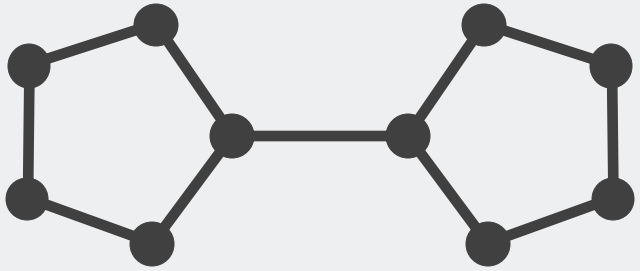
MAXIMALLY EXPRESSIVE GNNS FOR OUTERPLANAR GRAPHS

Franka Bause, Fabian Jogl, *Patrick Indri, Tamara Drucks, David Penz, Nils Kriege, Thomas Gärtner, Pascal Welke & Maximilian Thiessen*



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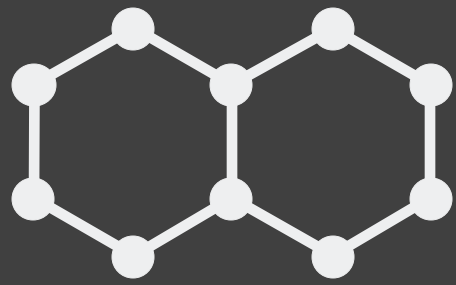

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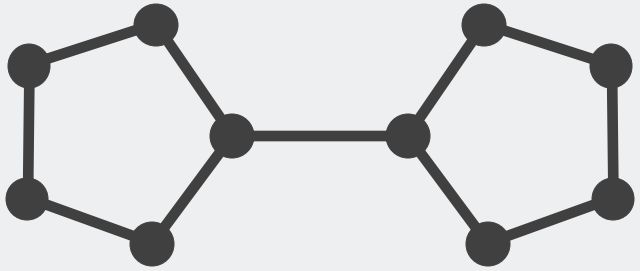

Bicyclopentyl

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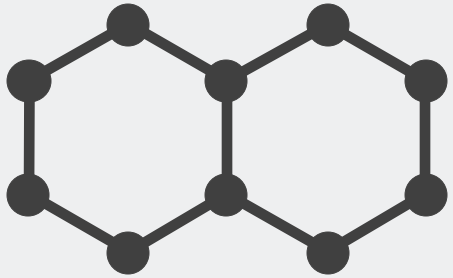

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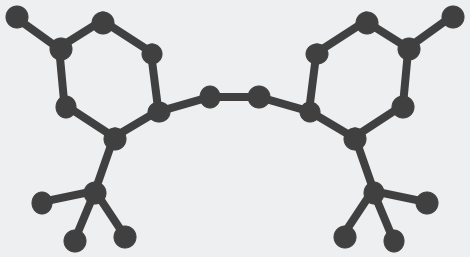
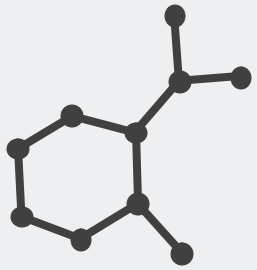
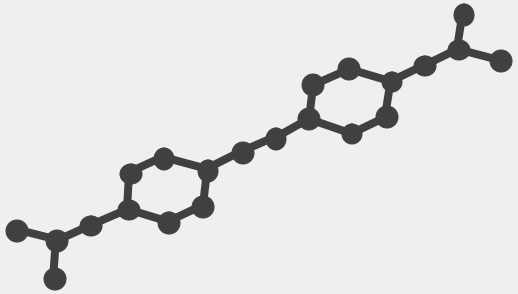
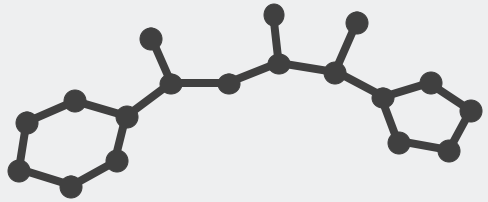
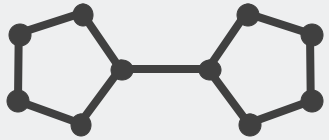
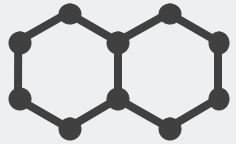
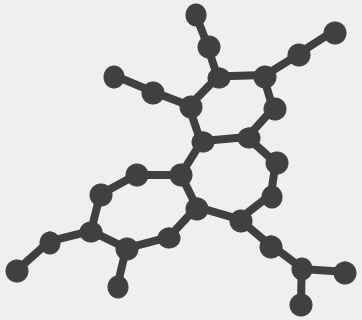
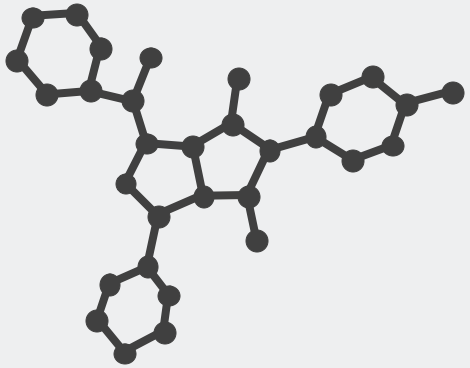
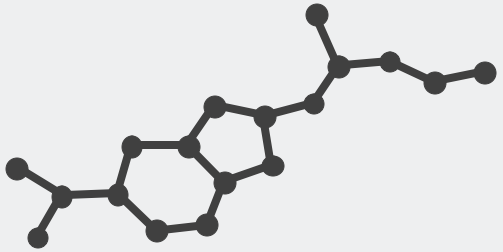
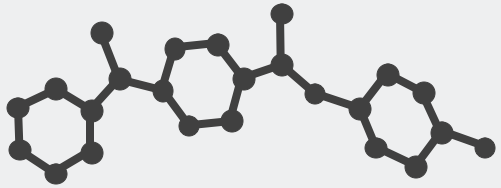
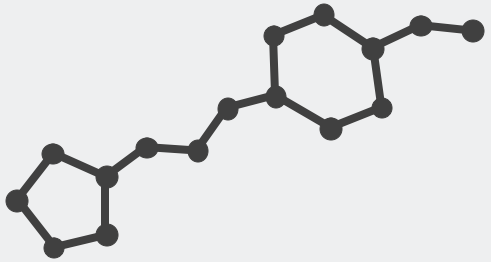
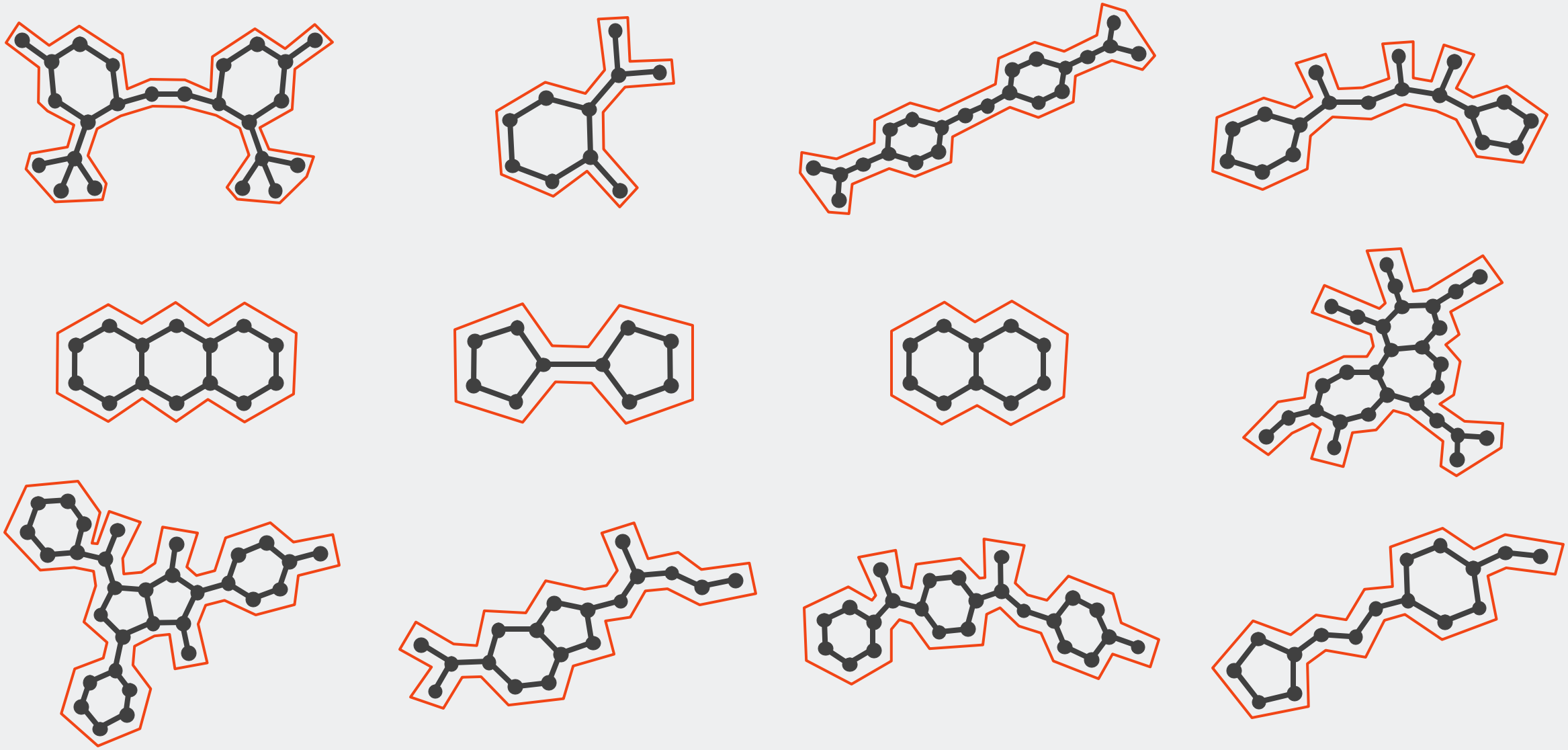
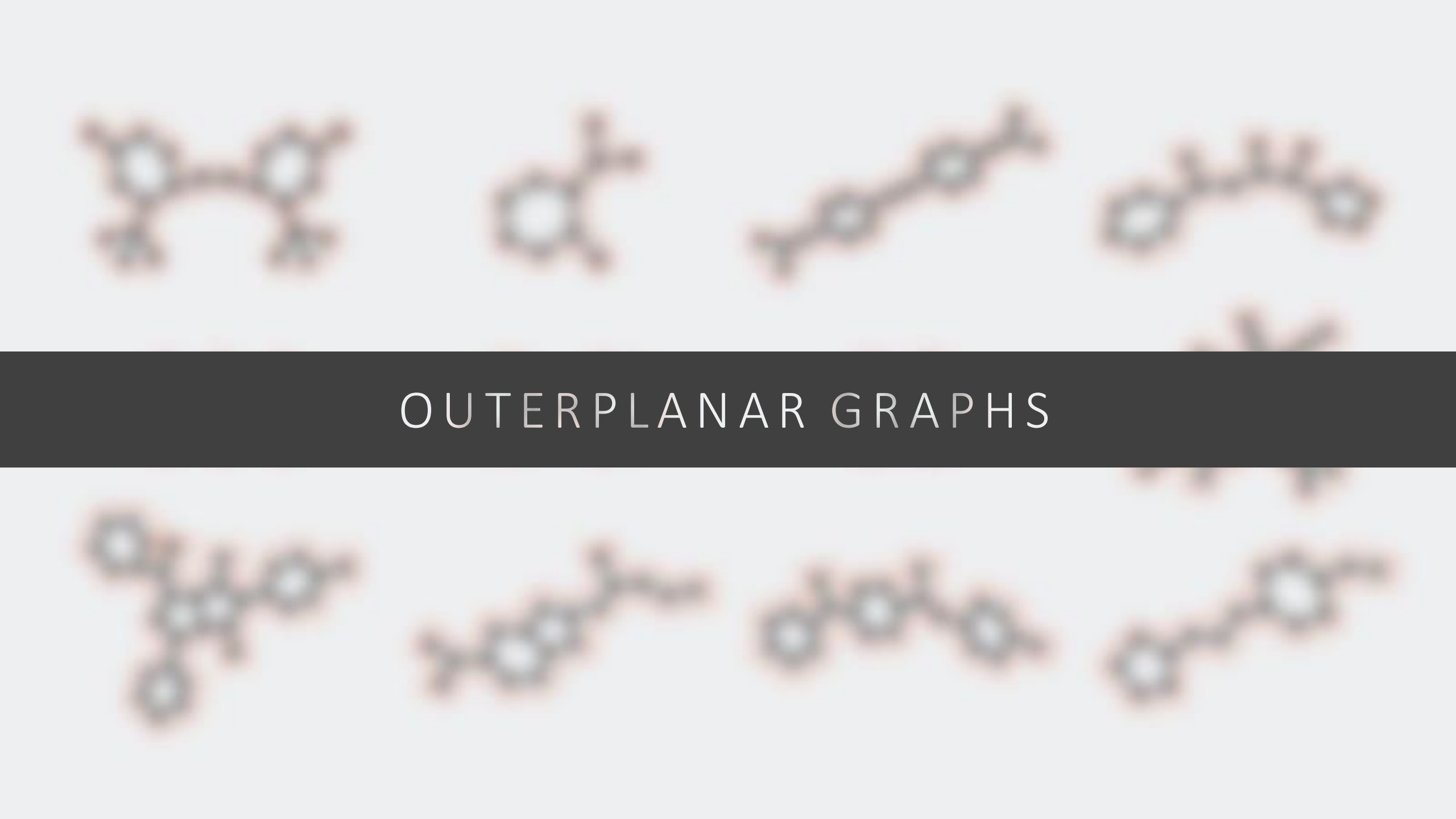





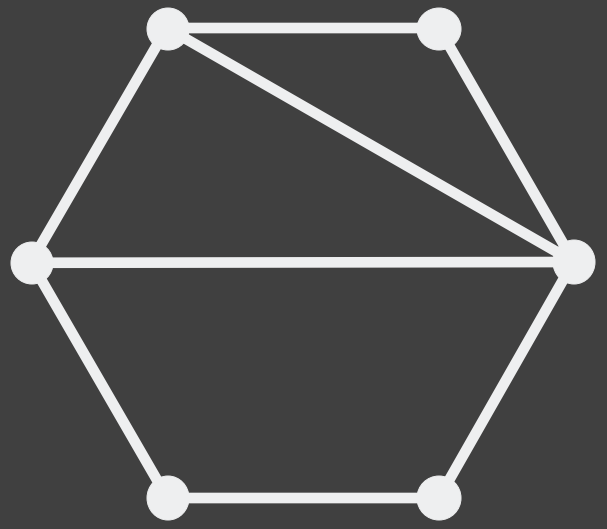








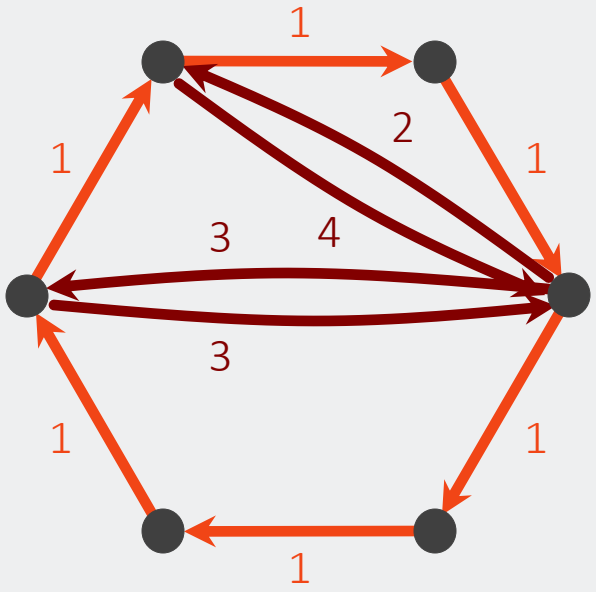


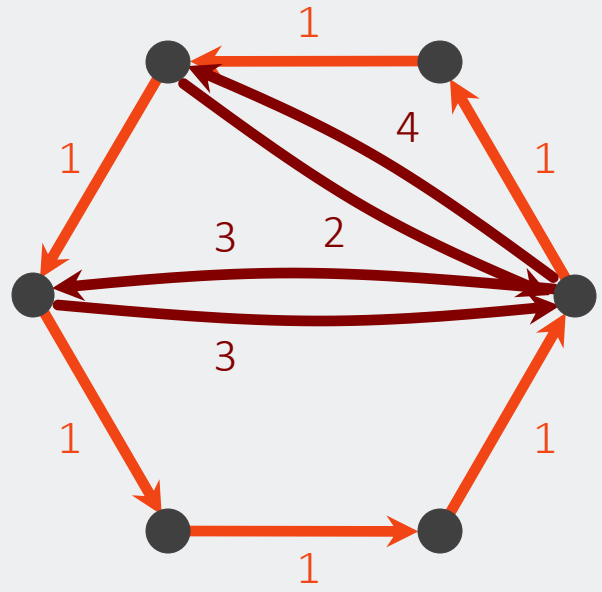


OUTERPLANAR GRAPHS

CAT*
TRANSFORMATION







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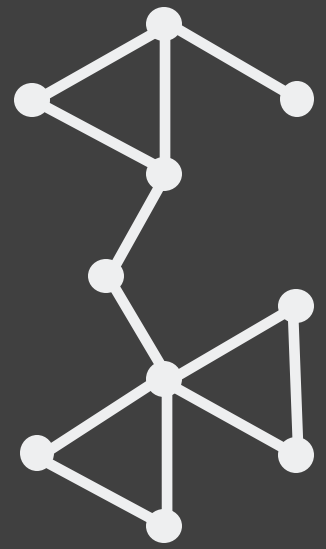

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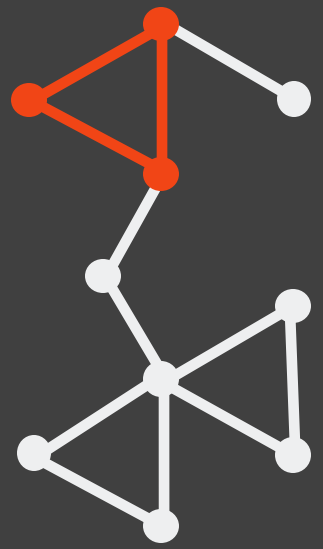
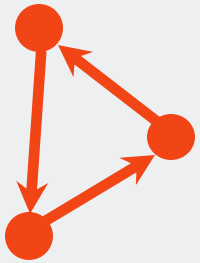
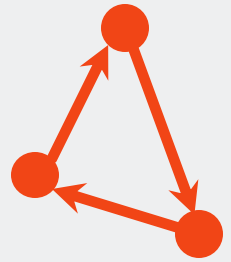


Apply CAT to all blocks*





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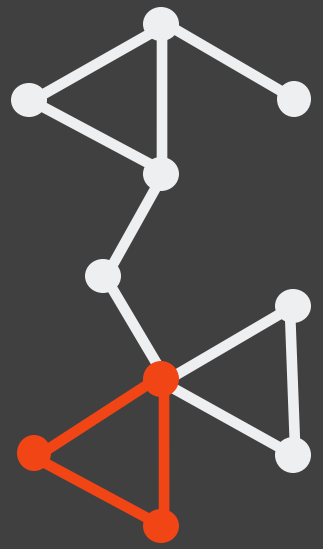

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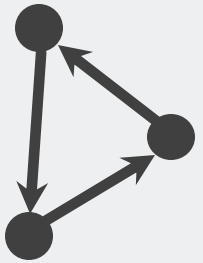

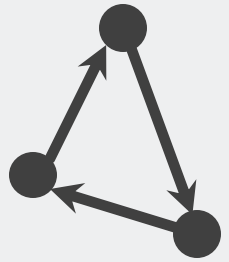

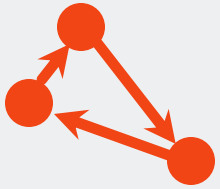

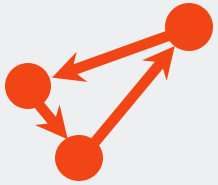

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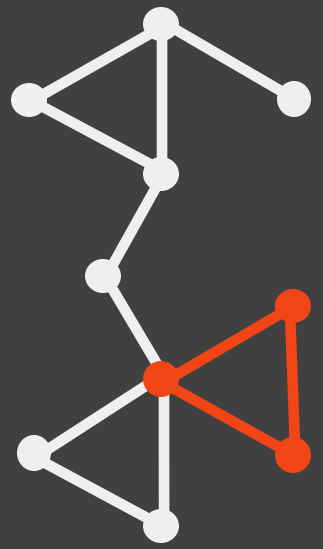

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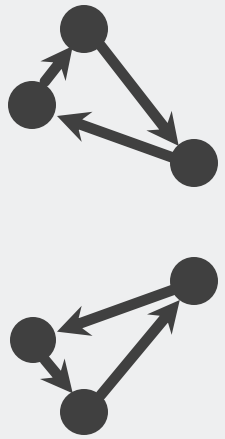

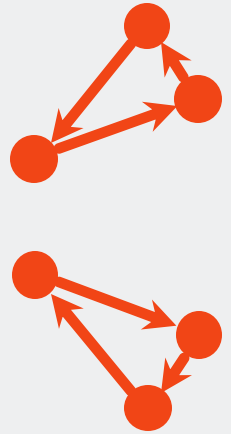

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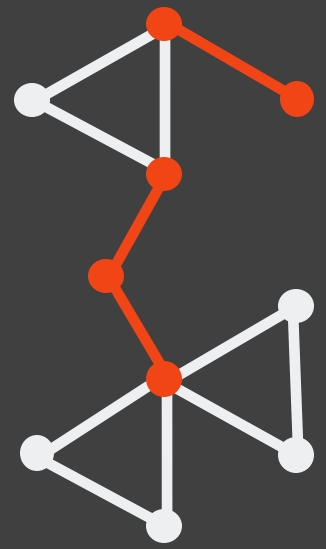
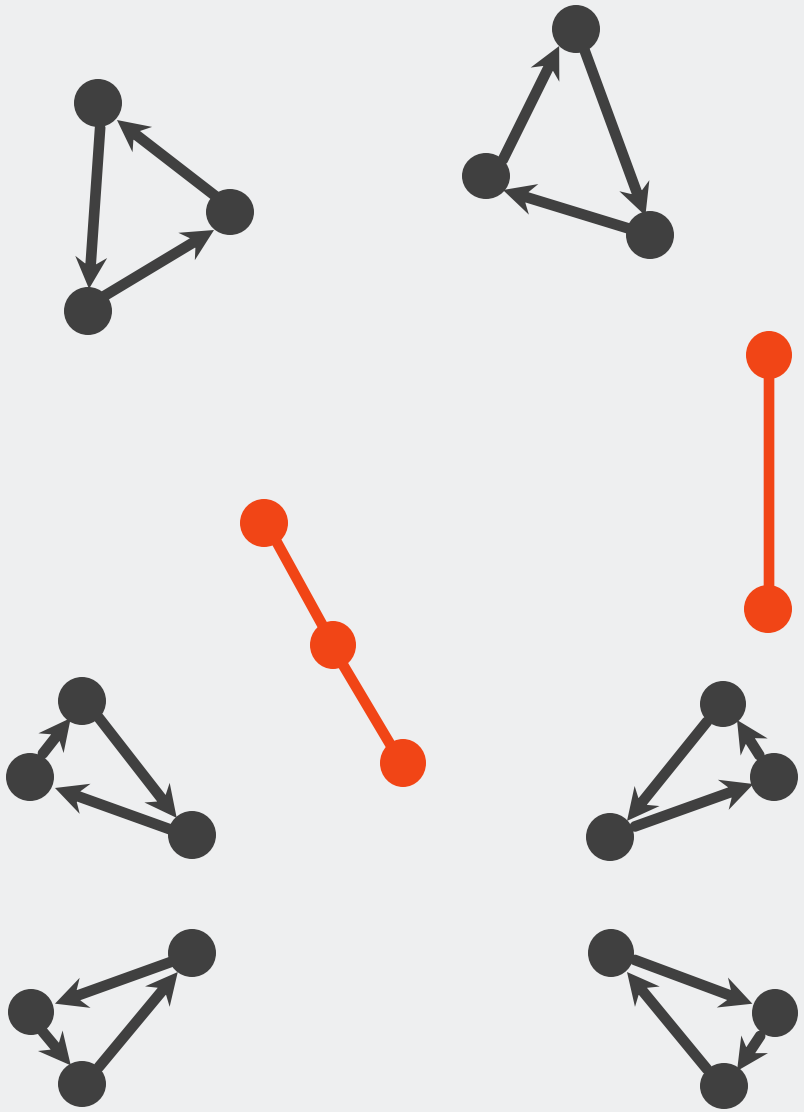


Add nodes & edges not in any block and nodes in more than 1 block



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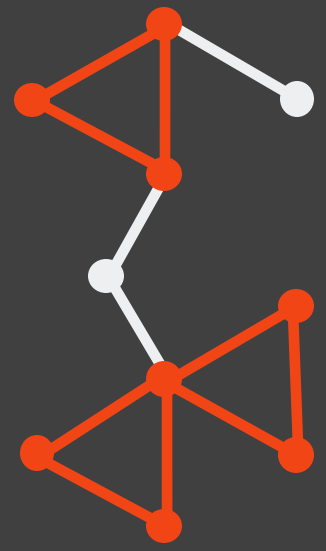
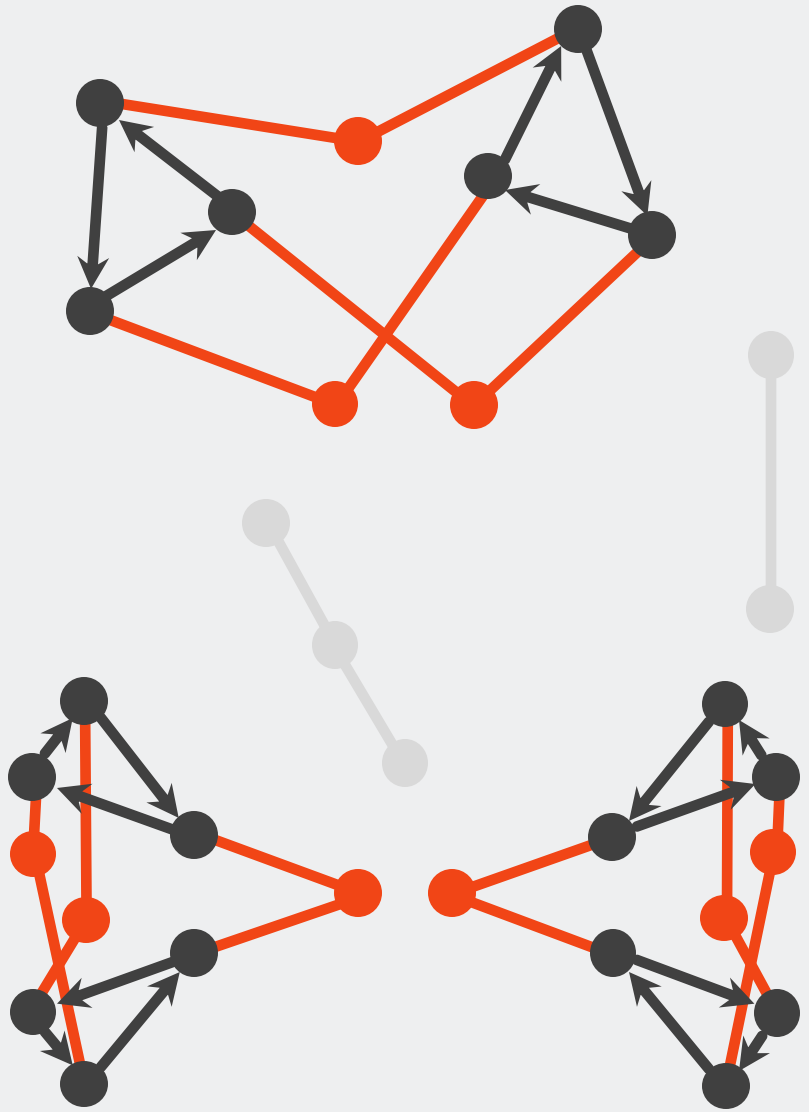


Add nodes connecting node pairs of each C and its reverse



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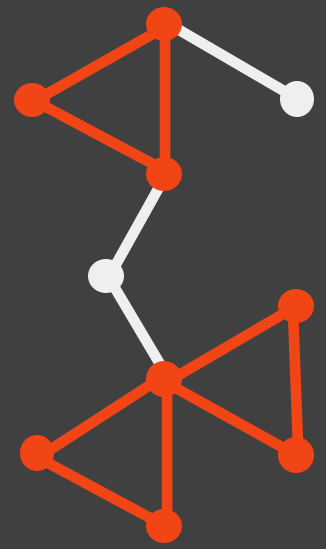
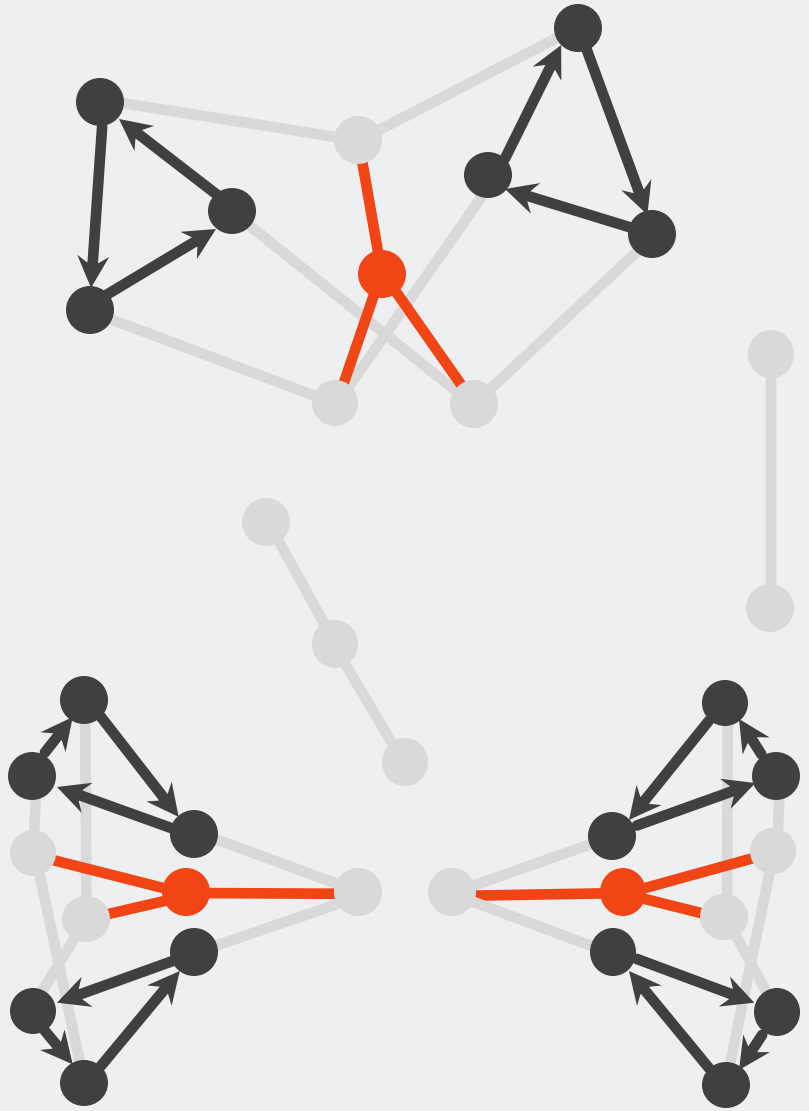


Add nodes connecting all previously introduced nodes of each block



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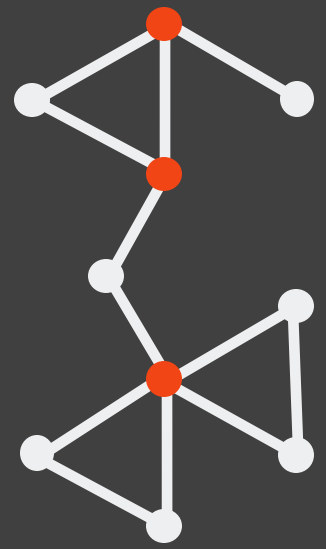
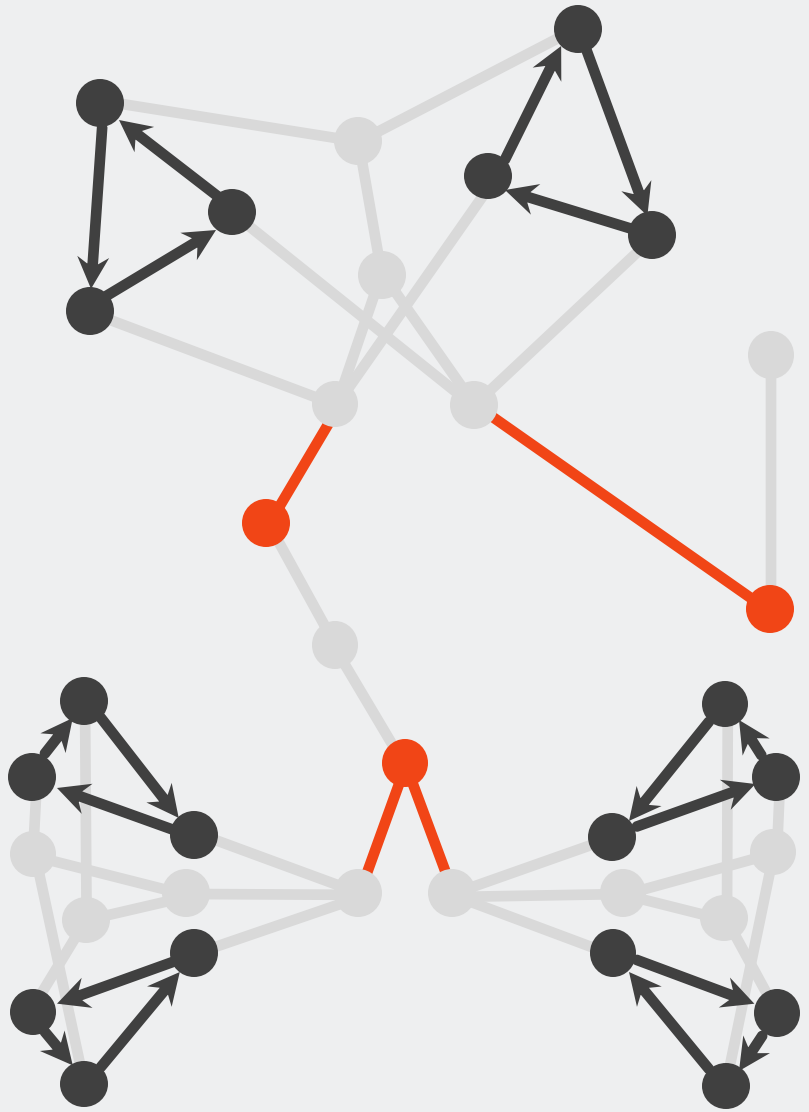


Add nodes for all nodes connecting multiple blocks



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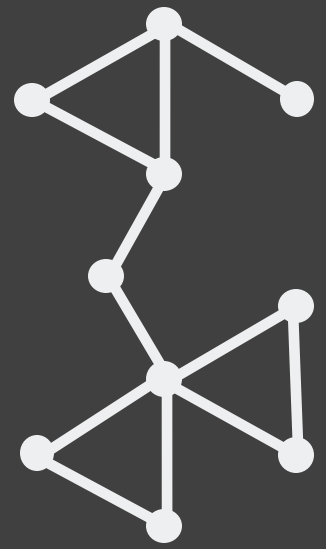

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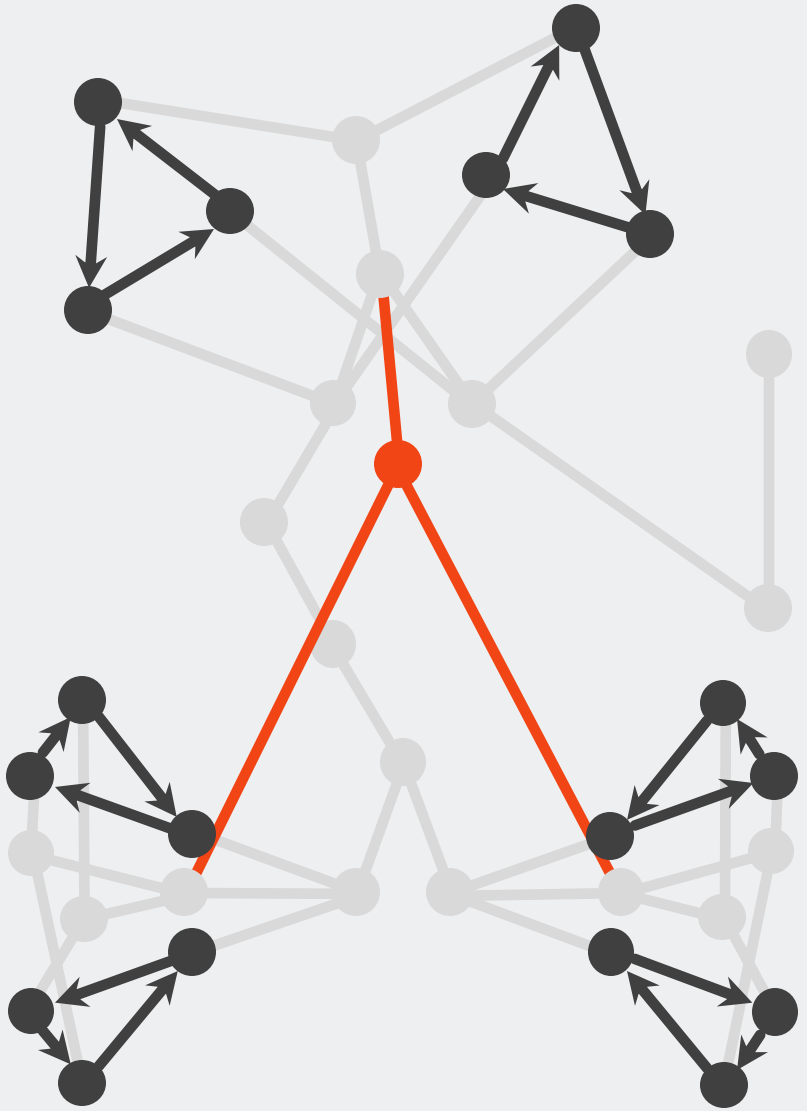

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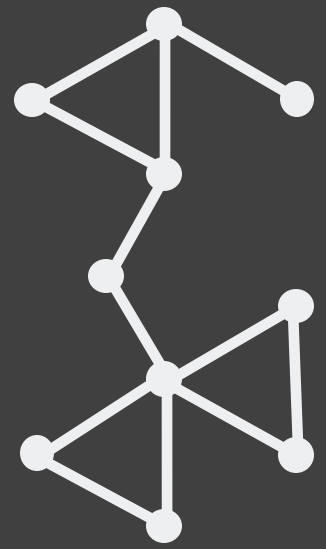
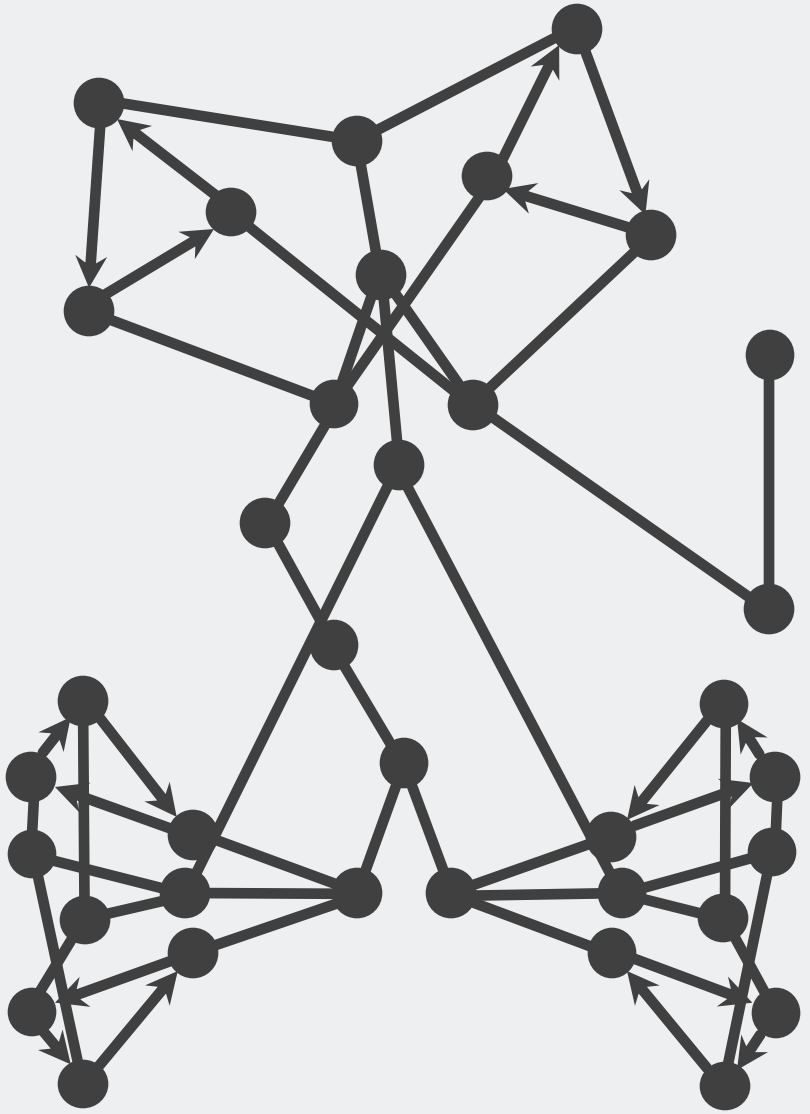


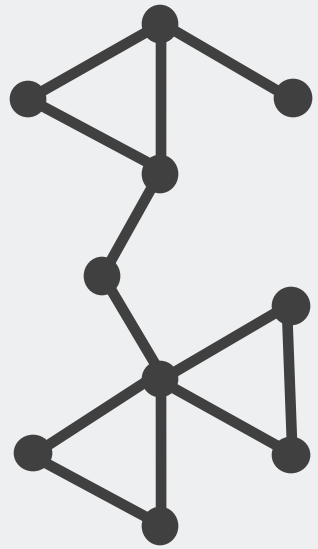
The transformation runs in linear time & is (together with MPNNs) maximally expressive on outerplanar graphs

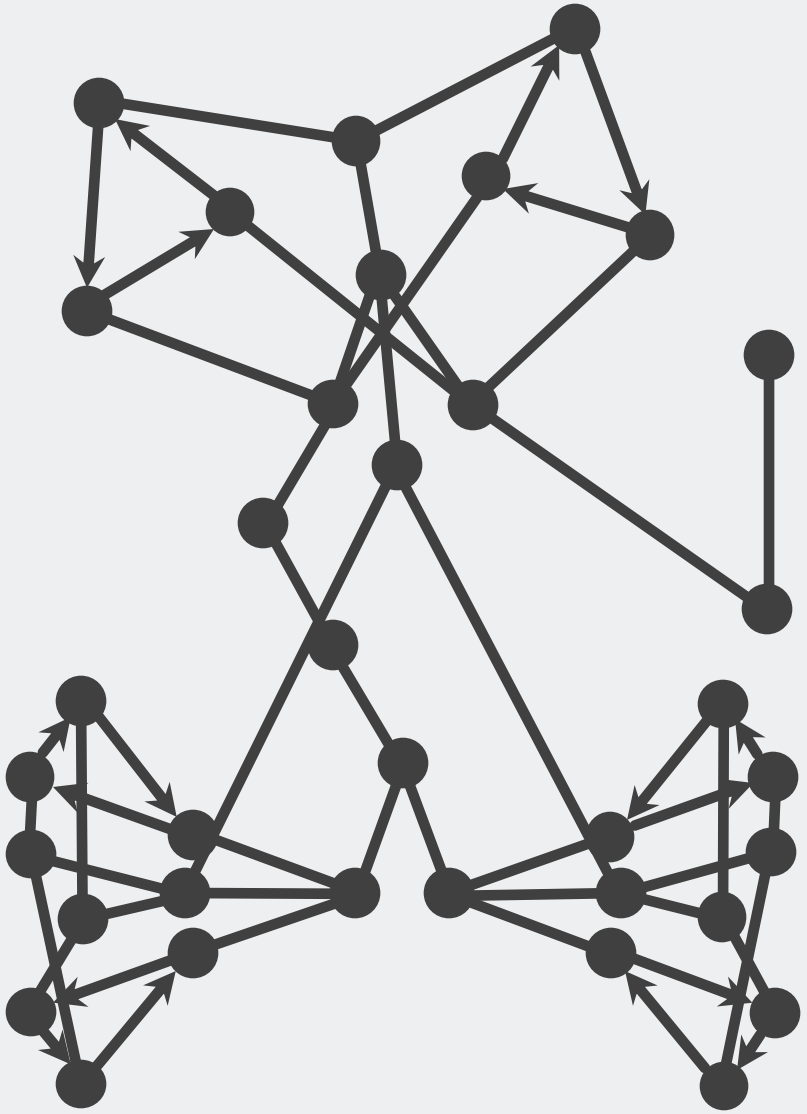


Dataset → ↓ Model	ZINC MAE (↓)	ZINC250k MAE (↓)	MOLHIV ROC-AUC (↑)	MOLBACE ROC-AUC (↑)	MOLBBBP ROC-AUC (↑)
GIN	0.168 ± 0.007	0.033 ± 0.003	77.9 ± 1.0	74.6 ± 3.2	66.0 ± 2.1
CAT+GIN	0.101 ± 0.004	0.034 ± 0.003	76.7 ± 1.8	79.5 ± 2.5	67.2 ± 1.8
GCN	0.184 ± 0.013	0.067 ± 0.005	76.7 ± 1.4	77.9 ± 1.7	66.1 ± 2.4
CAT+GCN	0.123 ± 0.008	0.034 ± 0.003	77.1 ± 1.6	79.2 ± 1.5	68.3 ± 1.7
GAT	0.375 ± 0.013	0.103 ± 0.004	76.6 ± 2.0	81.7 ± 2.3	66.2 ± 1.4
CAT+GAT	0.201 ± 0.022	0.046 ± 0.004	75.3 ± 1.6	79.3 ± 1.6	66.0 ± 1.9

Dataset → ↓ Model	MOLSIDER ROC-AUC (↑)	MOLESOL RMSE (↓)	MOLTOXCAST ROC-AUC (↑)	MOLLIPO RMSE (↓)	MOLTOX21 ROC-AUC (↑)
GIN	56.6 ± 1.0	1.105 ± 0.077	65.3 ± 0.6	0.717 ± 0.016	75.8 ± 0.7
CAT+GIN	58.2 ± 0.9	0.985 ± 0.055	65.6 ± 0.5	0.798 ± 0.031	74.8 ± 1.0
GCN	56.7 ± 1.5	1.053 ± 0.087	64.4 ± 0.4	0.748 ± 0.018	76.4 ± 0.3
CAT+GCN	57.9 ± 1.8	1.006 ± 0.036	66.2 ± 0.8	0.771 ± 0.023	74.9 ± 0.8
GAT	58.4 ± 1.0	1.037 ± 0.063	63.8 ± 0.8	0.728 ± 0.024	76.3 ± 0.6
CAT+GAT	58.3 ± 1.3	1.090 ± 0.048	64.5 ± 0.8	0.754 ± 0.021	75.4 ± 0.7

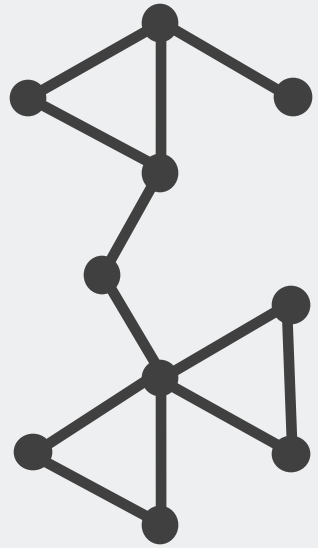
SUMMARY

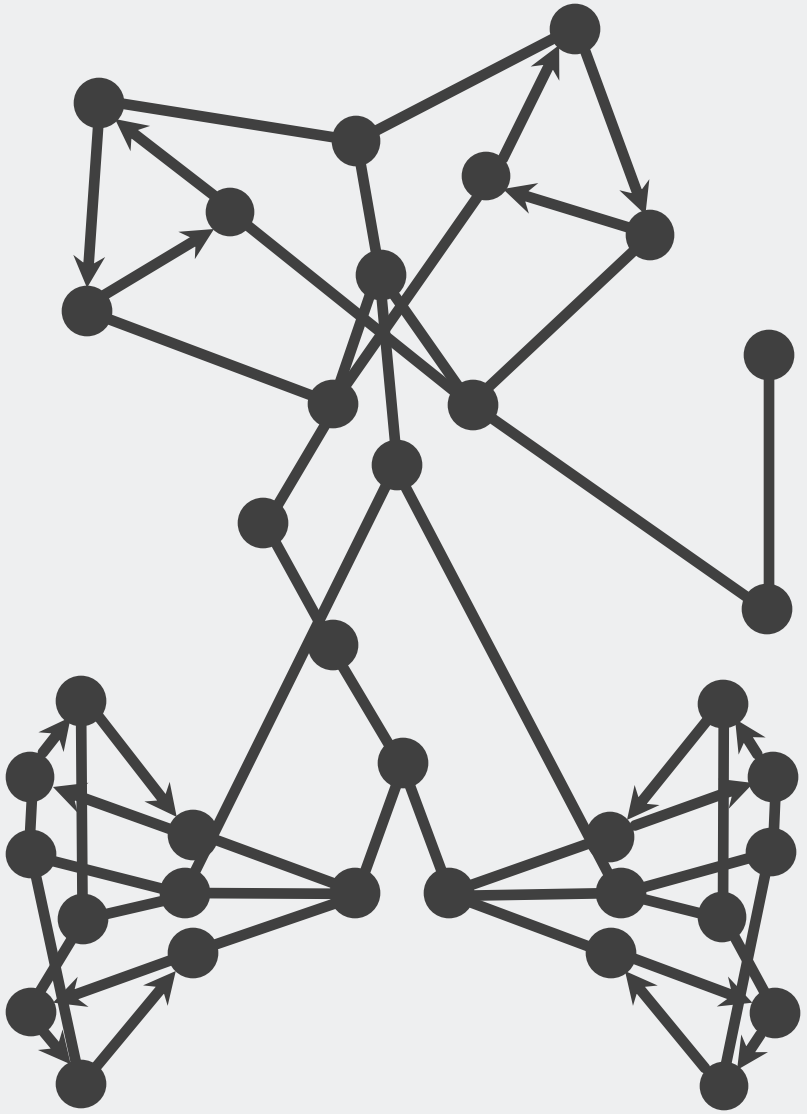




SUMMARY

Restricting graph class allows for faster and more expressive results



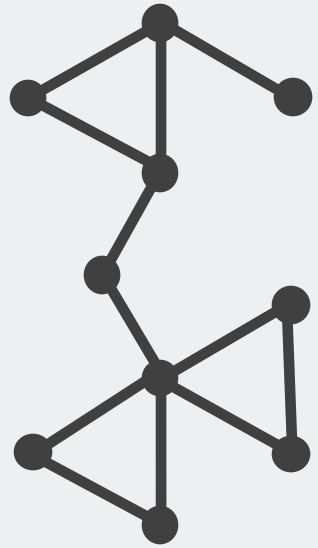


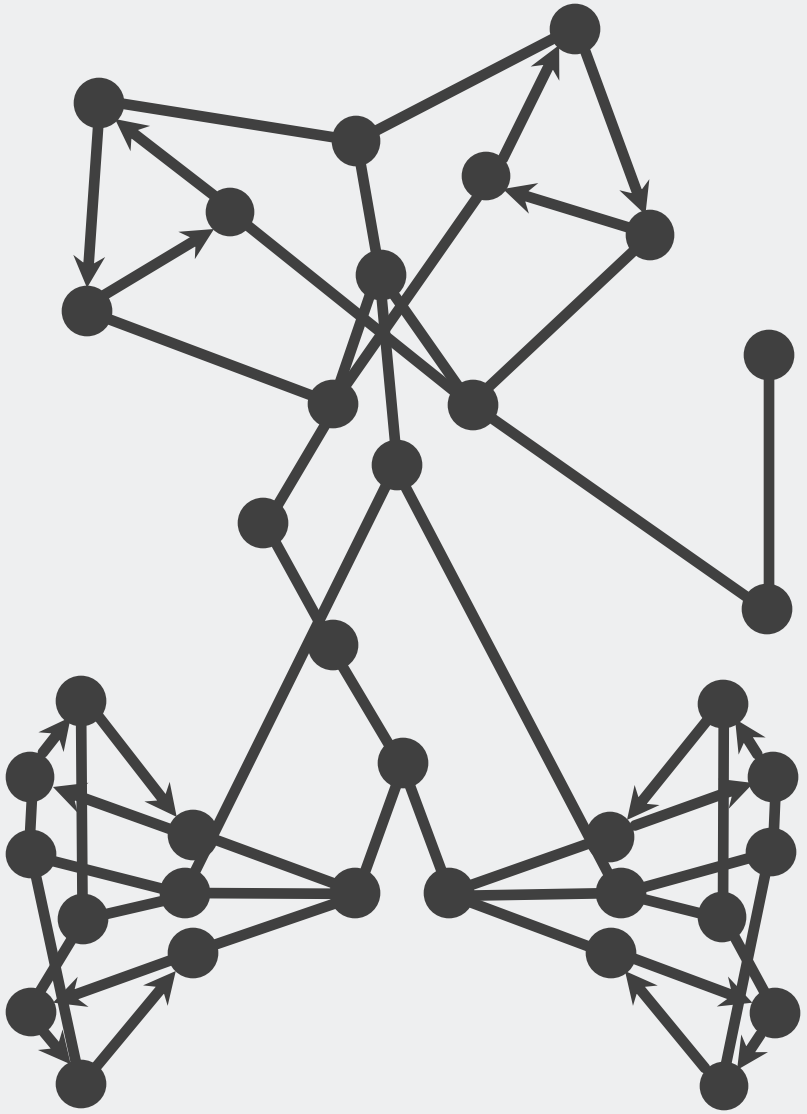
SUMMARY

Restricting graph class allows for faster and more expressive results

CAT transformation:

- a linear graph transformation
- enabling MPNNs to be maximally expressive
- on outerplanar graphs





SUMMARY

Restricting graph class allows for faster and more expressive results

CAT transformation:

- a linear graph transformation
- enabling MPNNs to be maximally expressive
- on outerplanar graphs

Boosts predictive performance of MPNNs on a variety of molecular benchmark datasets