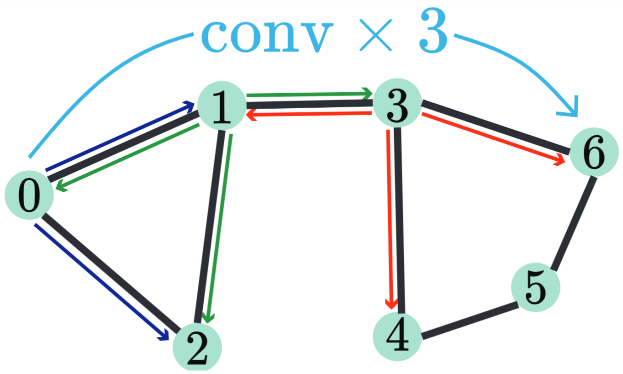
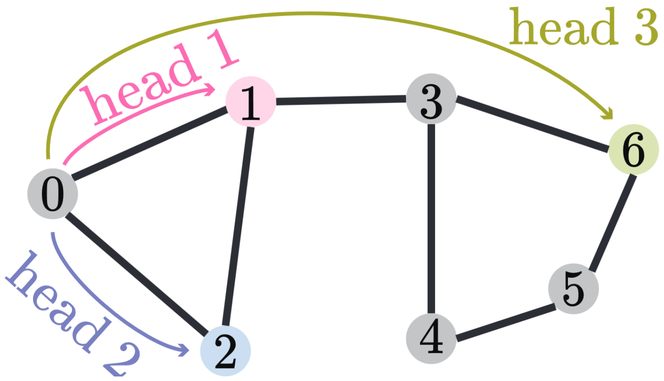
Graph Transformers vs. GCNs

- Long-distance, dynamic interaction
  - Not limited to neighbors
  - Attention weights are determined by the network
- Limitations of hand-crafted encodings/features
  - Positional-encoding based GTs (e.g., Graphormer)
    - Structural understanding ≈ as good as the used positional encoding
  - Geometric GTs (e.g., Equiformer)
    - Geometric understanding ≈ as good as the used geometric features
- **Goal: let the network form its <u>own</u> geometry / structure**



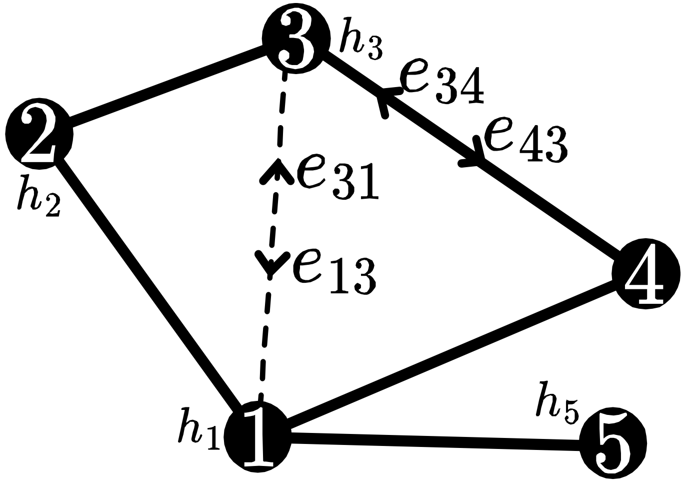
(a) Convolution



(b) Self-attention

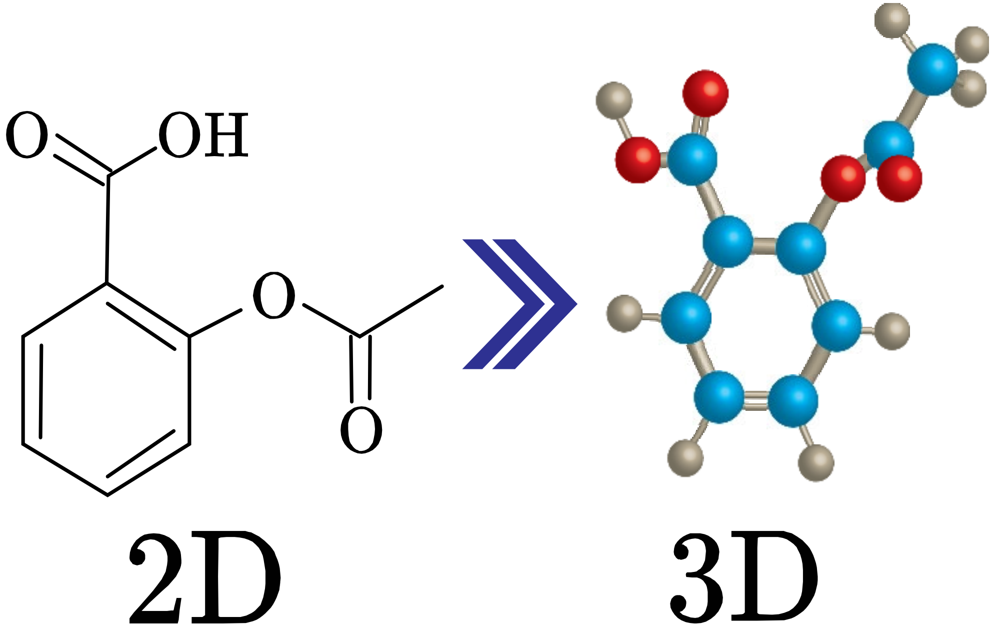
Graph Structure and Pair Representations

- Pairs → directed existing/non-existing edges
  - e.g., 3→4, 4→3, 3→1, 1→3
- For graphs pair representations (e_{ij}) can be as important as node representations (h_i)
  - Allow the structure of the graph to evolve over layers
  - Refine structure/topology internally in case of inaccuracies
  - Directly perform pair related task
    - Link prediction
    - Edge classification
    - Distance Prediction
- EGT (Edge-augmented Graph Transformer)
  - Make pairs (2-tuple) first class citizen, just like nodes
  - Break free of the input graph topology
  - **Limitation: only 2nd-order interaction**



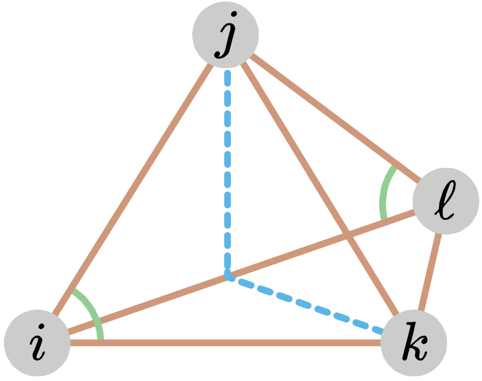
3D Molecular Geometry

- 2D
  - Bonds + Atoms (i.e., chemical formula)
- 3D
  - Coordinates
  - Often interatomic distances is enough
- 3D shape directly dictates molecular property
  - But costly to compute (QM simulation required)
- **Train a model: 2D→3D**
  - **i.e., predict the molecular geometry**



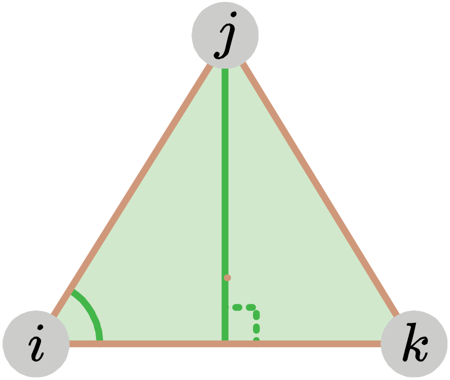
K-order interaction vs. K-order features

- **2nd Order (i, j): Pairwise distances**
- **3rd Order (i, j, k): Angles, area of triangles, etc.**
- **4th Order (i, j, k, ℓ): Dihedral angles, volume of tetrahedrons, etc.**



We need either higher order interactions or higher order features for full geometric understanding

- **Crucial for 3D geometry prediction**
- **Our contribution: Third order interaction**
  - Pairs $(i, j), (j, k), (i, k)$ within the 3-tuple (i, j, k)



Why higher order interactions?

- Using higher order features such as angles implies
  - An initial estimate of geometry is required
  - Features are only as accurate as the estimate
  - Specialized for geometric graphs only
- Using higher order interactions implies
  - No estimate of geometry is required, a simple graph is enough
  - The network can form representations that are more refined than the initial estimate
  - Applicable to both geometric and non-geometric graphs

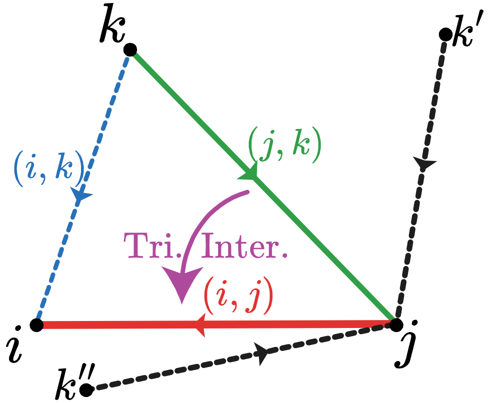
- **Our work improves geometric expressivity without losing generality**
- **We break free from the inaccuracies of the initial geometry (when given)**

Our Contribution

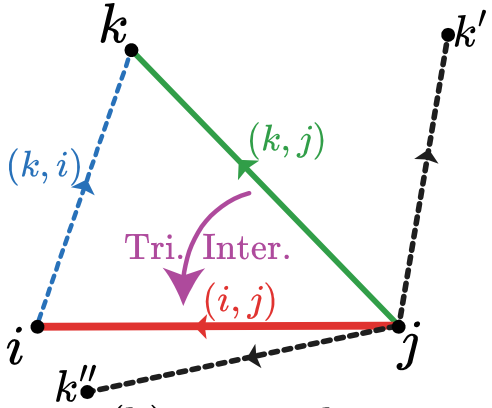
Triplet Graph Transformer

Triplet Interaction within a 3-tuple (i, j, k)

- Participants (inward): $(i, j), (j, k), (i, k)$
- (i, j) gathers information from (j, k)
- Without triplet interaction
  - $(j, k) \rightarrow j \rightarrow (i, j)$
  - Bottleneck at node j
- With triplet interaction
  - $(j, k) \xrightarrow{(i,k)} (i, j)$
- (i, k) also participates in this process
- Similarly: outward update



(a) inward



(b) outward

Triplet Interaction within a 3-tuple (i, j, k)

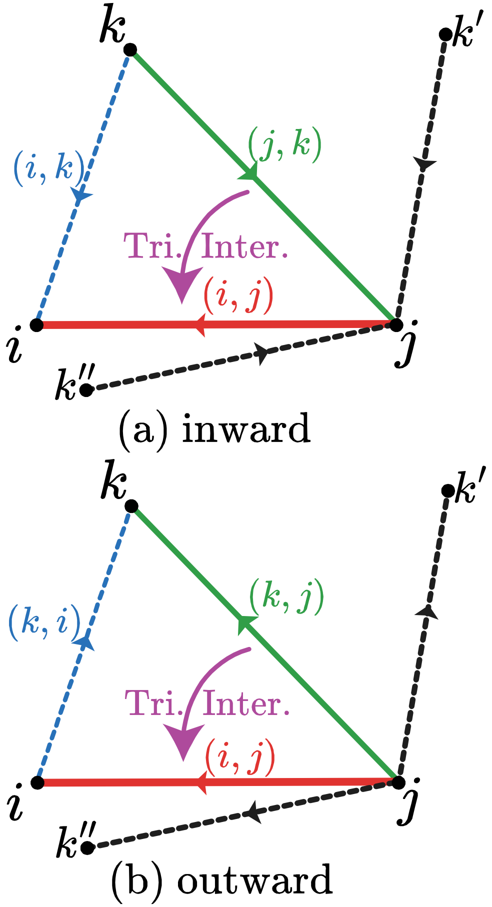
- Two mechanisms
  - Triplet Attention (TGT-At)

$$\mathbf{o}_{ij}^{\text{in}} = \sum_{k=1}^{N} a_{ijk}^{\text{in}} \mathbf{v}_{jk}^{\text{in}} \quad ; \quad a_{ijk}^{\text{in}} = \text{softmax}_k\left(\frac{1}{\sqrt{d}} \mathbf{q}_{ij}^{\text{in}} \cdot \mathbf{p}_{jk}^{\text{in}} + b_{ik}^{\text{in}}\right) \times \sigma(g_{ik}^{\text{in}})$$

    - More expressive, $O(N^3)$
  - Triplet Aggregation (TGT-Ag)

$$\mathbf{o}_{ij}^{\text{in}} = \sum_{k=1}^{N} a_{ik}^{\text{in}} \mathbf{v}_{jk}^{\text{in}} \; ; \qquad a_{ik}^{\text{in}} = \text{softmax}_k(b_{ik}^{\text{in}}) \times \sigma(g_{ik}^{\text{in}})$$

    - More efficient, $O(N^{2.37})$

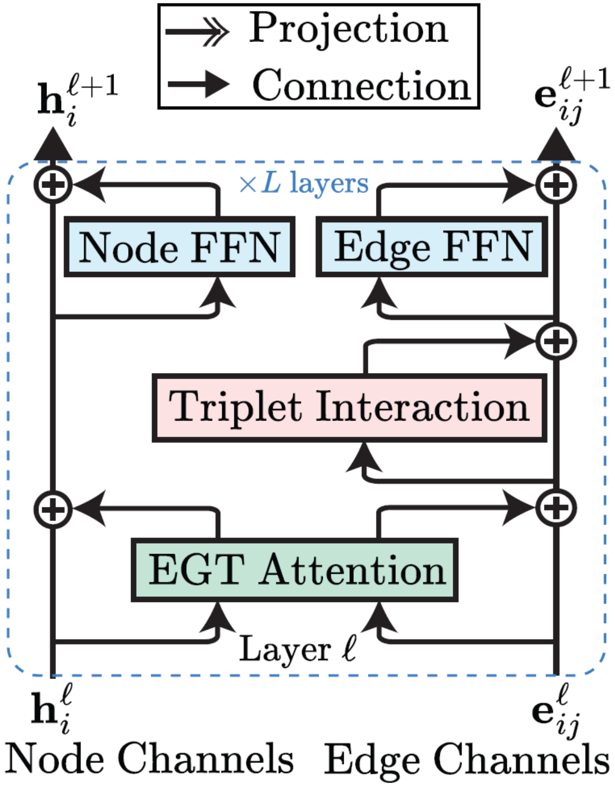


(a) inward

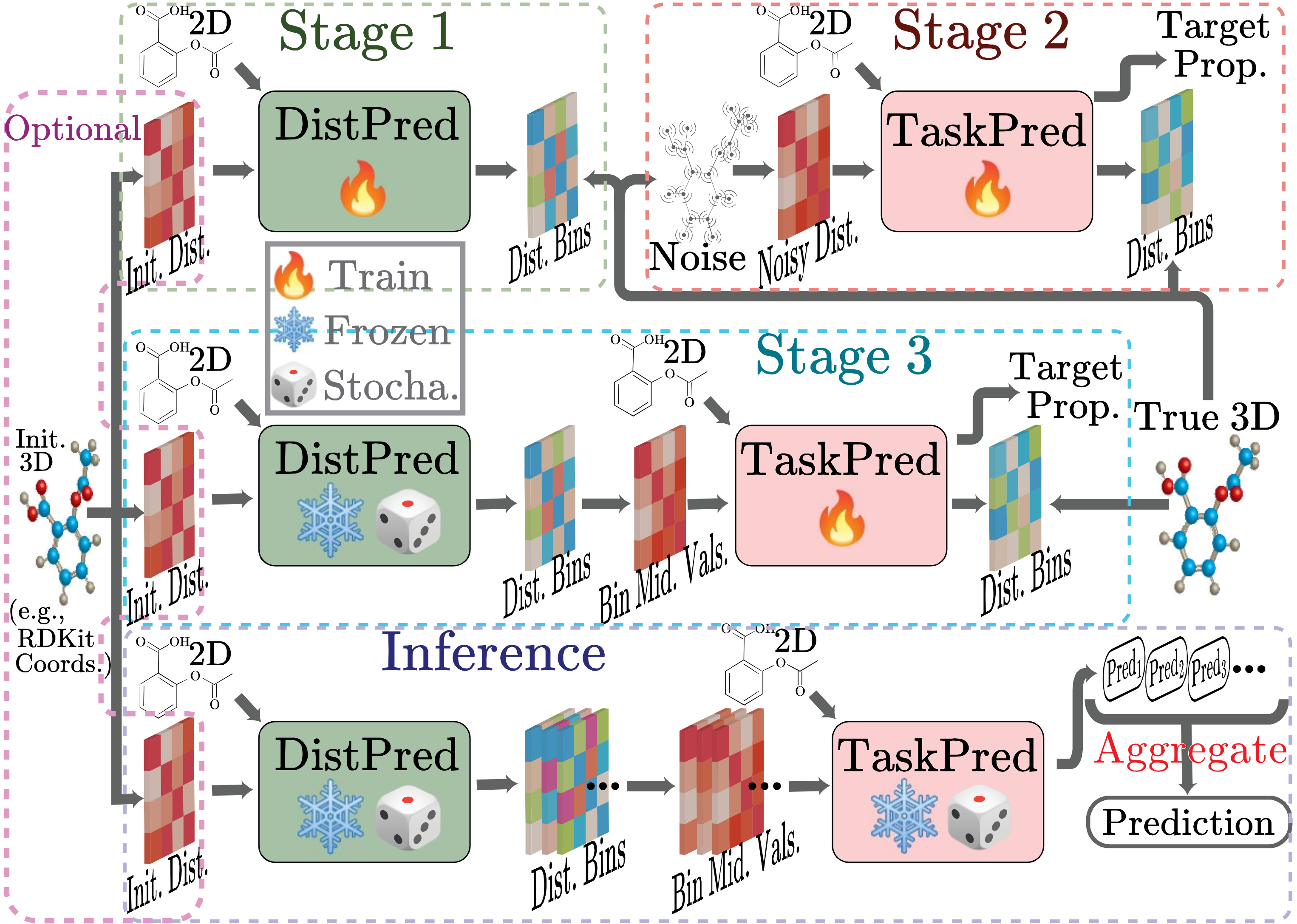
(b) outward

Network Architecture

- EGT (our previous work)
  - Node representations → Node channels
  - Pair representations → Edge channels
  - Only 2nd order interactions
- Triplet interaction (TGT)
  - Update pair representations based on each other
  - 3rd order interactions
- Pair embeddings are directly used for predicting (binned) pairwise atomic distances
- Useful for other geometric tasks as well (e.g., Traveling Salesman Problem)



Training and Inference

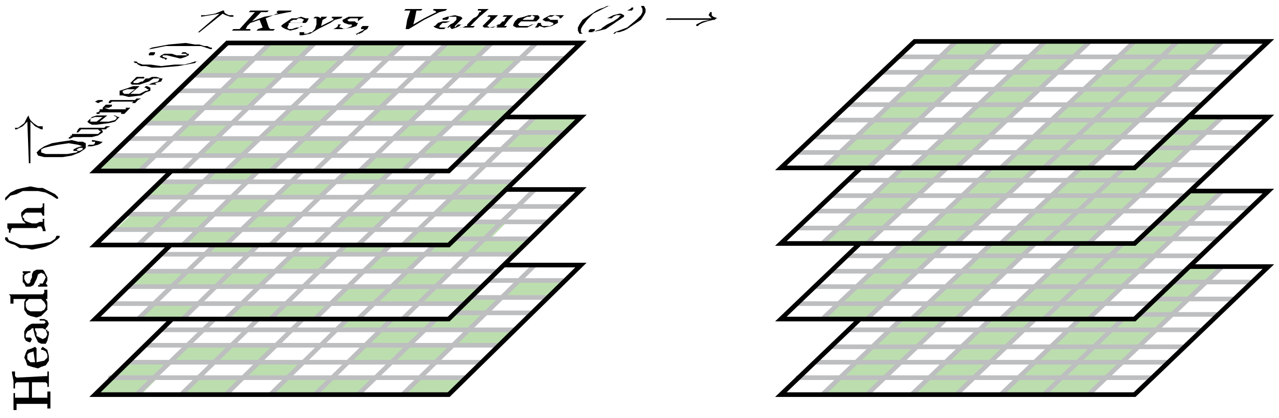


Other Contributions

- Locally smoothed 3D noise for pretraining the task predictor

$$\mathbf{r}'_i = \mathbf{r}_i + \sum_{j=1}^{N} e^{-\frac{\|\mathbf{r}_i - \mathbf{r}_j\|}{\nu}} \mathbf{u}_j; \text{ where } \mathbf{u}_j \sim \mathcal{N}(0, \sigma^2 \mathbf{I})$$

- Source dropout: Stronger regularization for graph transformers



(a)Attention Dropout **(b)Source Dropout**

Key Contributions

- Triplet Graph Transformer (TGT)
  - Novel triplet interaction mechanisms for direct pair-to-pair communication
  - Accurately models geometry in graphs
- Two-stage model
  - Separate distance and task predictors
  - Eliminates need for initial 3D coordinates
- Three-stage training procedure and stochastic inference
  - Significantly improves training efficiency and predictive performance
- TGT for graph learning
  - Traveling Salesman Problem

Quantum Chemistry (Large-scale)

- Predict in absence of ground truth 3D

(a) PCQM4Mv2 (Molecules)

Model	MAE↓ (meV)
EGT	86.2
Transformer-M	78.2
Uni-Mol+ (+RDKit)	70.5
TGT-At	69.8
TGT-At (+RDKit)	**68.3**

(b) OC20 IS2RE (Crystals)

	MAE↓	EwT↑
Model	**(meV)**	**(%)**
SphereNet	618.8	3.32
EquiFormer	466	5.66
Uni-Mol+	**414.3**	8.23
TGT-At	**414.7**	**8.3**

Quantum Chemistry (Transfer Learning)

- Ground truth 3D is provided
- Fine-tuned from PCQM4Mv2

(a) QM9 (Molecules)

Method	μ	α	ϵ_H	ϵ_L	$\Delta\epsilon$	**ZPVE**	C_v
3D Infomax	0.034	0.075	29.8	25.7	48.8	1.67	0.033
SphereNet	0.025	0.053	22.8	18.9	31.1	**1.12**	0.024
Equiformer	**0.011**	0.046	15	14	30	1.26	0.023
Transformer-M	0.037	0.041	17.5	16.2	27.4	1.18	0.022
TGT-Ag	0.025	**0.040**	**9.9**	**9.7**	**17.4**	1.18	**0.020**

Molecular Property (Transfer Learning)

- Non-quantum property prediction and drug discovery
- Use frozen (not finetuned) distance predictor from PCQM4Mv2
  - Provides more accurate 3D information than RDKIT

MOLPCBA (Property)

Model	AP↑ (%)
PHC-GNN	29.47
Graphormer	31.40
TGT-Ag+RDKit	31.44
TGT-Ag+DP	**31.67**

LITPCBA (Drugs)

Model	ROC-AUC↑ (%)
GEM	78.4
GEM-2+RDKit	**81.5**
EGT+RDKit	81.2
EGT+DP	**81.5**

Traveling Salesman Problem(Graph Learning)

- Points on a 2D plane
- Edge classification

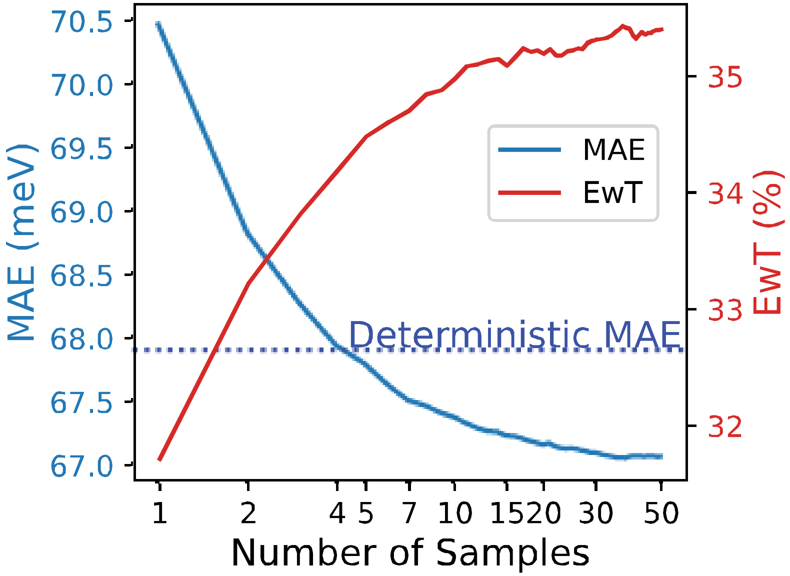
TSP

Model	**F1↑ (%)**
GatedGCN	83.8
ARGNP	85.5
EGT	85.3
TGT-Agx4	**87.1**

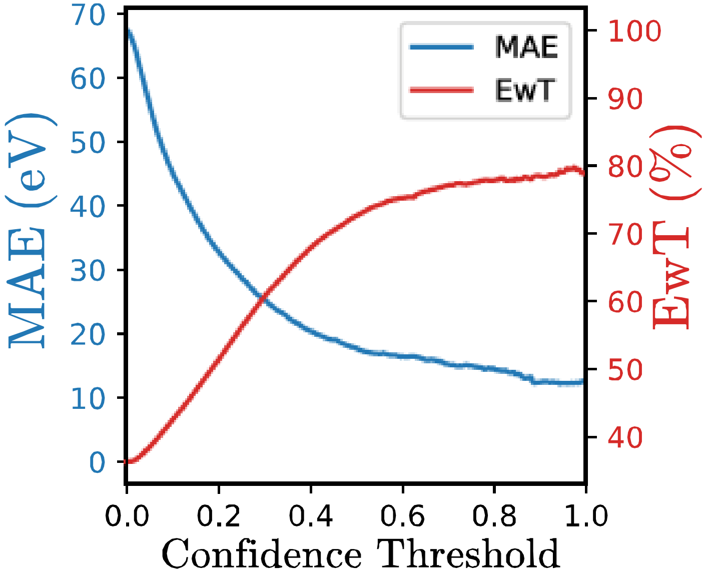
- Demonstrate the generality of our model

Merits of Stochastic Inference

- Outperforms deterministic inference with only ~4 samples
- Higher confidence implies higher accuracy



#Samples vs Performance



Confidence vs Performance

Future Work

- Explore use of triplet interaction for other graph learning tasks
    - Molecule and conformation generation
    - Link prediction
    - Combinatorial Problem
    - Self-supervised/semi-supervised/generative graph learning
- Improve compute and memory efficiency of triplet interaction
    - Sparsity
    - Linearity

Thank You

Please check out our paper for more details.

Paper: https://arxiv.org/abs/2402.04538

Implementation: https://github.com/shamim-hussain/tgt