NEURAL INFORMATION PROCESSING SYSTEMS

PlanE: Representation Learning over Planar Graphs

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Expressiveness of GNNs

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GNNs learn **incomplete** graph invariants

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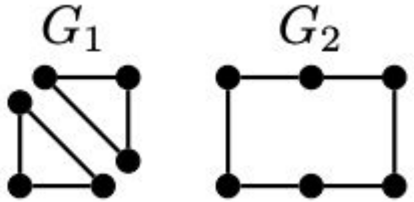
- MPNNs are bounded by 1-WL



Indistinguishable by **1-WL**

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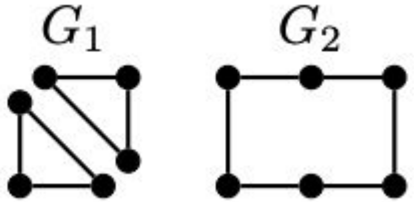

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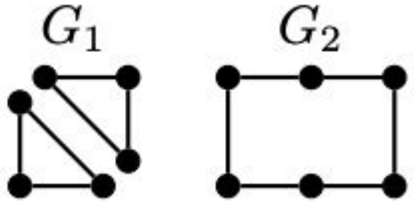

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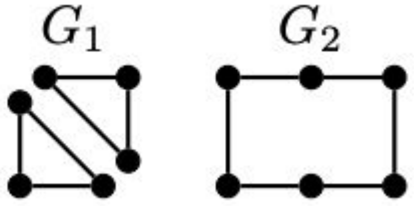

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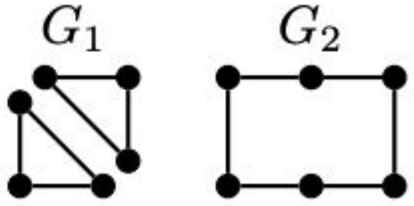


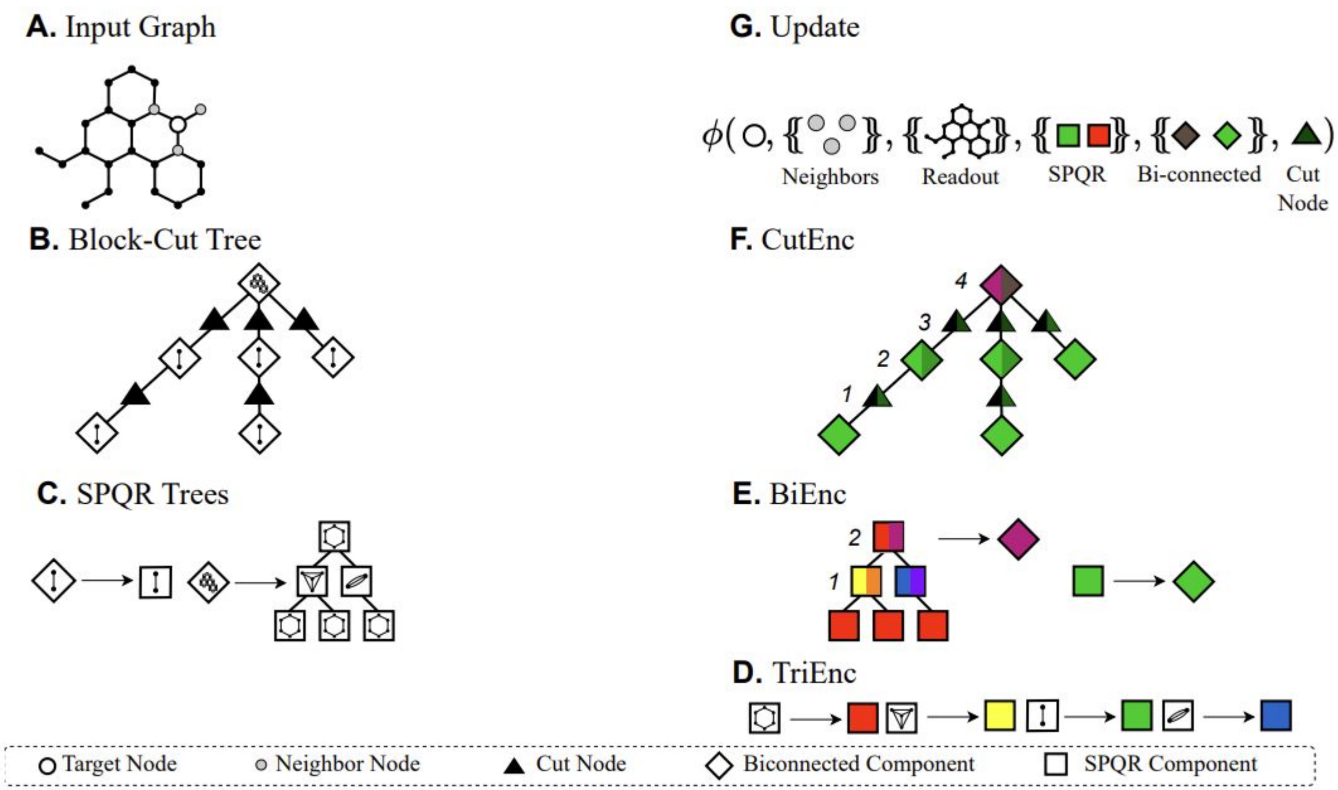
Indistinguishable by **1-WL**

Efficient algorithms for **planar** graph isomorphism exist

- **Weinberg, 1968**: Triconnected planar graphs in $O(|V|^2)$
- **Tarjan & Hopcroft, 1971**: Extend to all planar graphs

Can we efficiently learn **complete** planar graph invariants?

The PlanE framework



BasePlanE: a simple instance of PlanE

TriEnc: $$\widehat{\boldsymbol{h}}_C^{(\ell)} = \text{MLP}\left(\sum_{i=1}^{|\omega|} \text{MLP}\left(\boldsymbol{h}_{\omega[i]}^{(\ell-1)} \| \boldsymbol{p}_{\kappa[i]} \| \boldsymbol{p}_i\right)\right)$$

Encoder based on Weinberg's Algorithm

BiEnc: $$\widetilde{\boldsymbol{h}}_{\gamma_C}^{(\ell)} = \text{MLP}\left(\widehat{\boldsymbol{h}}_C^{(\ell)} + \sum_{C' \in \chi(C)} \text{MLP}\left(\widetilde{\boldsymbol{h}}_{\gamma_{C'}}^{(\ell)} \| \boldsymbol{p}_{\theta(C,C')}\right)\right)$$

Hierarchical Encoder over SPQR tree

CutEnc: $$\overline{\boldsymbol{h}}_{\delta_u}^{(\ell)} = \text{MLP}\left(\boldsymbol{h}_u^{(\ell-1)} + \sum_{B \in \chi(u)} \text{MLP}\left(\widetilde{\boldsymbol{h}}_B^{(\ell)} + \sum_{v \in \chi(B)} \overline{\boldsymbol{h}}_{\delta_v}^{(\ell)}\right)\right)$$

Hierarchical Encoder over Block-Cut tree

Update: Node-level by readout from each of these encoders.

BasePlanE: a simple Instance of PlanE

The runtime of one BasePlanE layer is $O(|V|d^2)$, with a **one-off** pre-processing of $O(|V|^2)$.

BasePlane requires a **logarithmic** number of layers:

Theorem 6.1. *For any planar graphs $G_1 = (V_1, E_1, \zeta_1)$ and $G_2 = (V_2, E_2, \zeta_2)$, there exists a parametrization of* BasePlanE *with at most $L = \lceil \log_2(\max\{|V_1|, |V_2|\}) \rceil + 1$ layers, which computes a complete graph invariant, that is, the final graph-level embeddings satisfy $\boldsymbol{z}_{G_1}^{(L)} \neq \boldsymbol{z}_{G_2}^{(L)}$ if and only if G_1 and G_2 are not isomorphic.*

Empirical Evaluation

Expressiveness experiments: EXP & P3R

We evaluate on EXP consisting of planar graphs representing SAT instances.

We propose a new synthetic dataset P3R:
Learning the equivalence classes of 3-regular planar graphs with 10 nodes.

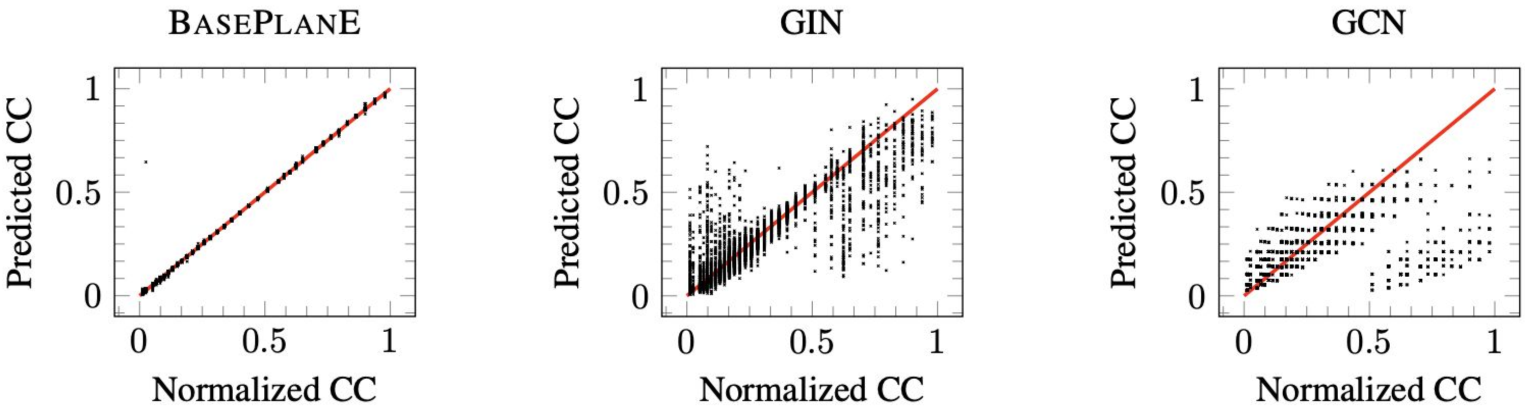
EXP	
Model	Accuracy (%)
GCN	50.0±0.00
GCN-RNI(N)	98.0±1.85
3-GCN	**99.7**±0.004
BASEPLANE	**100**±0.00

P3R	
Model	Accuracy (%)
GIN	11.1 ±0.00
PPGN	**100** ±0.00
BASEPLANE	**100** ±0.00

Structure detection experiment: $QM9_{CC}$

We evaluate the ability of detecting structural graph information without explicit access to the target structure. The task we propose is:

Given a subset of graphs from QM9, predict the graph-level **clustering coefficient** (CC).



Scalability experiment: TIGER

BasePlanE manages to scale to large planar graphs, while competitive models suffer from memory constraints.

		BasePlanE		PPGN		ESAN	
Dataset	#Nodes	Pre.	Train	Pre.	Train	Pre.	Train
TIGER-Alaska-2K	2000	9.8 sec	0.1 sec	3.4 sec	5.9 sec	4.6 sec	87.73 sec
TIGER-Alaska-10K	10000	50 sec	0.33 sec	OOM	OOM	OOM	OOM
TIGER-Alaska-93K	93366	3.7 h's	2.2 sec	OOM	OOM	OOM	OOM

Real-world dataset: QM9

Property	R-GIN		R-GAT		R-SPN		BASEPLANE
	base	+FA	base	+FA	$k = 5$	$k = 10$	
mu	2.64±0.11	2.54±0.09	2.68±0.11	2.73±0.07	2.16±0.08	2.21±0.21	**1.97**±0.03
alpha	4.67±0.52	2.28±0.04	4.65±0.44	2.32±0.16	1.74±0.05	1.66±0.06	**1.63**±0.01
HOMO	1.42±0.01	1.26±0.02	1.48±0.03	1.43±0.02	1.19±0.04	1.20±0.08	**1.15**±0.01
LUMO	1.50±0.09	1.34±0.04	1.53±0.07	1.41±0.03	1.13±0.01	1.20±0.06	**1.06**±0.02
gap	2.27±0.09	1.96±0.04	2.31±0.06	2.08±0.05	1.76±0.03	1.77±0.06	**1.73**±0.02
R2	15.63±1.40	12.61±0.37	52.39±42.5	15.76±1.17	10.59±0.35	10.63±1.01	**10.53**±0.55
ZPVE	12.93±1.81	5.03±0.36	14.87±2.88	5.98±0.43	3.16±0.06	**2.58**±0.13	2.81±0.16
U0	5.88±1.01	2.21±0.12	7.61±0.46	2.19±0.25	1.10±0.03	**0.89**±0.05	0.95±0.04
U	18.71±23.36	2.32±0.18	6.86±0.53	2.11±0.10	1.09±0.05	**0.93**±0.03	0.94±0.04
H	5.62±0.81	2.26±0.19	7.64±0.92	2.27±0.29	1.10±0.03	**0.92**±0.03	**0.92**±0.04
G	5.38±0.75	2.04±0.24	6.54±0.36	2.07±0.07	1.04±0.04	**0.83**±0.05	0.88±0.04
Cv	3.53±0.37	1.86±0.03	4.11±0.27	2.03±0.14	1.34±0.03	1.23±0.06	**1.20**±0.06
Omega	1.05±0.11	0.80±0.04	1.48±0.87	0.73±0.04	0.53±0.02	0.52±0.02	**0.45**±0.01

Real-world datasets: ZINC & MolHIV

Edge Features	ZINC(12k) No	ZINC(12k) Yes	ZINC(Full) Yes
GCN	0.278±0.003	-	-
GIN(-E)	0.387±0.015	0.252±0.014	0.088±0.002
PNA	0.320±0.032	0.188±0.004	0.320±0.032
ESAN	-	0.102±0.003	-
GSN	0.140±0.006	0.101±0.010	-
CIN	**0.115**±0.003	0.079±0.006	**0.022**±0.002
HIMP	-	0.151±0.006	0.036±0.002
(E-)BasePlanE	0.124±0.004	**0.076**±0.003	0.028±0.002

	MolHIV (OGB)
GCN	75.58±0.97
GIN	77.07±1.40
PNA	79.05±1.32
ESAN	78.00±1.42
GSN	80.39±0.90
CIN	**80.94**±0.57
HIMP	78.80±0.82
E-BasePlanE	80.04±0.50

Summary and outlook

We propose PlanE as a framework for planar representation learning, and we show that the BasePlanE instance can learn **complete** graph invariants over planar graphs.

We evaluate BasePlanE on synthetic datasets for **expressiveness** (EXP & P3R), **scalability** (TIGER-Alaska), and detecting **structural information** ($QM9_{CC}$).

We show that BasePlanE is competitive on **molecular** real-world datasets (QM9, Zinc, MolHIV).

Implementation: https://github.com/ZZYSonny/PlanE
Paper: https://arxiv.org/abs/2307.01180