Transformers over Directed Acyclic Graphs

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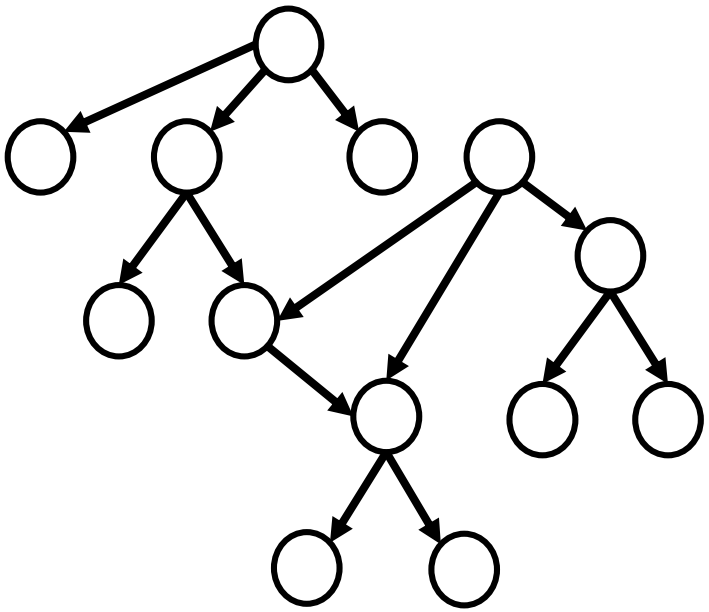
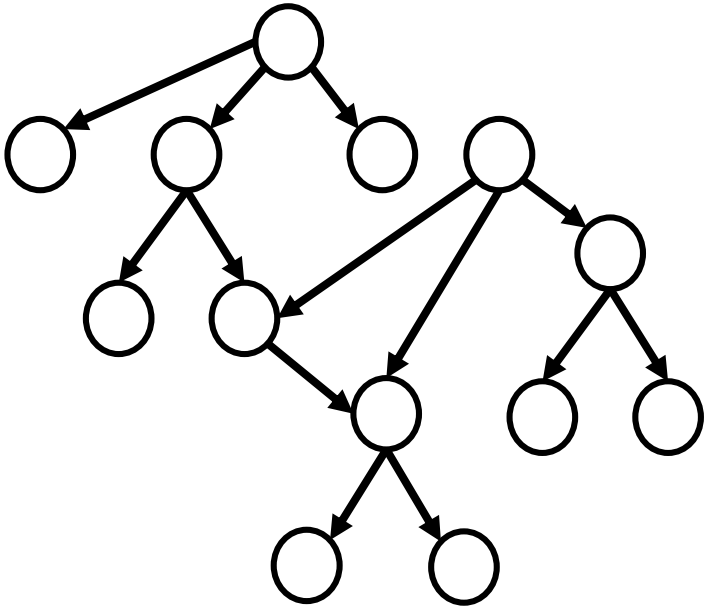
Directed Acyclic Graphs (DAGs)



- Directed acyclic graph (DAG) :

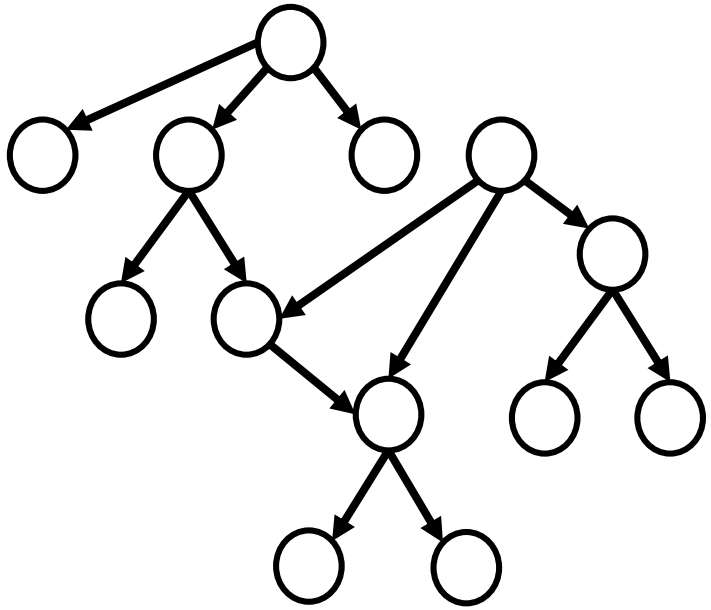
  a directed graph without directed cycles.

Directed Acyclic Graphs (DAGs)



- Can define a unique strong partial order $\preccurlyeq$ on the node set V,
- such that, for all pairs of nodes $u, v \in V$, $u \preccurlyeq v$ if and only if there is a directed path from u to v.

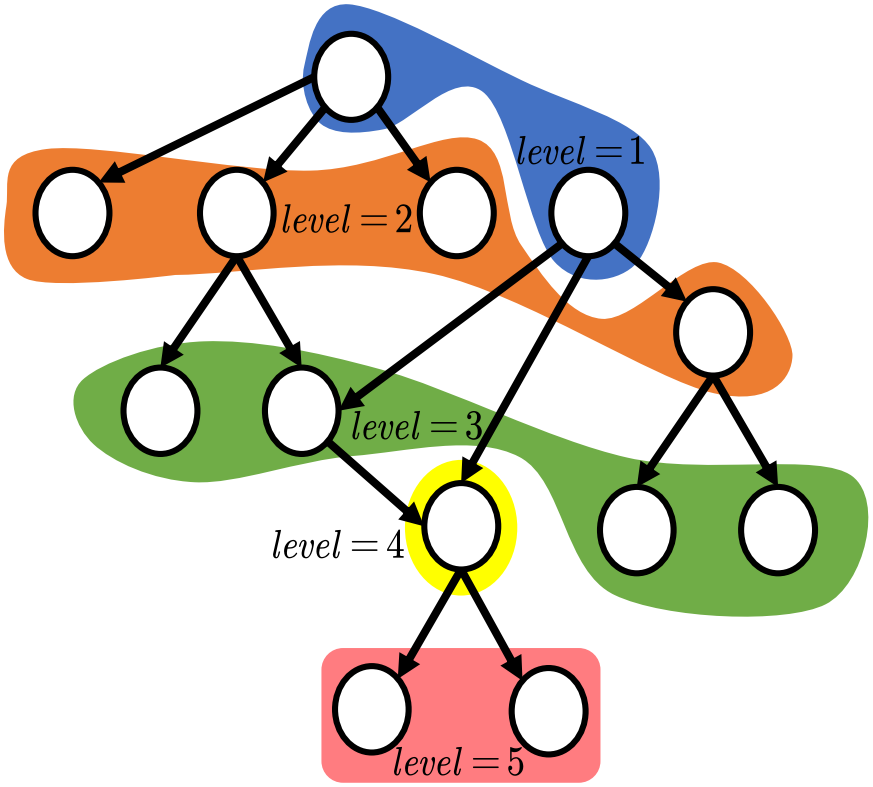
Directed Acyclic Graphs (DAGs)



- DAGs appear across various domains:

Source code, logical formulas, probabilistic graphical models, neural architectures (NNs), citation networks.

SOTA: Recursive neural networks over DAGs



- The node embedding is computed by iterating over the DAG nodes in an asynchronous way.
- At every node v, information is aggregated from the direct predecessors.

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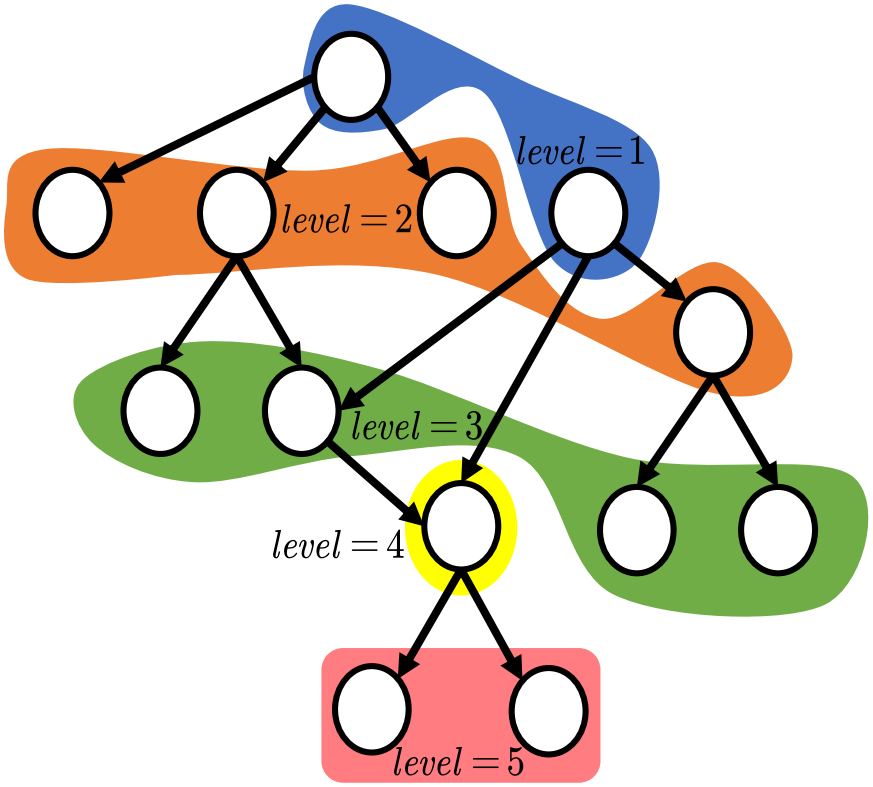

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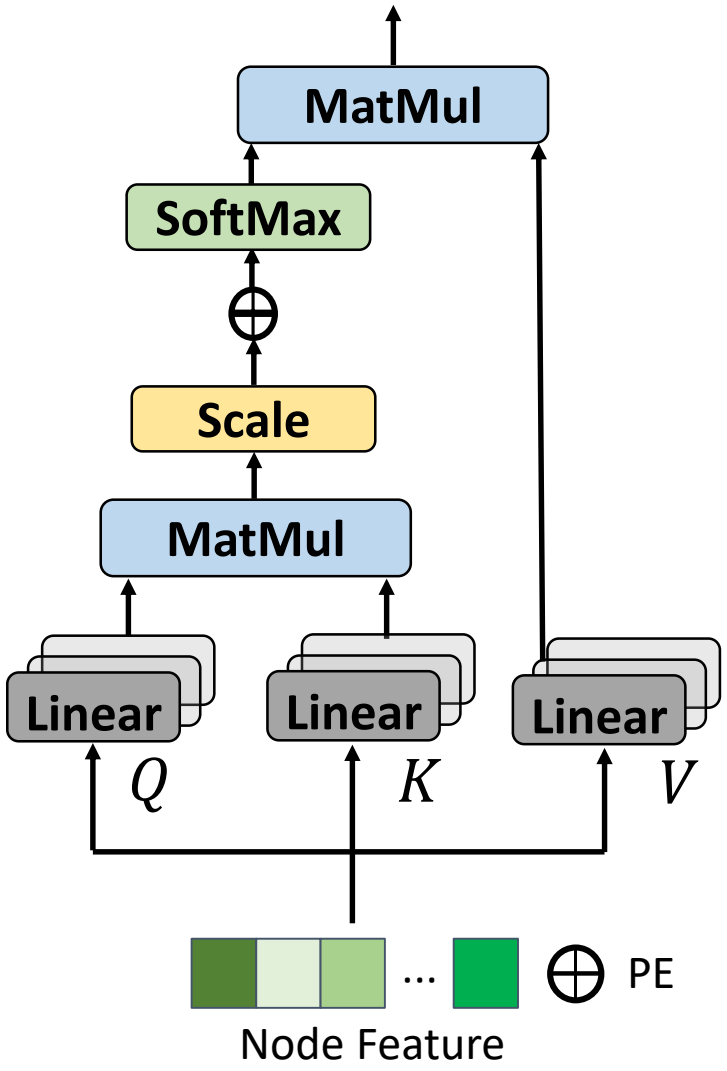
These recursive DAG models are yielding SOTA results, but their asynchronous nature leads to very slow performance.

Transformers on Graphs

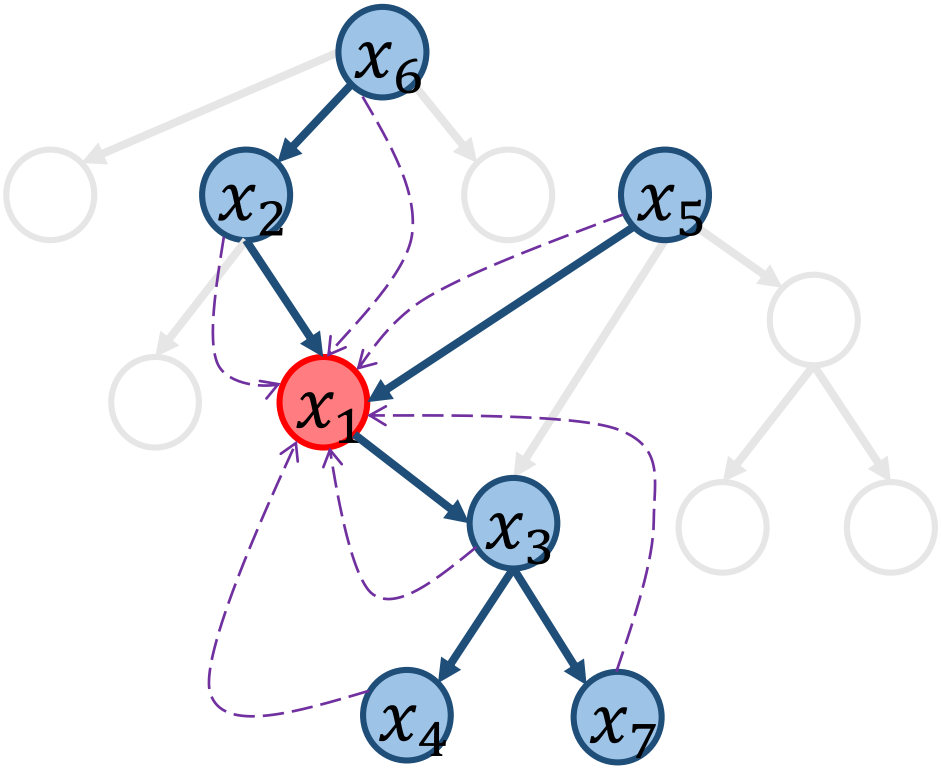
Note: DAGs are sequential in nature! And the parallelism of Transformers actually matches well the shortcomings of DAG neural networks.



Attention based on DAG Reachability (DAGRA)

- We restrict the receptive field of each node based on reachability:

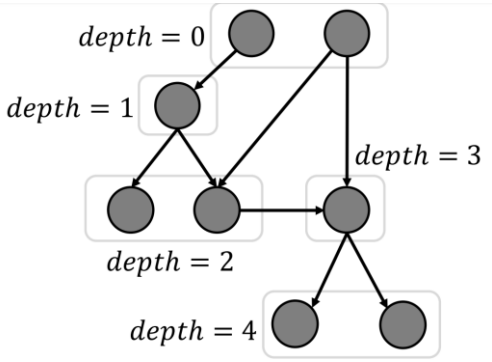
$$N(v) = \{(u,v) \in \leqslant\} \cup \{(v,u) \in \leqslant\}$$



PEs based on DAG Depth (DAGPE)

- Our positional encoding encodes (only) node depth.

$$depth(v) = \begin{cases} 0 & \text{if } v \text{ is a source node} \\ 1 + \max\limits_{(u,v)\in E} depth(u) & \text{otherwise} \end{cases}$$



$$PE_{(v,2i)} = \sin\left(\frac{depth(v)}{10000^{\frac{2i}{d}}}\right)$$

$$PE_{(v,2i+1)} = \cos\left(\frac{depth(v)}{10000^{\frac{2i}{d}}}\right)$$

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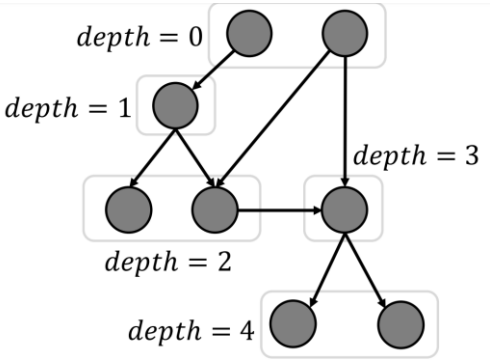

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- Combining DAGRA and DAGPE, we obtain DAG Attention:

$$\text{Attention}(x_v) = \sum_{u\in N(v)} \frac{\kappa(x_v + PE_v, x_u + PE_u)}{\sum\limits_{w\in N(v)} \kappa(x_v + PE_v, x_w + PE_w)} f(x_u)$$

DAG Attention

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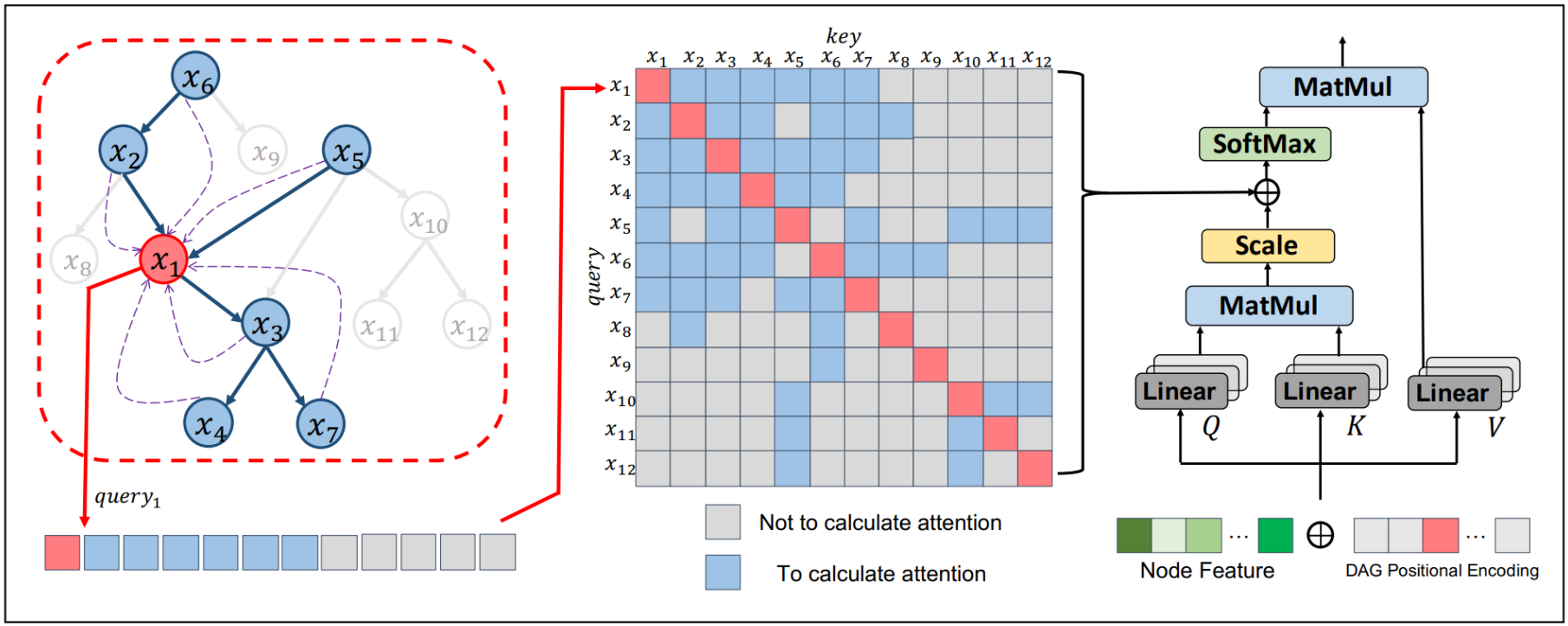
This can be flexibly applied on top of existing graph transformers and tailor them to DAGs.

DAG Attention

- DAG attention using a mask that masks out node pairs based on the DAG reachability relation. $O(|V|^2 d)$



- DAG Attention using Message Passing $O(|V| \times N \times d)$

Aggregating messages using the *torch* <u>*scatter add*</u> method

Evaluation

Table 2: **Code graph classification** on ogbg-code2. The baseline results were taken from the OGB leaderboard.

Model	Valid F1 (%)	Test F1 (%)	Time(epoch)
GIN	13.7 ± 0.2	14.9 ± 0.2	181s
GCN	14.0 ± 0.2	15.1 ± 0.2	127s
GIN-Virtual	14.4 ± 0.3	15.8 ± 0.2	155s
GCN-Virtual	14.6 ± 0.1	16.0 ± 0.2	198s
GAT	14.4 ± 0.2	15.7 ± 0.2	134s
PNA	14.5 ± 0.3	15.7 ± 0.3	427s
DAGNN	16.1 ± 0.4	17.5 ± 0.5	6018s
PACE	16.3 ± 0.3	17.8 ± 0.2	2410s
Transformer	15.5 ± 0.2	16.7 ± 0.2	1817s
DAG+Transformer	**17.4** ± 0.1	**18.8** ± 0.2	591s
GraphTrans	16.6 ± 0.1	18.3 ± 0.2	1117s
DAG+GraphTrans	**17.0** ± 0.2	**18.7** ± 0.2	526s
GraphGPS	17.4 ± 0.2	18.9 ± 0.2	1919s
DAG+GraphGPS	**17.6** ± 0.1	**19.3** ± 0.2	608s
SAT (SOTA)	17.7 ± 0.2	19.4 ± 0.3	2437s
DAG+SAT	**18.5** ± 0.1	**20.2** ± 0.2	681s

Table 3: **Node classification** results for the self-citation dataset; AP (%) and ROC-AUC (%).

Model	AP ↑	ROC-AUC ↑
GIN	57.7 ± 1.8	79.7 ± 0.2
GCN	58.8 ± 0.4	79.9 ± 0.2
GIN-Virtual	57.4 ± 1.2	79.5 ± 0.4
GCN-Virtual	58.9 ± 0.2	80.0 ± 0.1
GAT	55.3 ± 3.7	77.9 ± 1.4
PNA	62.4 ± 0.7	81.0 ± 0.4
DAGNN	61.2 ± 0.6	81.0 ± 0.3
PACE	52.1 ± 1.8	75.9 ± 0.7
Transformer	56.8 ± 1.8	78.7 ± 0.3
DAG+Transformer	**63.8** ± 0.8	**82.2** ± 0.5
GraphGPS	61.6 ± 2.6	**81.3** ± 0.6
DAG+GraphGPS	**63.5** ± 1.2	80.8 ± 0.5
SAT	59.8 ± 1.7	79.8 ± 0.7
DAG+SAT	**62.7** ± 1.5	**80.6** ± 0.7
NodeFormer	39.6 ± 0.6	69.4 ± 0.3
DAG+NodeFormer	**64.9** ± 0.8	**81.7** ± 0.8

Evaluation

Table 4: **Node classification accuracy** (%).The baseline results were taken from [Wu et al., 2022].

Model	Cora	Citeseer	Pubmed
GCN	87.06 ± 0.34	75.75 ± 0.37	88.16 ± 0.14
GAT	86.85 ± 0.30	75.92 ± 0.26	86.90 ± 0.22
MixHop	87.59 ± 0.52	73.64 ± 0.73	89.32 ± 0.25
IDGL	87.88 ± 0.34	74.32 ± 0.51	89.22 ± 0.14
LDS-GNN	87.82 ± 0.62	75.22 ± 0.23	OOM
PACE	79.47 ± 0.63	73.65 ± 1.23	OOM
Transformer	75.92 ± 0.86	72.23 ± 1.06	OOM
DAG+Transformer	**87.80** ± 0.53	**74.42** ± 0.22	**89.01** ± 0.13
SAT	75.18 ± 0.62	74.88 ± 0.73	OOM
DAG+SAT	**87.48** ± 0.37	**76.64** ± 0.26	**89.17** ± 0.15
NodeFormer	88.80 ± 0.26	76.33 ± 0.59	89.32 ± 0.25
DAG+NodeFormer	**90.49** ± 0.17	**78.24** ± 0.33	**89.44** ± 0.24

Table 5: **Regression.** Predictive performance of latent representations over NA.

Model	RMSE ↓	Pearson's r ↑
GCN	0.482 ± 0.003	0.871 ± 0.001
S-VAE	0.521 ± 0.002	0.847 ± 0.001
D-VAE	0.375 ± 0.003	0.924 ± 0.001
DAGNN	0.264 ± 0.004	0.964 ± 0.001
PACE	0.254 ± 0.002	0.964 ± 0.001
Transformer	0.285 ± 0.004	0.957 ± 0.001
GT	0.275 ± 0.003	0.961 ± 0.001
DAG+Transformer	**0.253** ± 0.002	**0.966** ± 0.001
GraphGPS	0.306 ± 0.004	0.950 ± 0.001
DAG+GraphGPS	**0.267** ± 0.005	**0.964** ± 0.001
SAT	0.298 ± 0.003	0.952 ± 0.001
DAG+SAT	**0.262** ± 0.004	**0.964** ± 0.001

- Over all datasets, our DAG attention makes the transformers outperform

  (1) the original transformers and

  (2) the neural networks tailored to DAGs.

Conclusions

Our proposal proves effective in:

- Making graph transformers generally outperform neural networks tailored to DAGs
- Improving SOTA graph transformer performance in terms of both quality and efficiency.

https://github.com/LUOyk1999/DAGformer

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Thanks for listening!

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