ETH zürich

Maximally Expressive GNNs for Outerplanar Graphs

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Seminar in Deep Neural Networks (FS 2024)

12 March 2024, Zurich

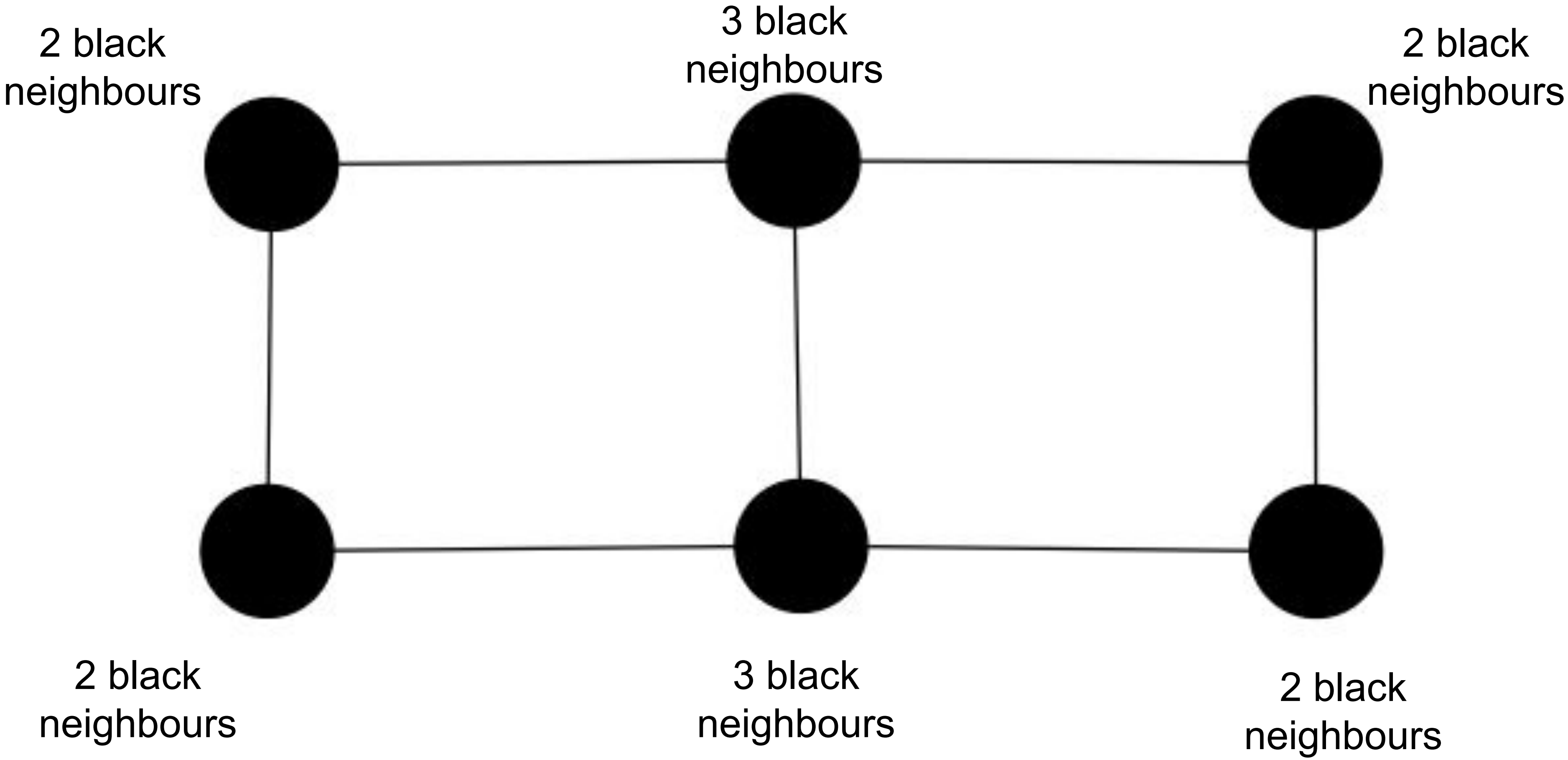
GNNs

MPNN: $u_{l+1}\ \Phi(u_l, \Psi(Nei_l(u)))$

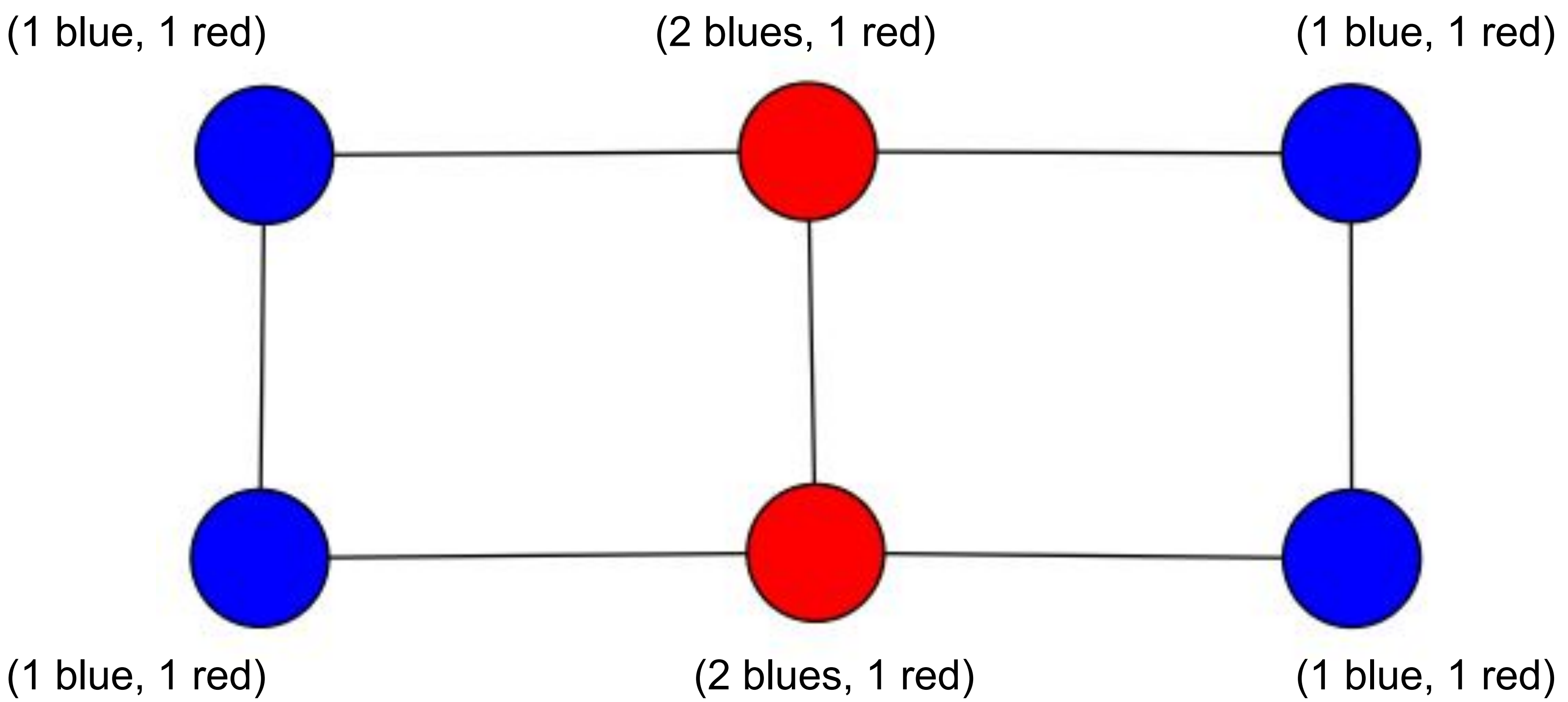
Graph Neural Network’s goal would be to only consider the isomorphism class of a graph (i.e. 2 isomorphic graphs should give the same output).

1-WL Test

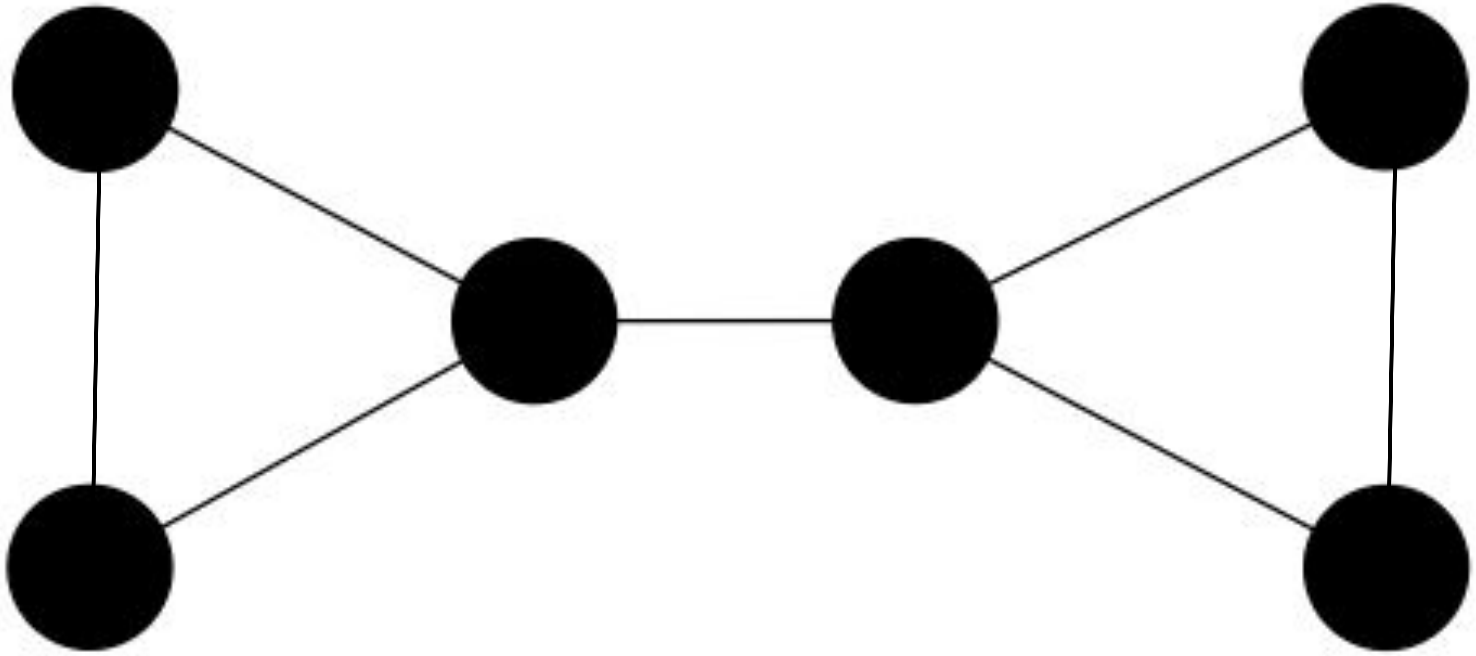
$$u_{t+1} \leftarrow (u_t, Nei_t(u))$$



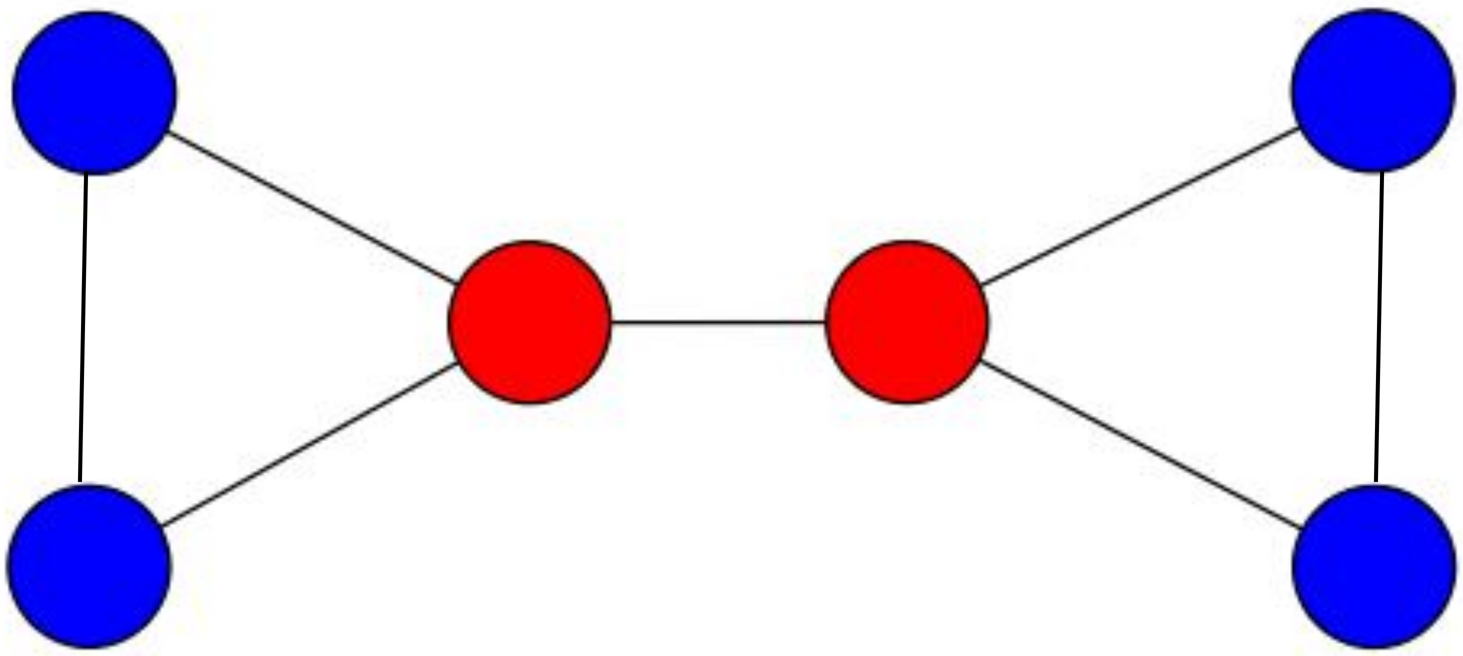
1-WL Test


(1 blue, 1 red)
(2 blues, 1 red)
(1 blue, 1 red)
(1 blue, 1 red)
(2 blues, 1 red)
(1 blue, 1 red)

1-WL Test



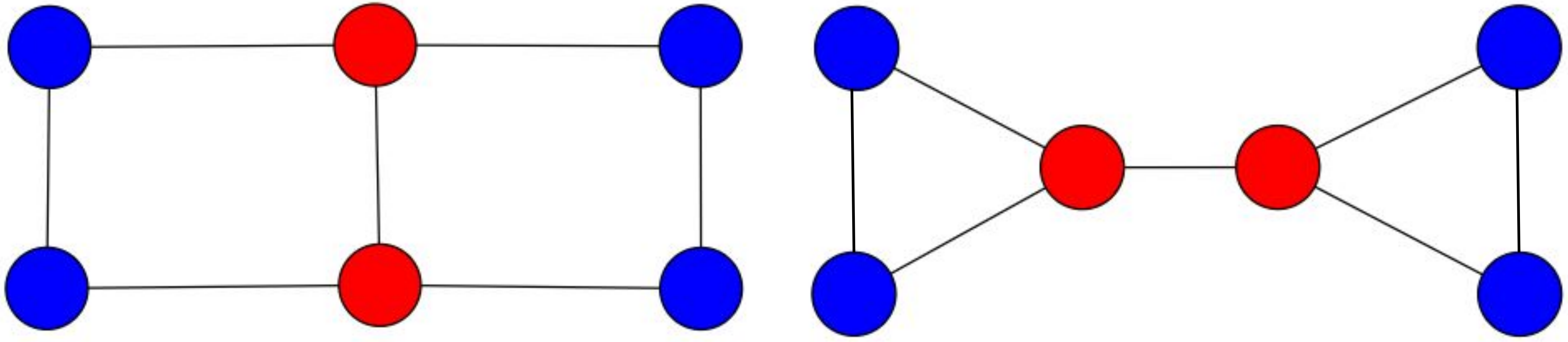
1-WL Test



1-WL Test

If WL(G) ≠ WL(H), then G and H are not isomorphic

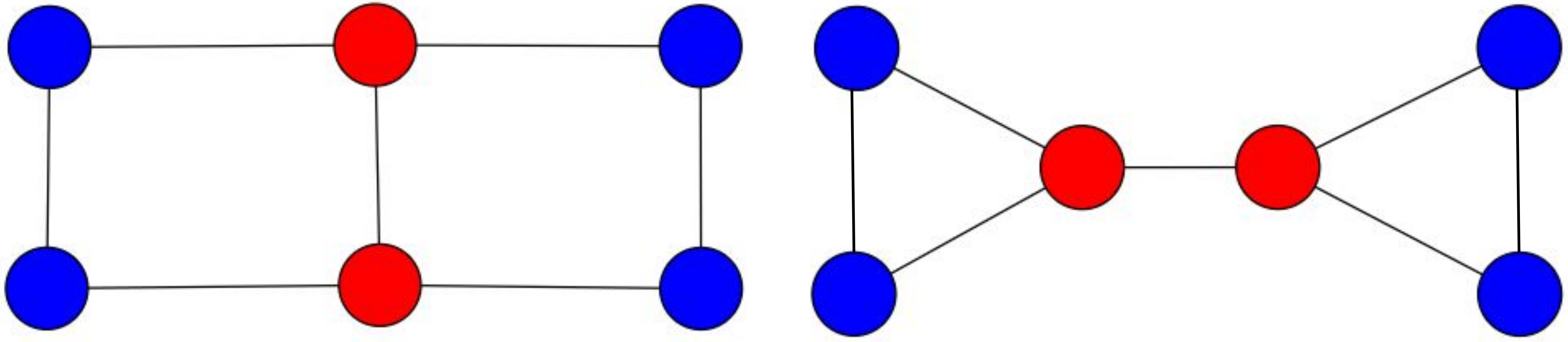
However, if WL(G) = WL(H), G and H might not be isomorphic



{4 blue, 2 red} = {4 blue, 2 red}

GNNs

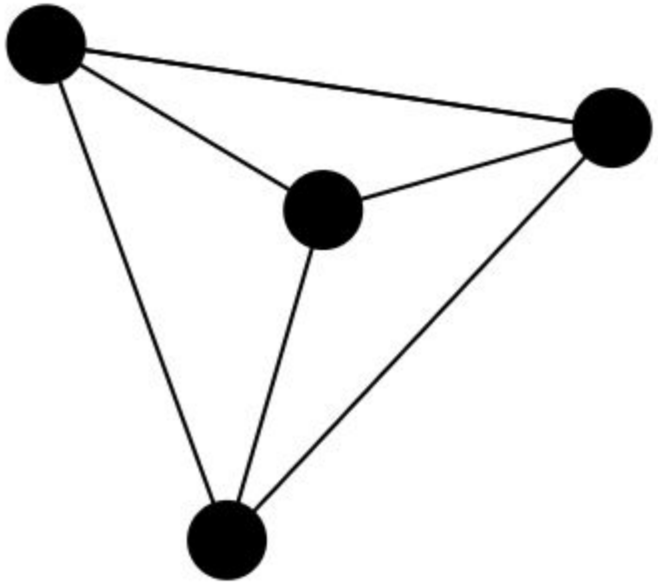
Problem: MPNN’s expressiveness is bounded by the 1-WL test.
In particular, GINs (Graph Isomorphism Networks) are proven to be as expressive as the 1-WL test.



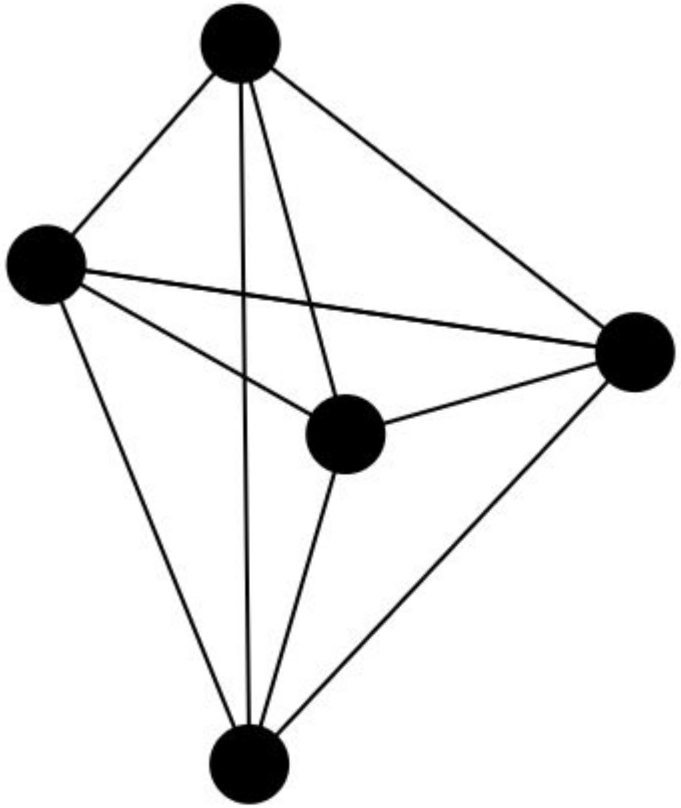
GNNs
Can we restrict ourselves to a simpler subclass of graphs?

Planar graphs
Can be drawn on the plane in such a way that no edges cross each other

Planar

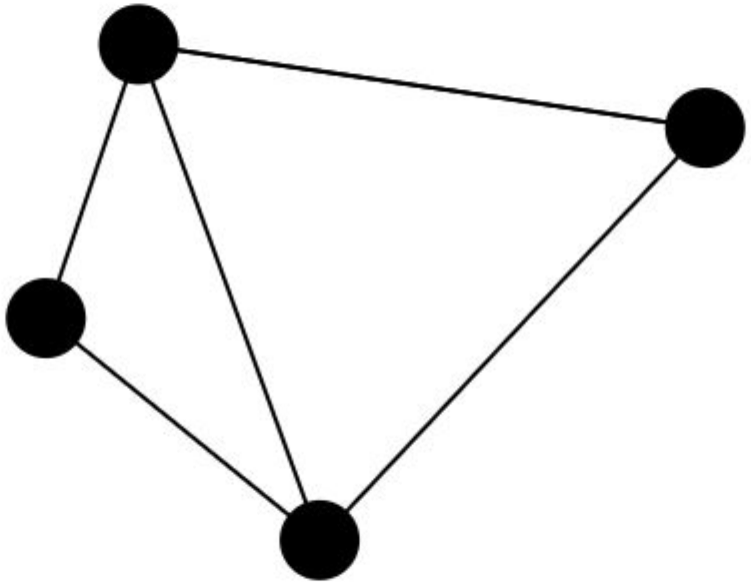


Non-planar

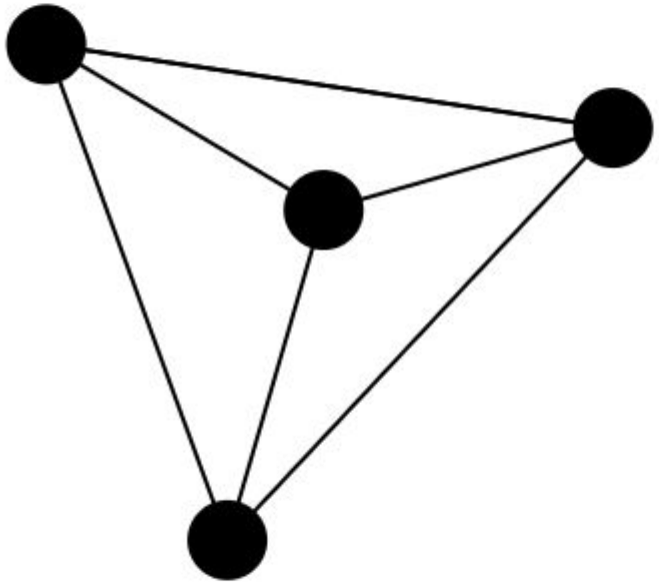


Outerplanar graphs
Planar graph that can be drawn so that no vertex is “trapped” inside the edges of the graph

Outerplanar



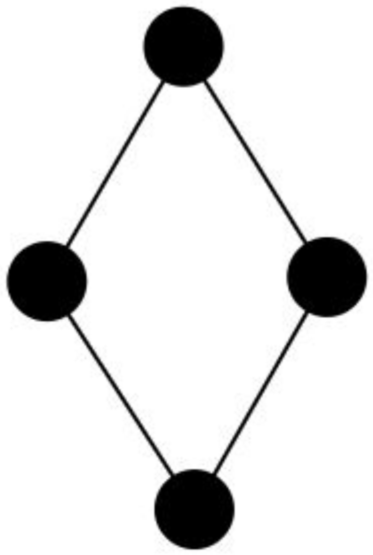
Non-outerplanar



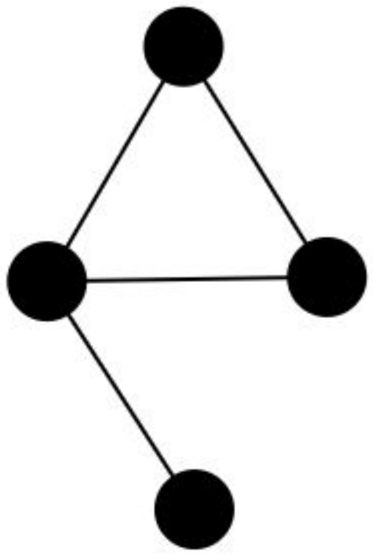
Biconnected graph

Connected graph that is not broken into disconnected pieces by deleting any single vertex

Biconnected



Non-biconnected



Biconnected graph

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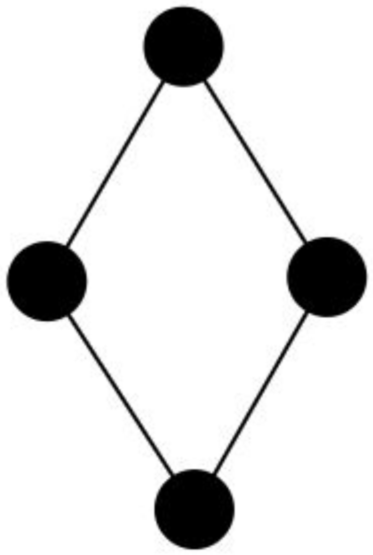
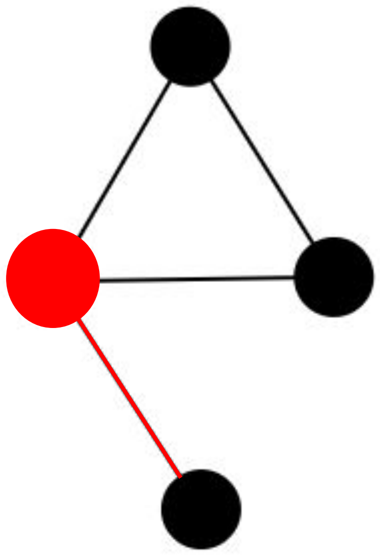
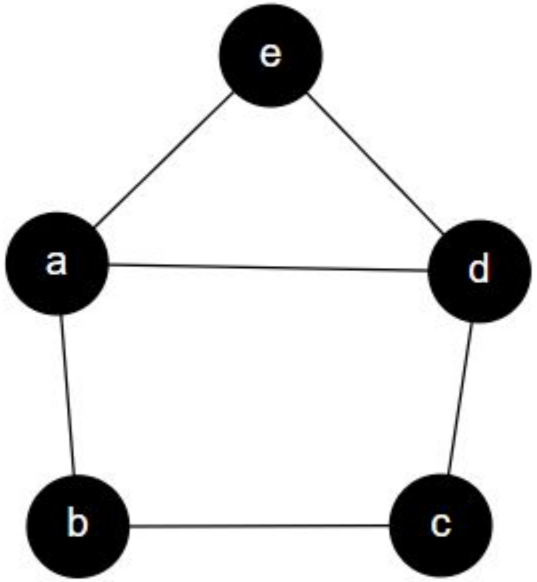
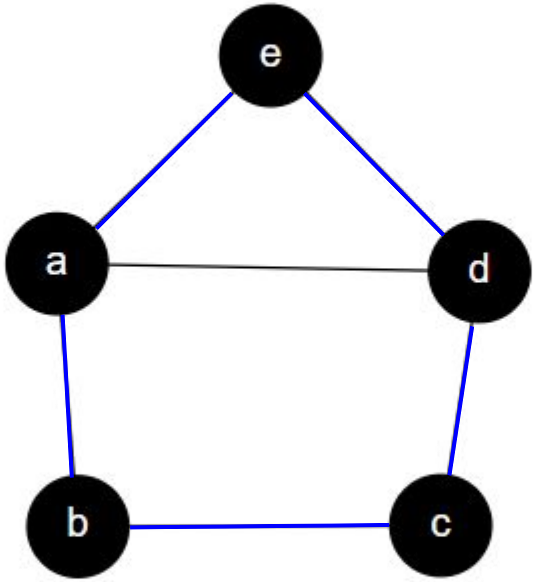


Non-biconnected



Hamiltonian cycle
Cycle which goes over each node exactly once

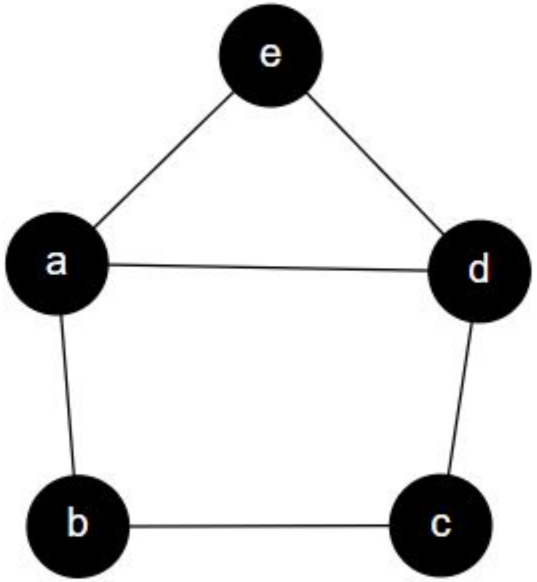


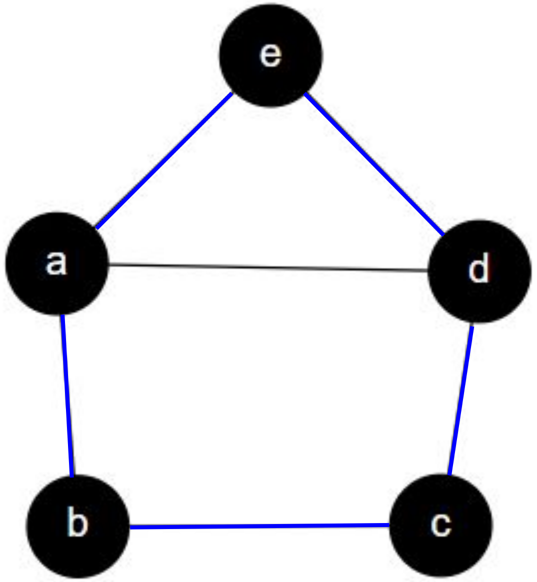


Hamiltonian cycle

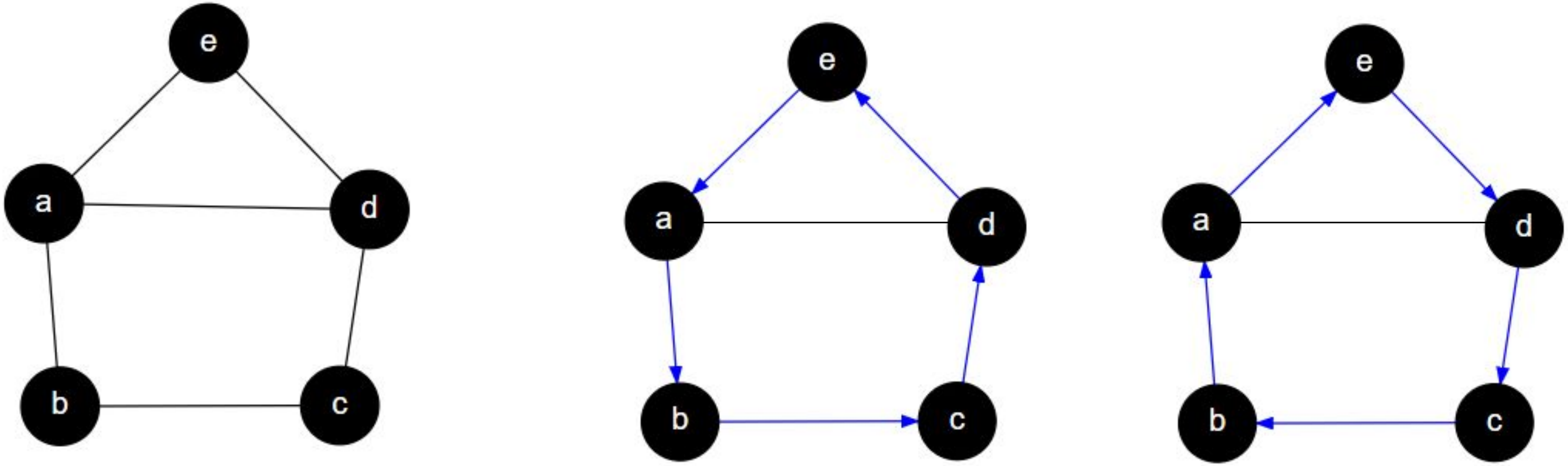
Cycle which goes over each node exactly once

Theorem 1: Biconnected outerplanar graphs have a unique Hamiltonian cycle that can be found in linear time





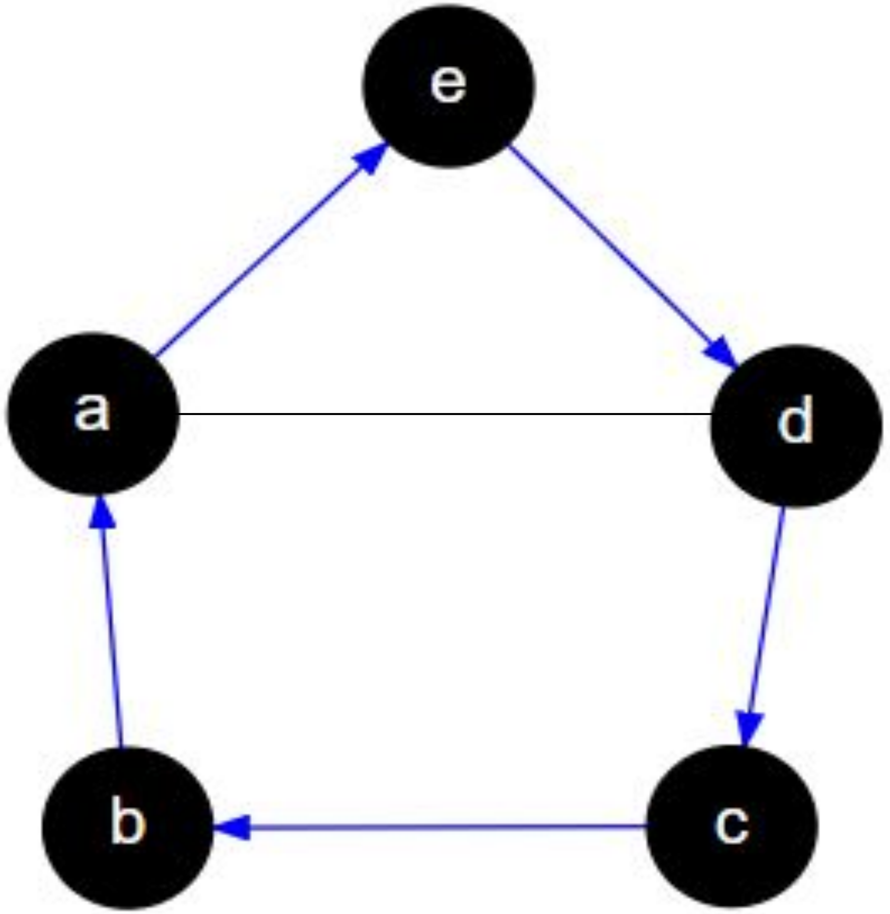
Hamiltonian cycle (2 directed variants)



HALs (Hamiltonian Adjacency Lists)

Annotating each node with the sorted distances d_c to all its neighbors on the two directed variants of the Hamiltonian cycle C.

1



$d_c(e, d) = 1$

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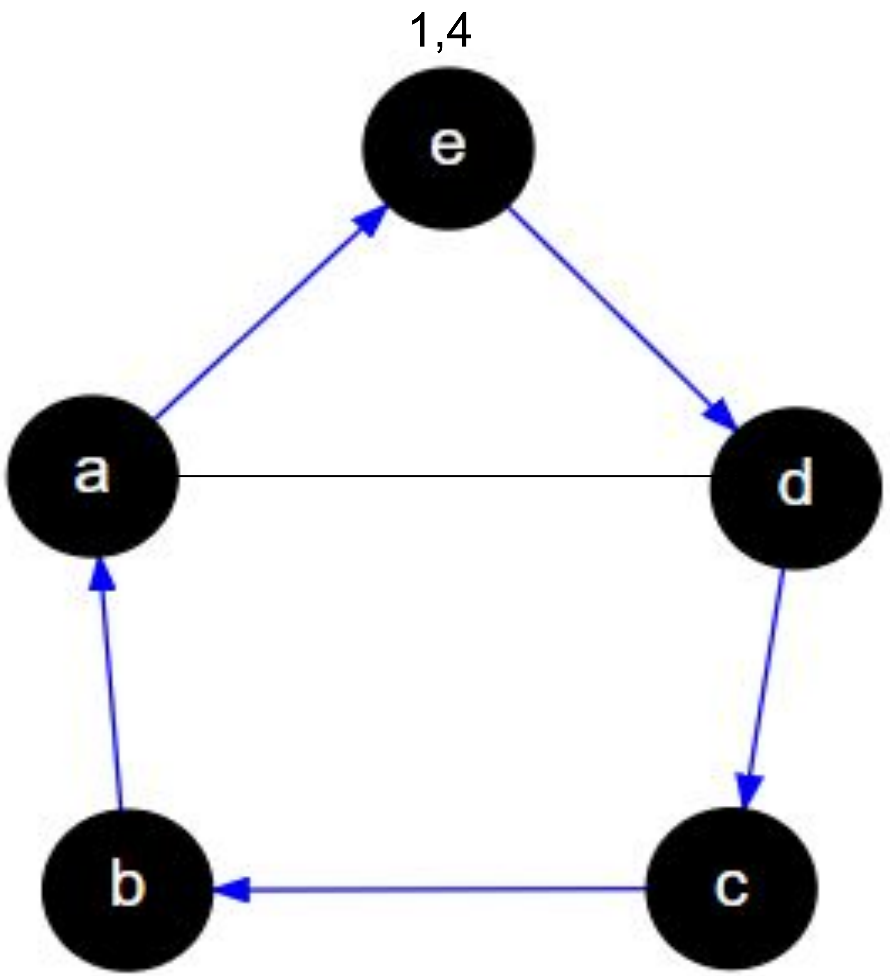

$d_c(e, a) = 4$

HALs (Hamiltonian Adjacency Lists)

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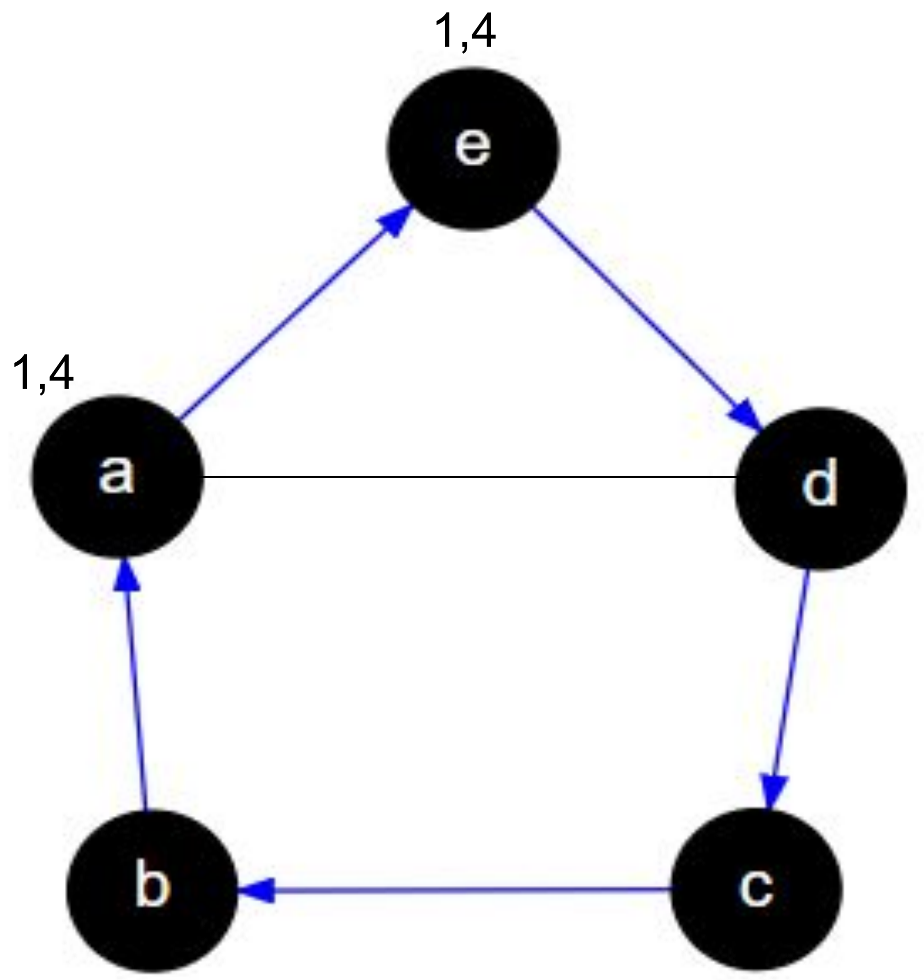
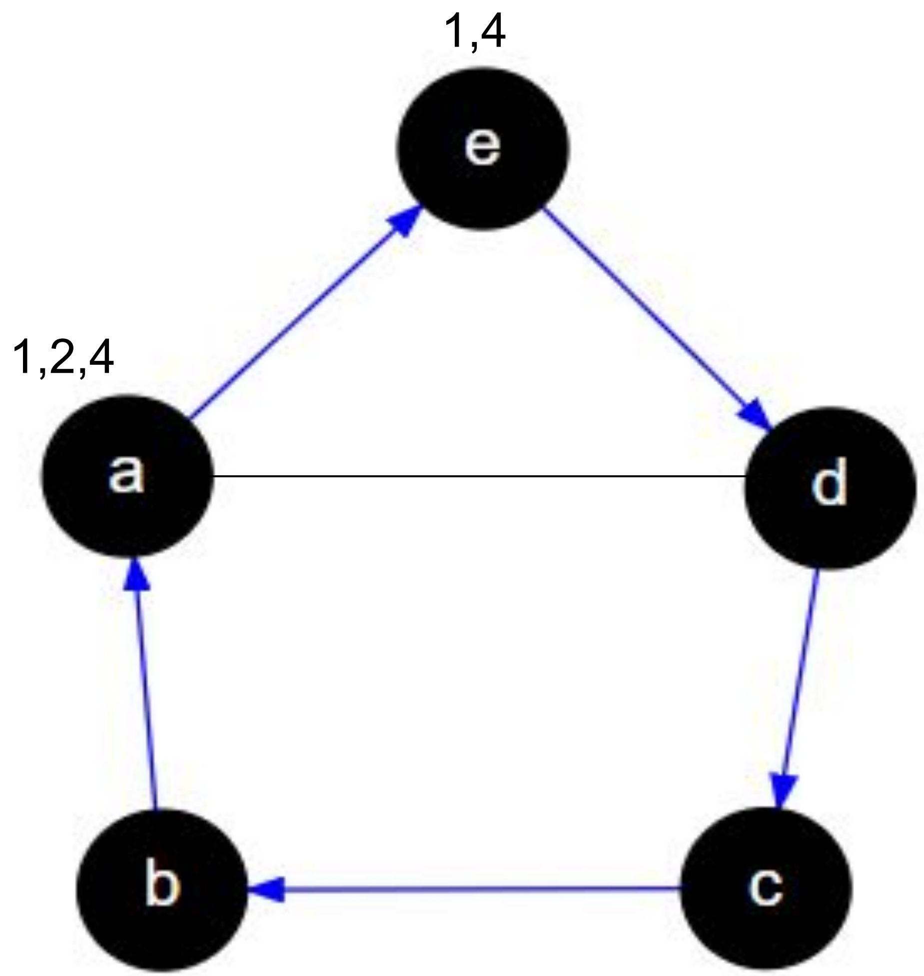


$d_c(a, e) = 1$
$d_c(a, b) = 4$

HALs (Hamiltonian Adjacency Lists)

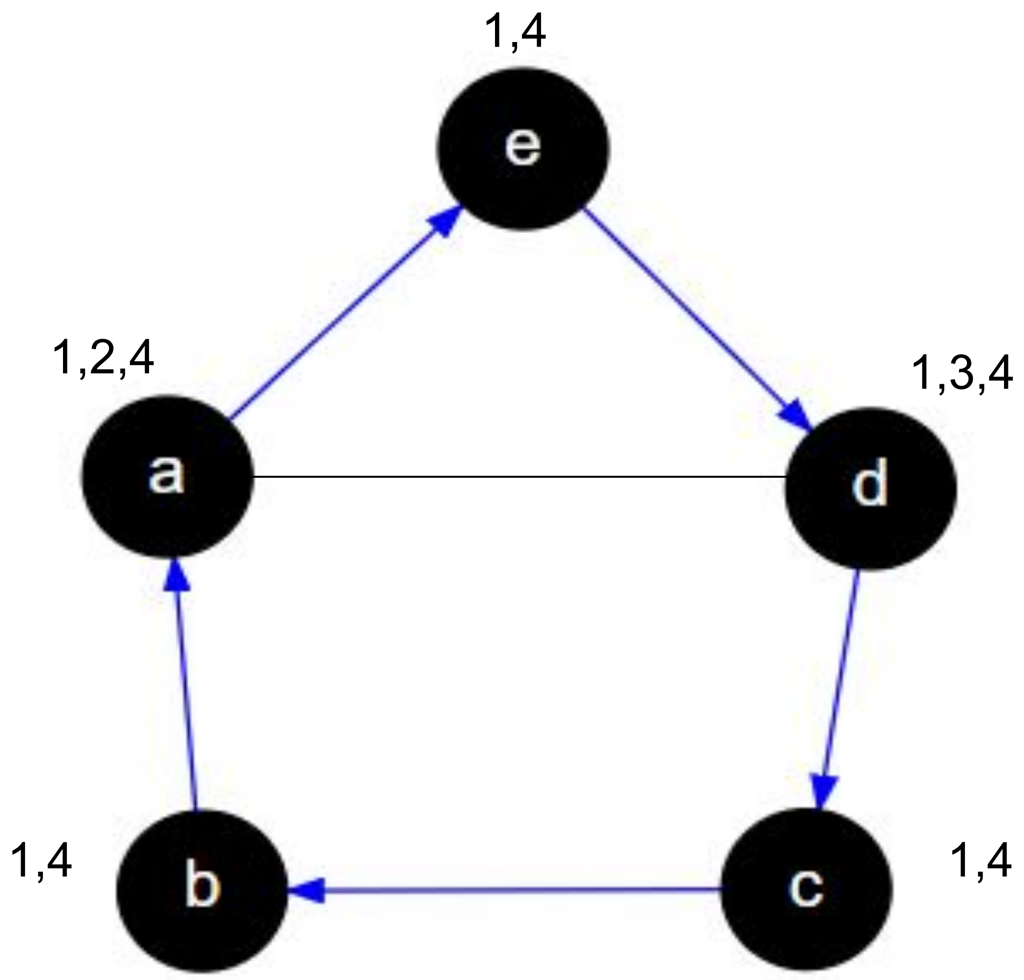
Annotating each node with the sorted distances d_c to all its neighbors on the two directed variants of the Hamiltonian cycle C.



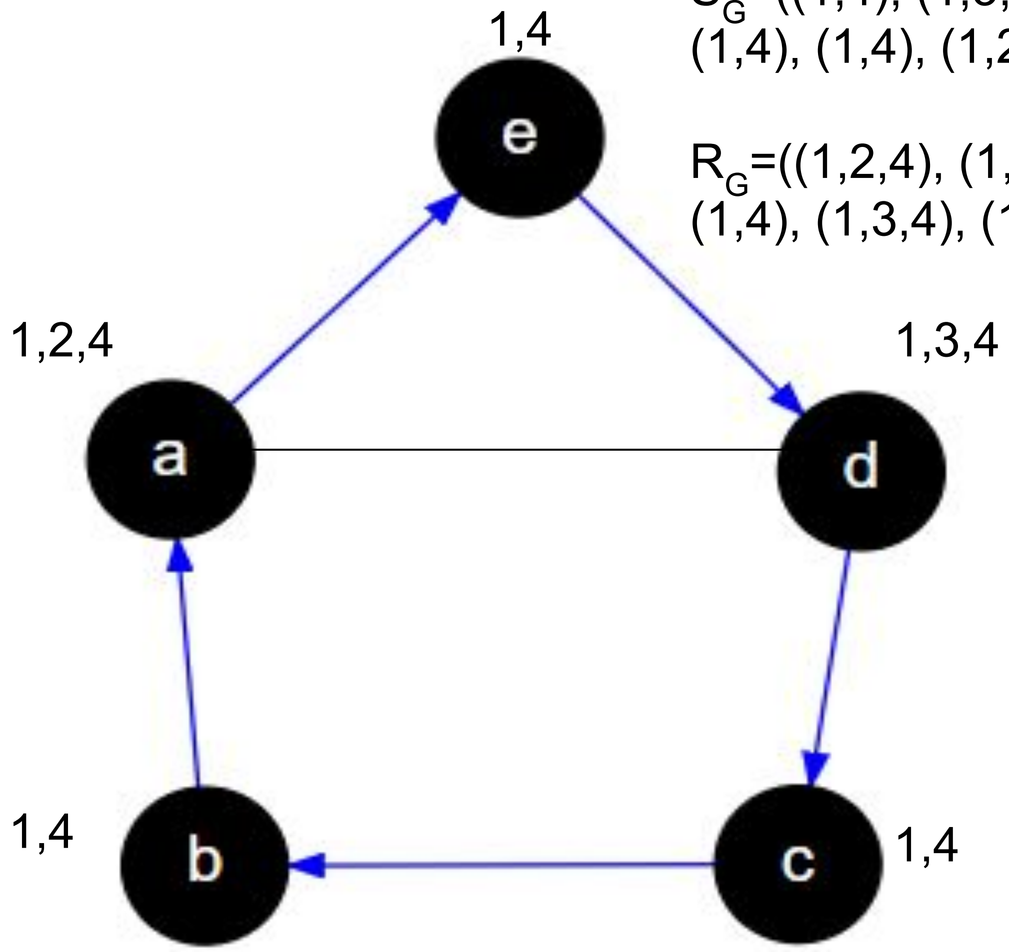
$d_c(a, d) = 2$

HALs (Hamiltonian Adjacency Lists)

Annotating each node with the sorted distances d_c to all its neighbors on the two directed variants of the Hamiltonian cycle C.

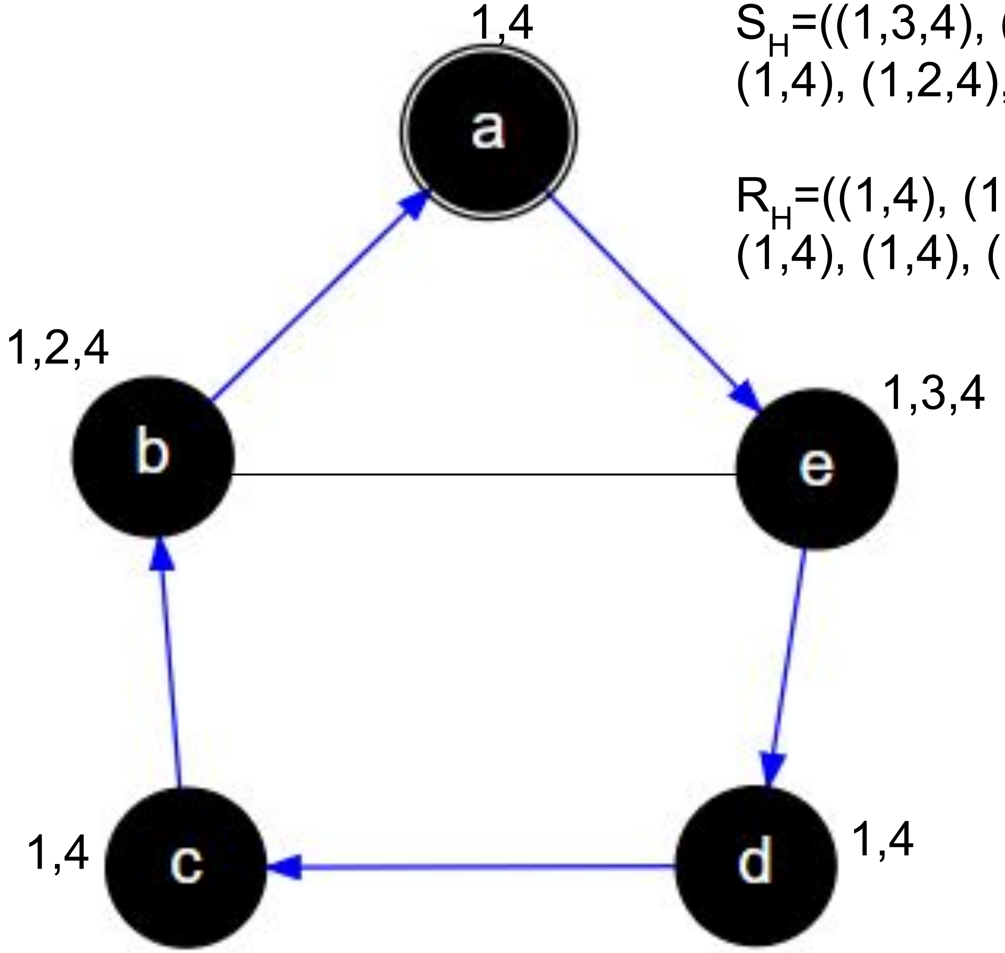


Theorem 2: Two biconnected outerplanar graphs G and H with HAL and reverse sequences S_G, S_H and R_G, R_H are isomorphic, iff S_G is a cyclic shift of S_H or R_H.



S_G=((1,4), (1,3,4), (1,4), (1,4), (1,2,4))

R_G=((1,2,4), (1,4), (1,4), (1,3,4), (1,4))



S_H=((1,3,4), (1,4), (1,4), (1,2,4), (1,4))

R_H=((1,4), (1,2,4), (1,4), (1,4), (1,3,4))

S = (e, d, c, b, a), R = (a, b, c, d, e)

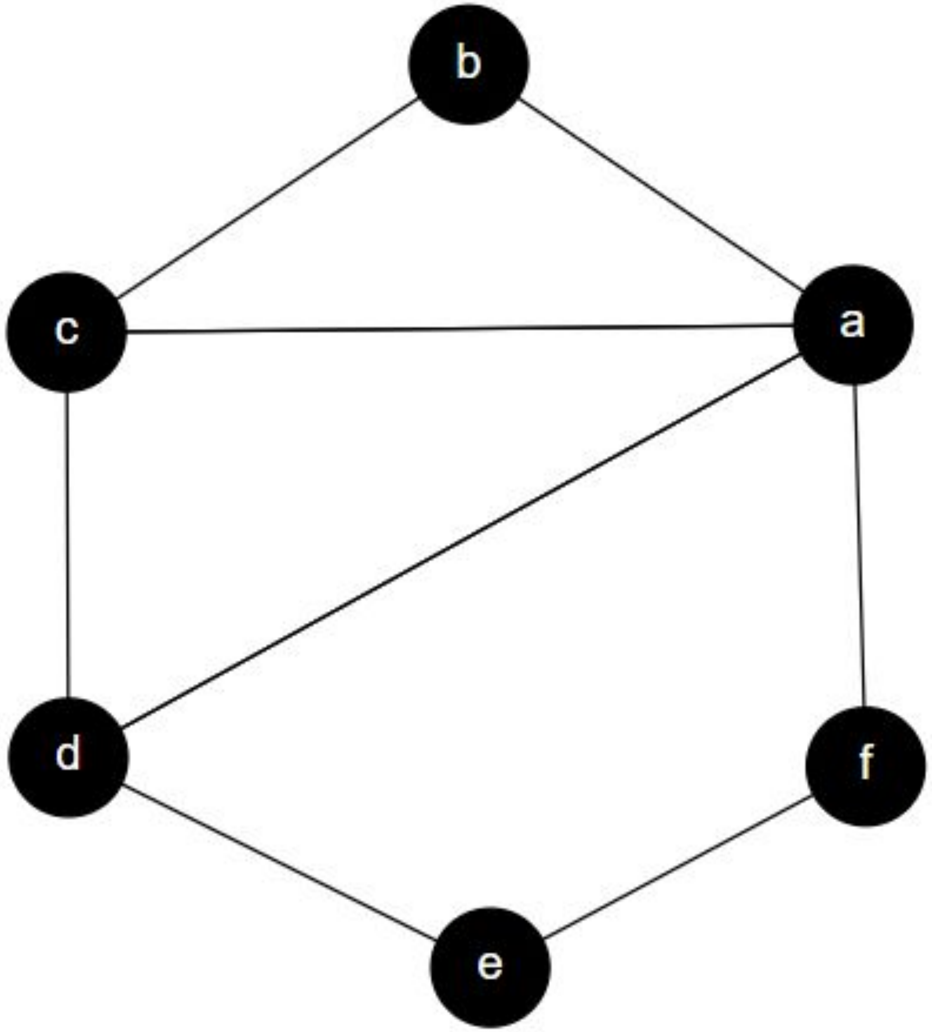
Idea

Let's build a transformation to make S_G and R_G recognizable by WL test

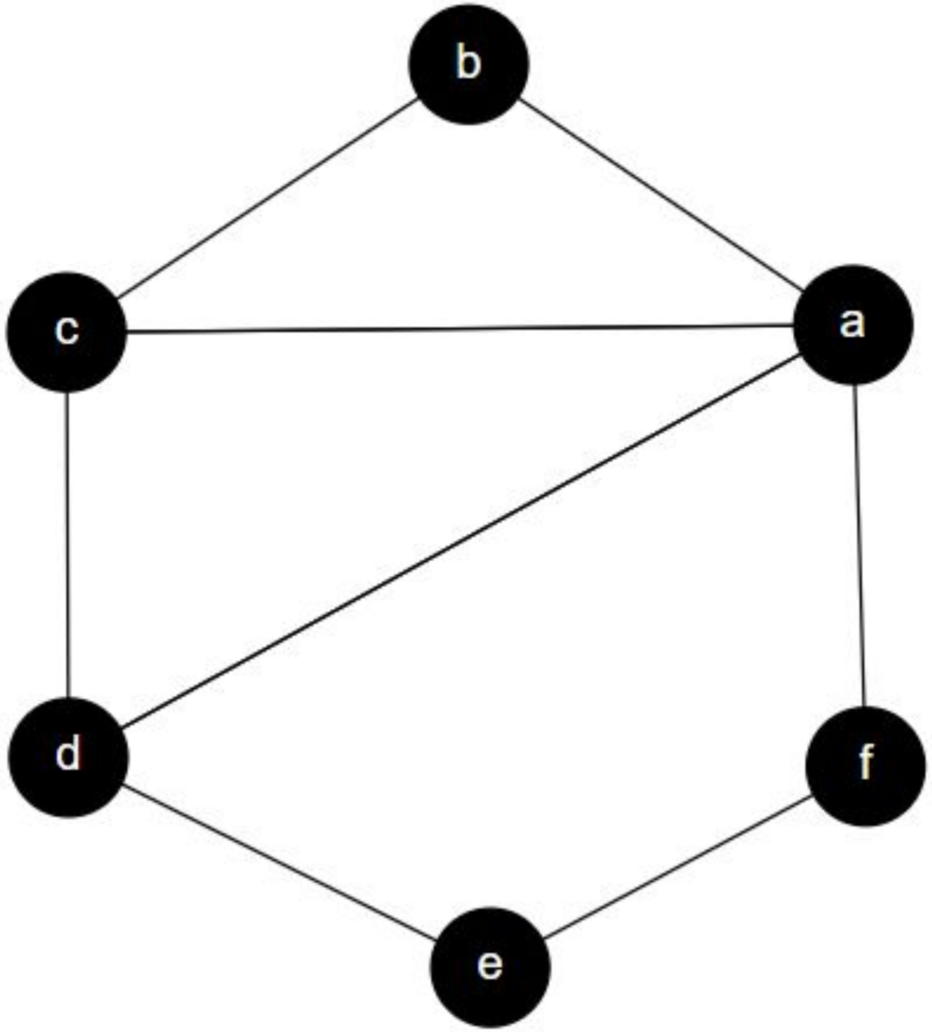
Agenda

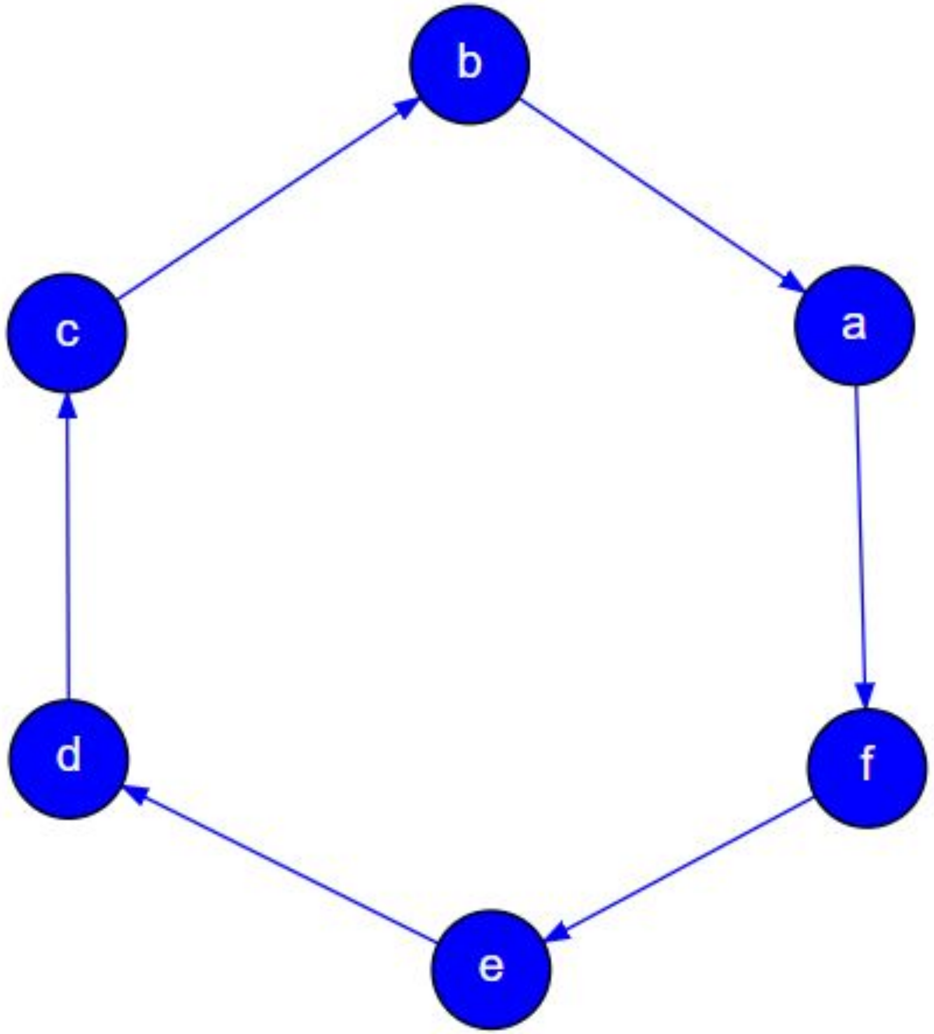
1. Find transformation CAT* that guarantees maximal expressiveness for biconnected outerplanar graphs
2. Extend CAT* to build transformation CAT that covers all outerplanar graphs
3. Use CAT to boost expressiveness of GNNs

CAT*
Transformation of a biconnected outerplanar graph

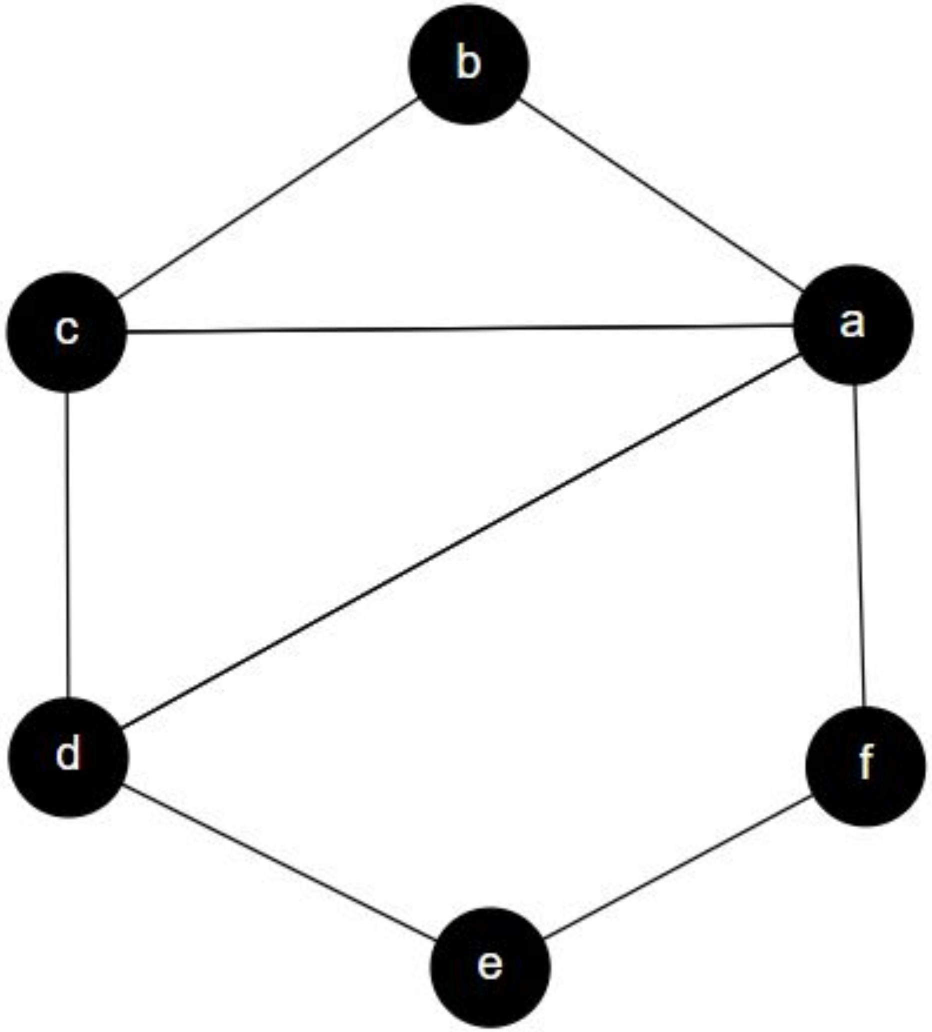


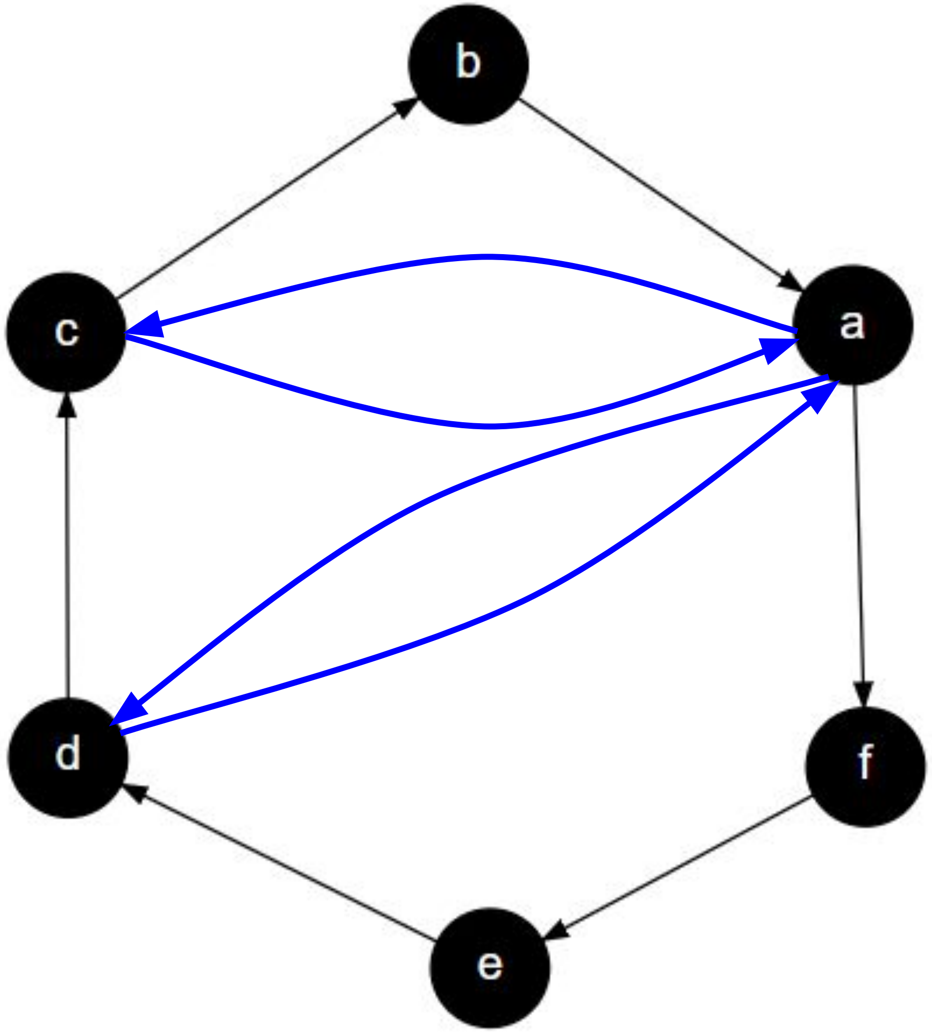
CAT*
1. Find directed Hamiltonian cycle C





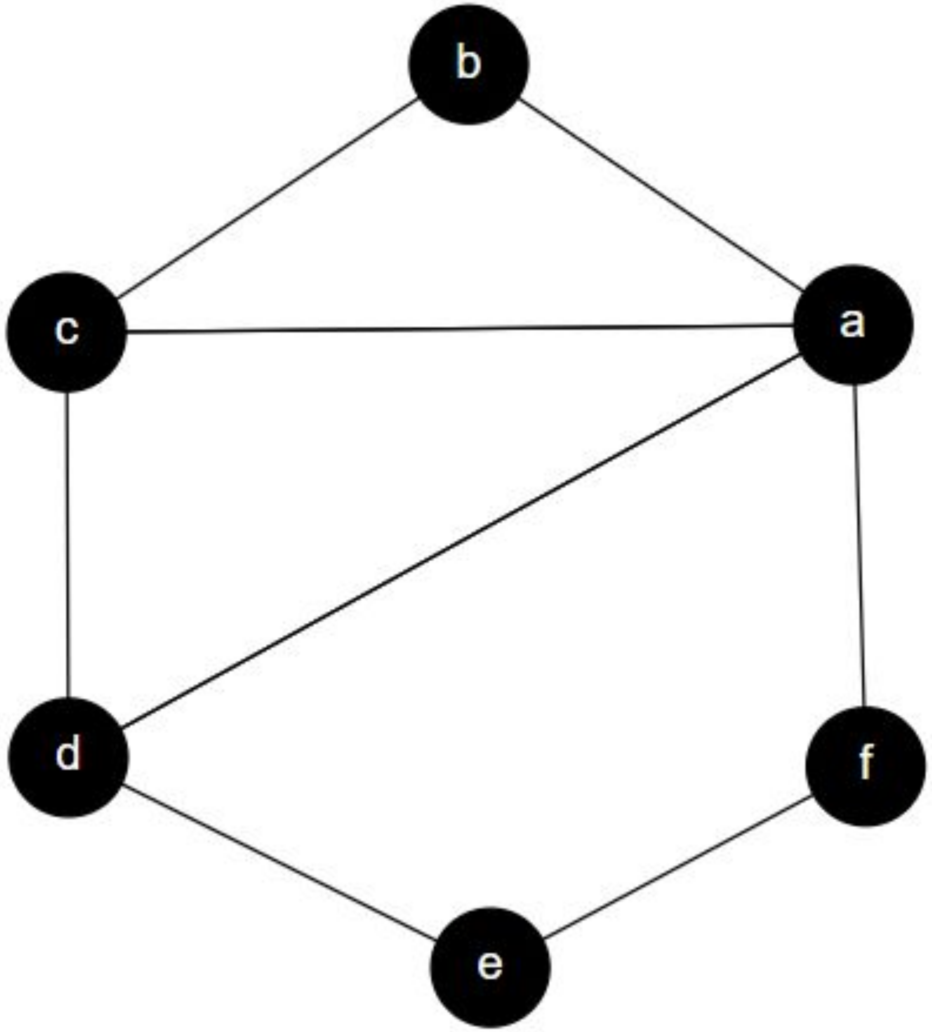
CAT*
3. Add edges not in the Hamiltonian cycle in both directions



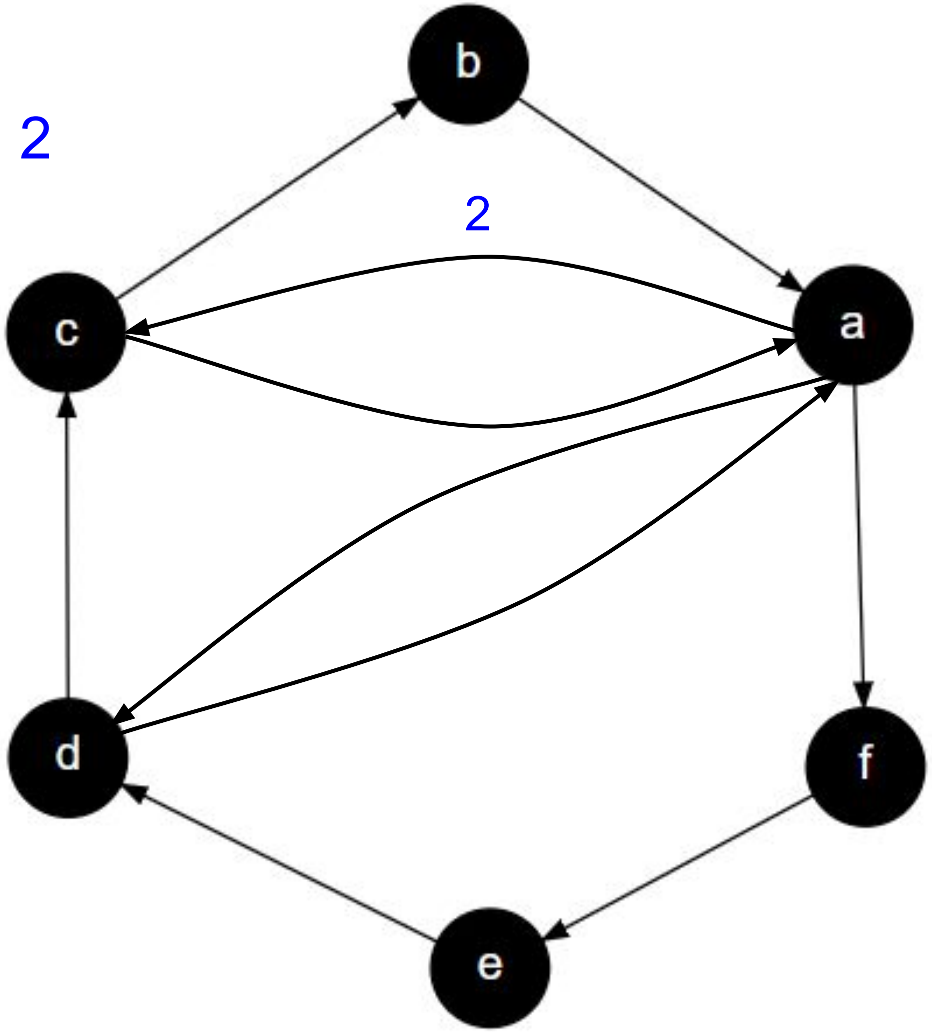


CAT*

4. Label the new edges (u, v) with their distance $d_C(v, u)$ according to HAL



$d_C(c, a) = 2$



CAT*

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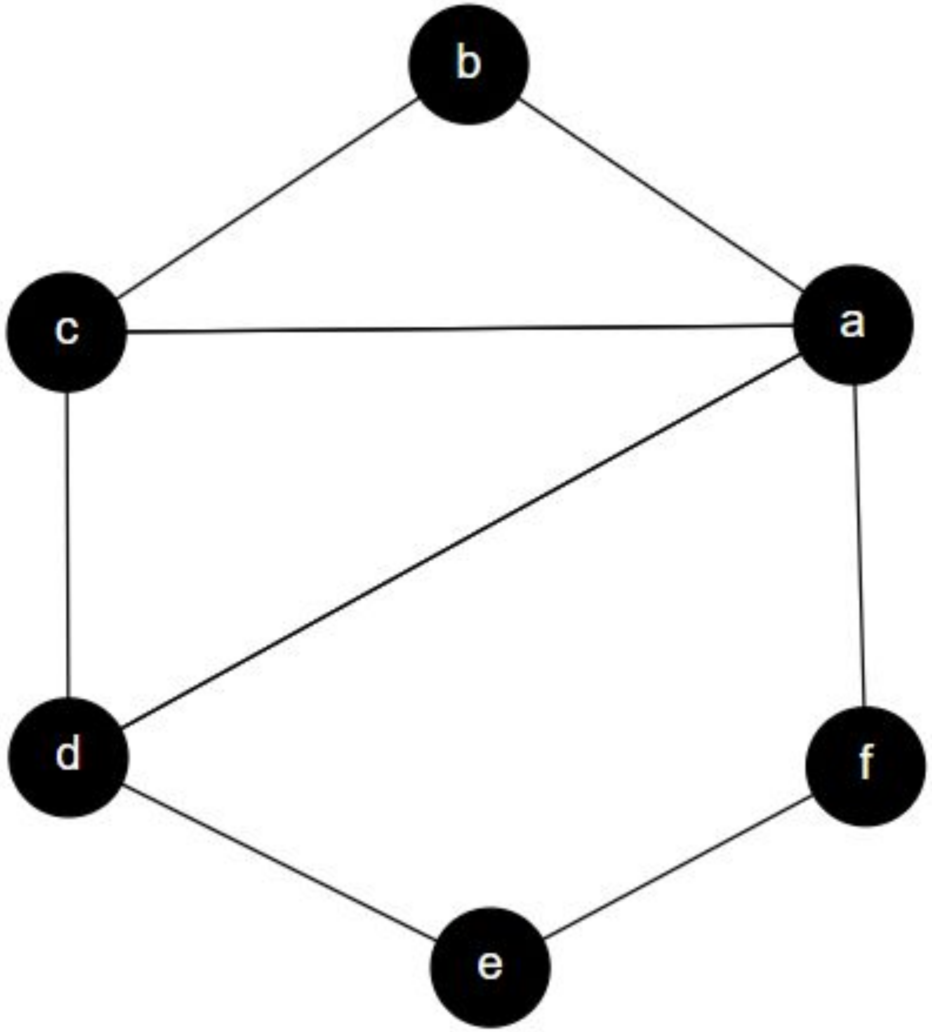
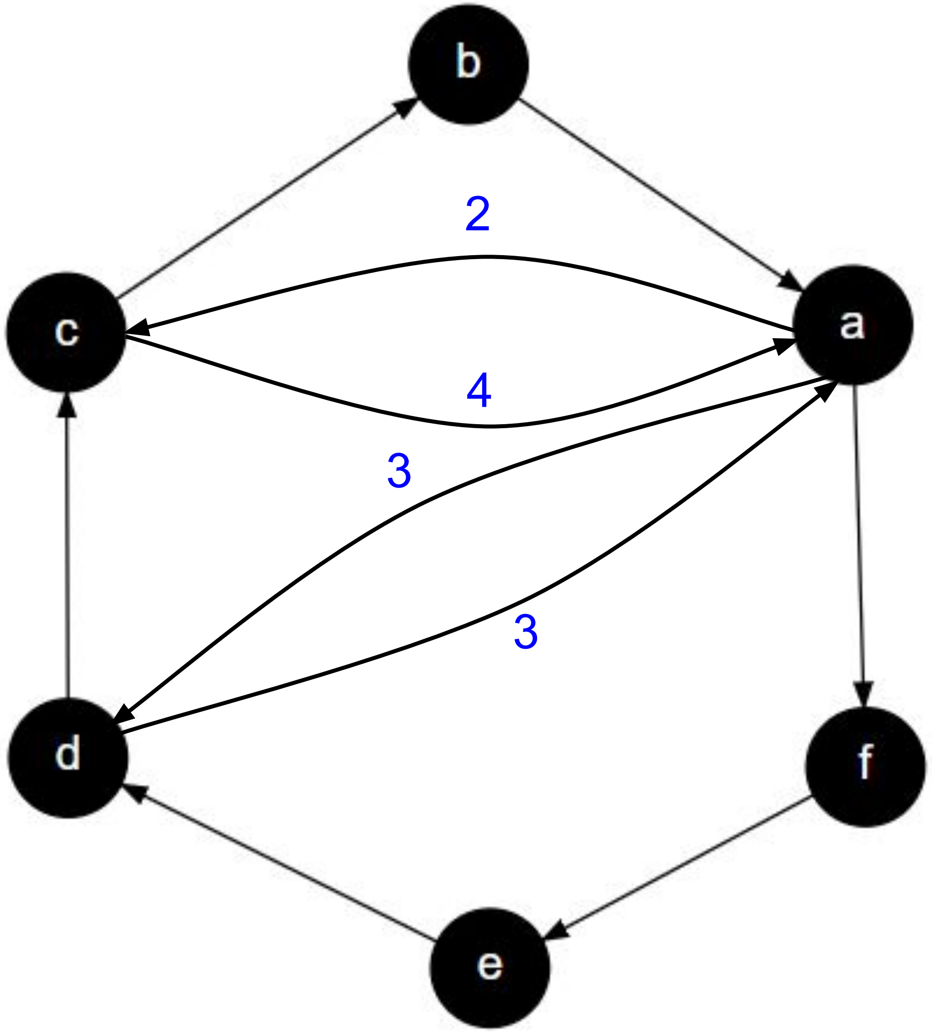
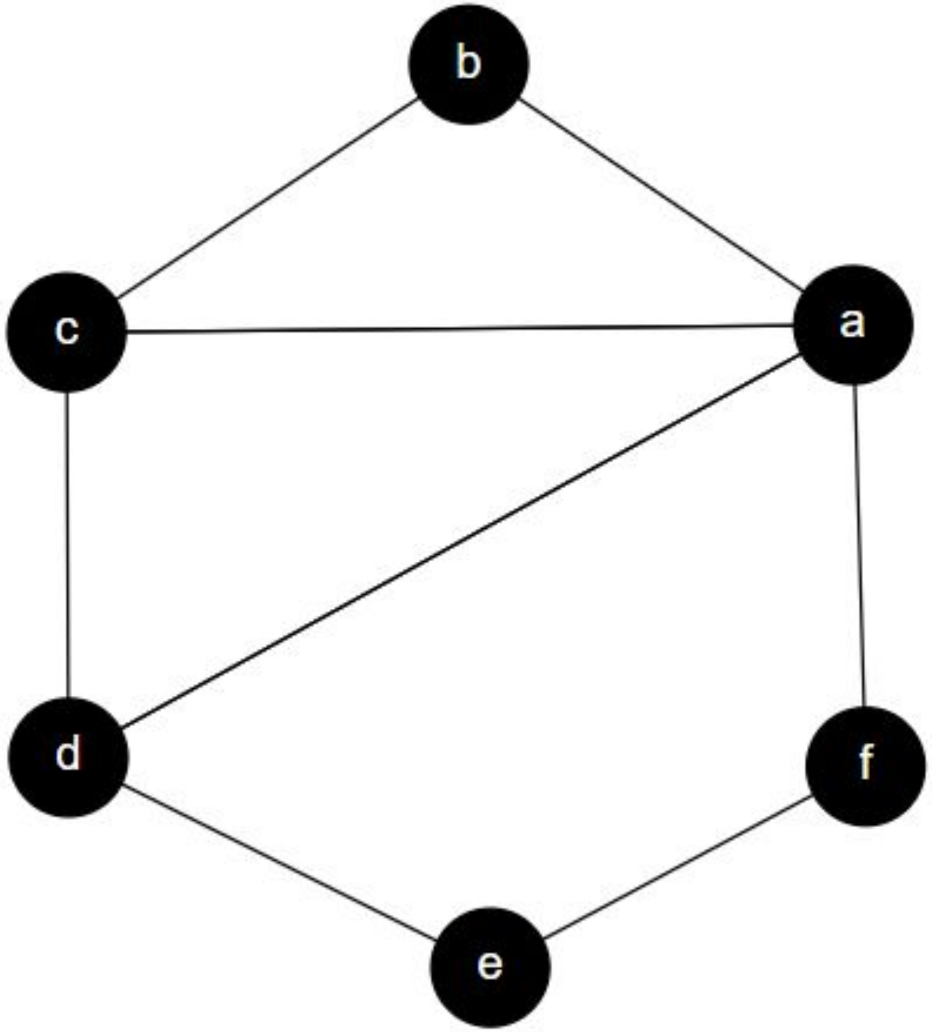
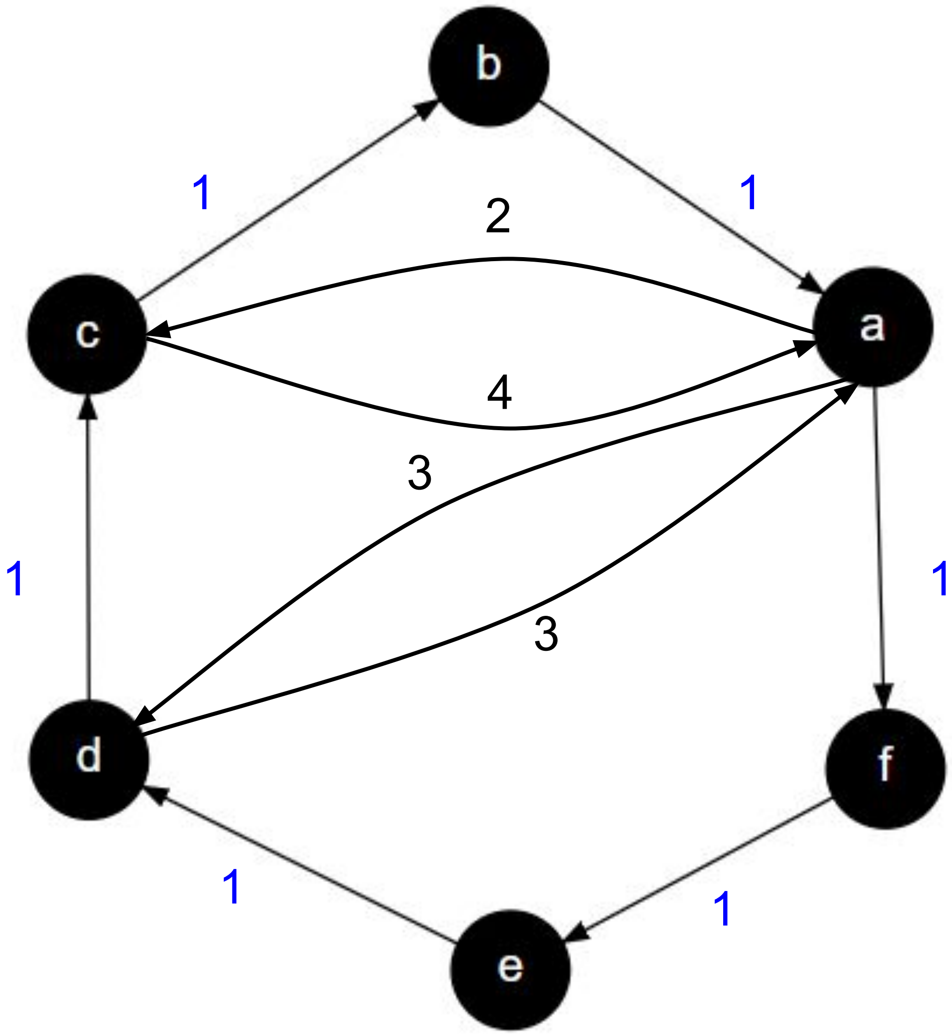




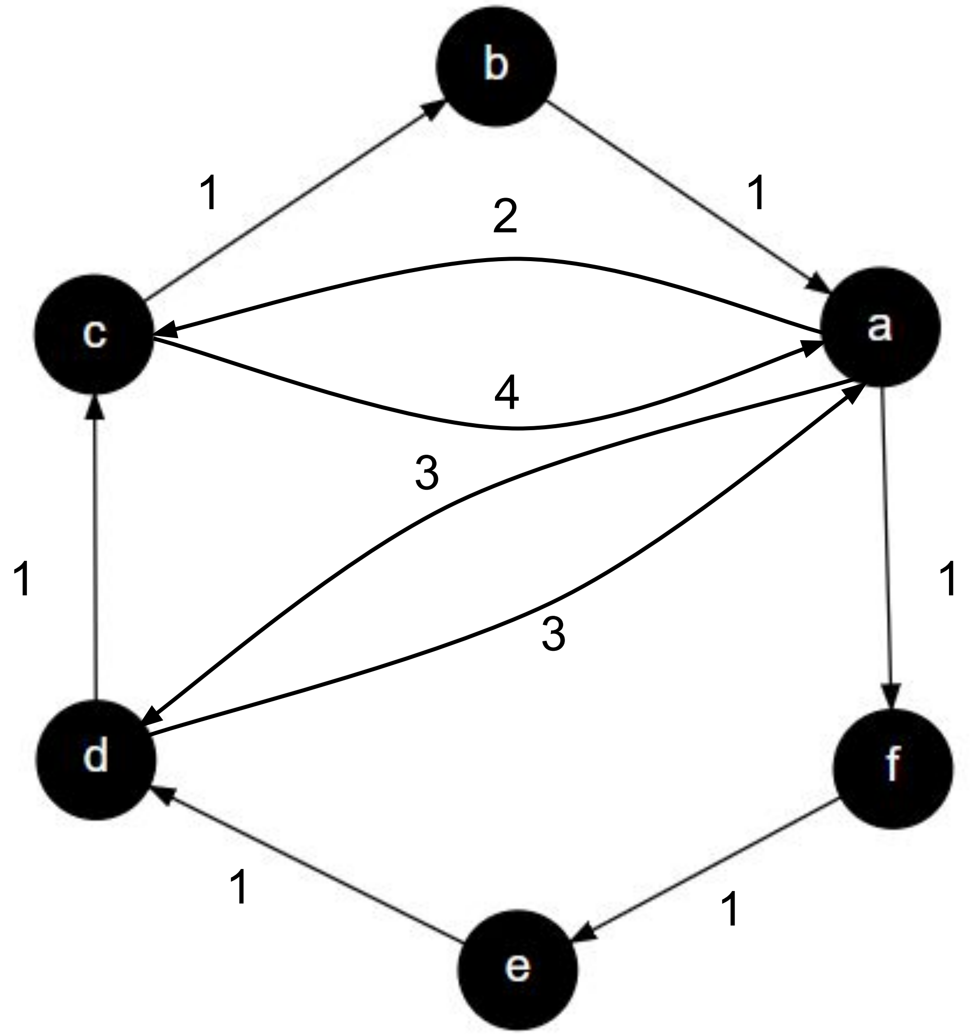
CAT*

2. Give on the directed Hamiltonian cycle C all the edges weight 1



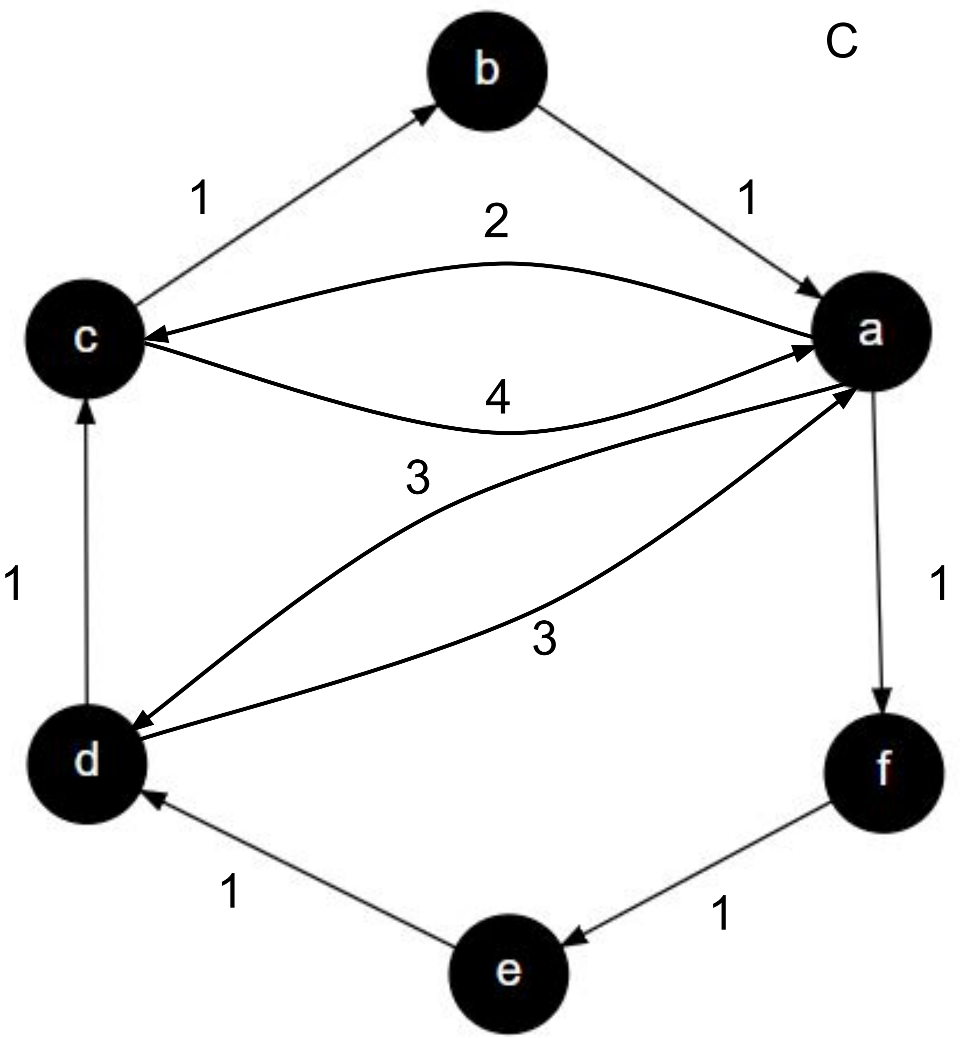


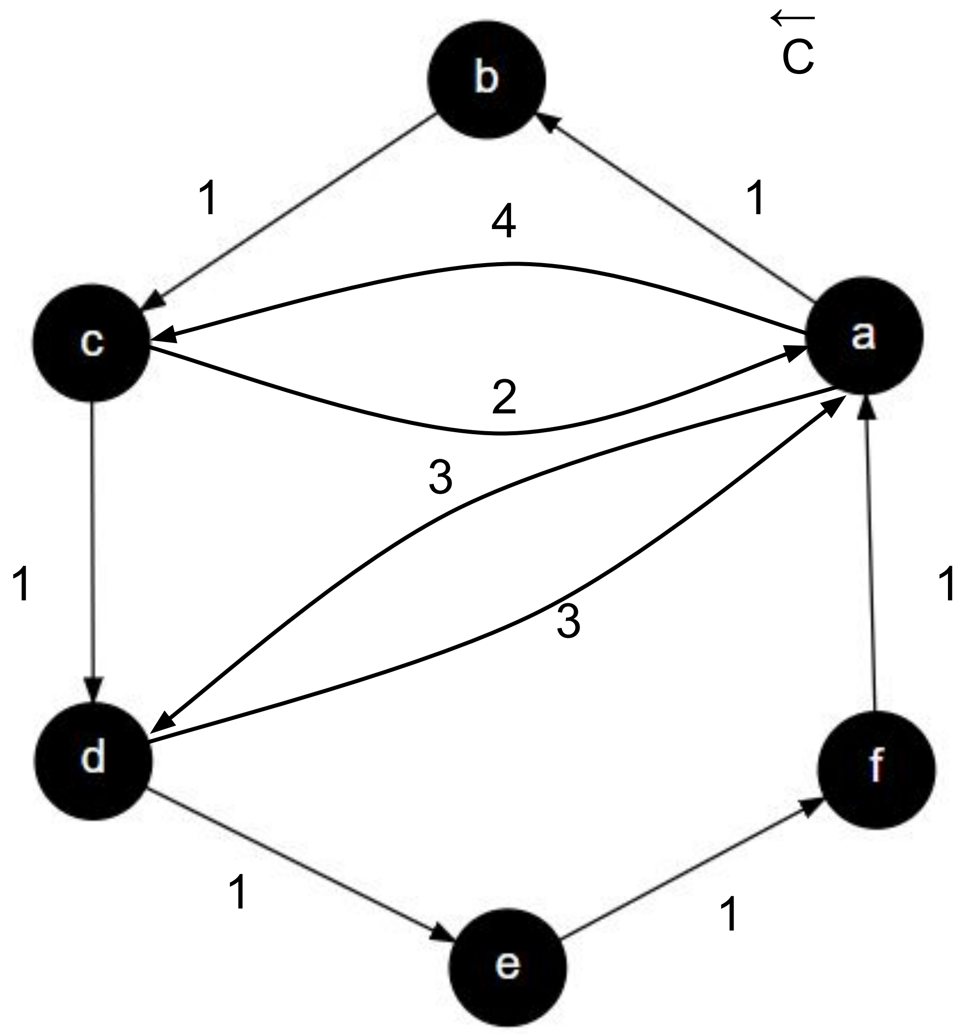
CAT*



CAT*

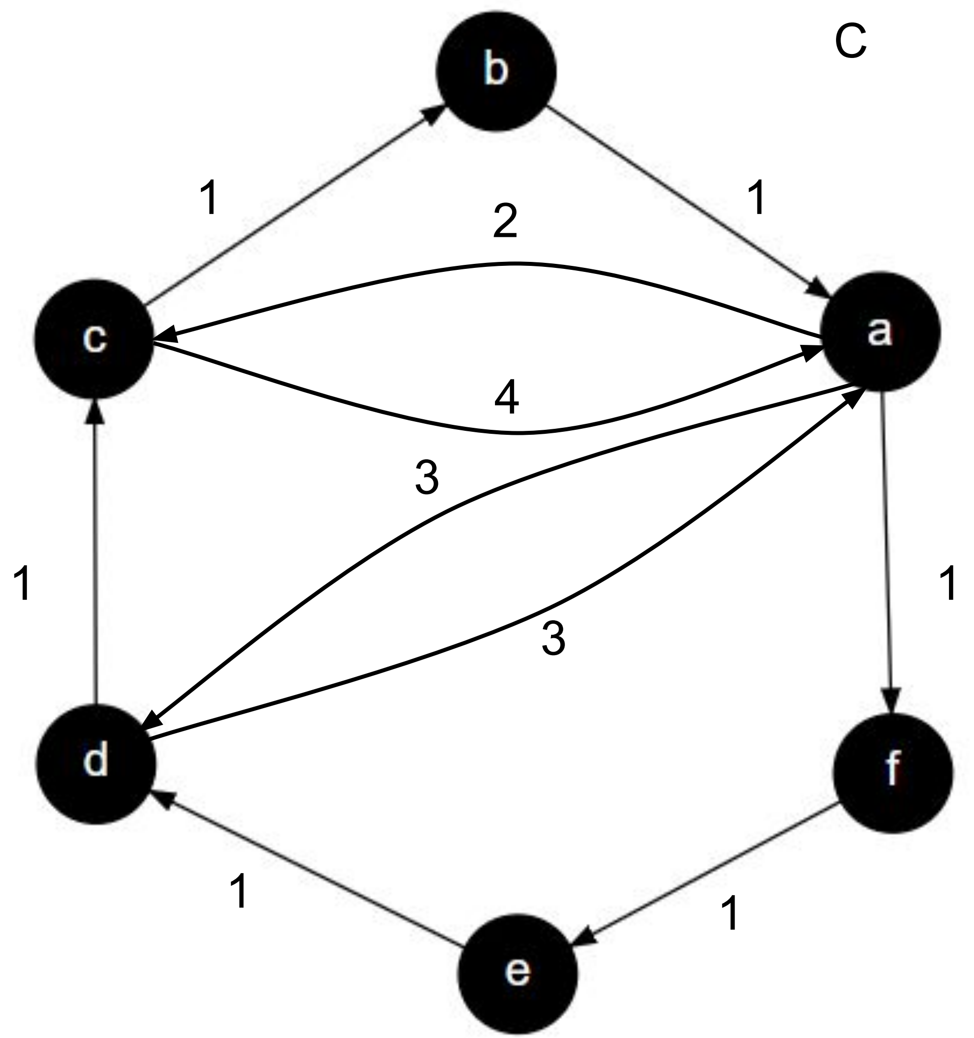
Repeat the whole procedure on the reverse hamiltonian cycle $\overleftarrow{C}$

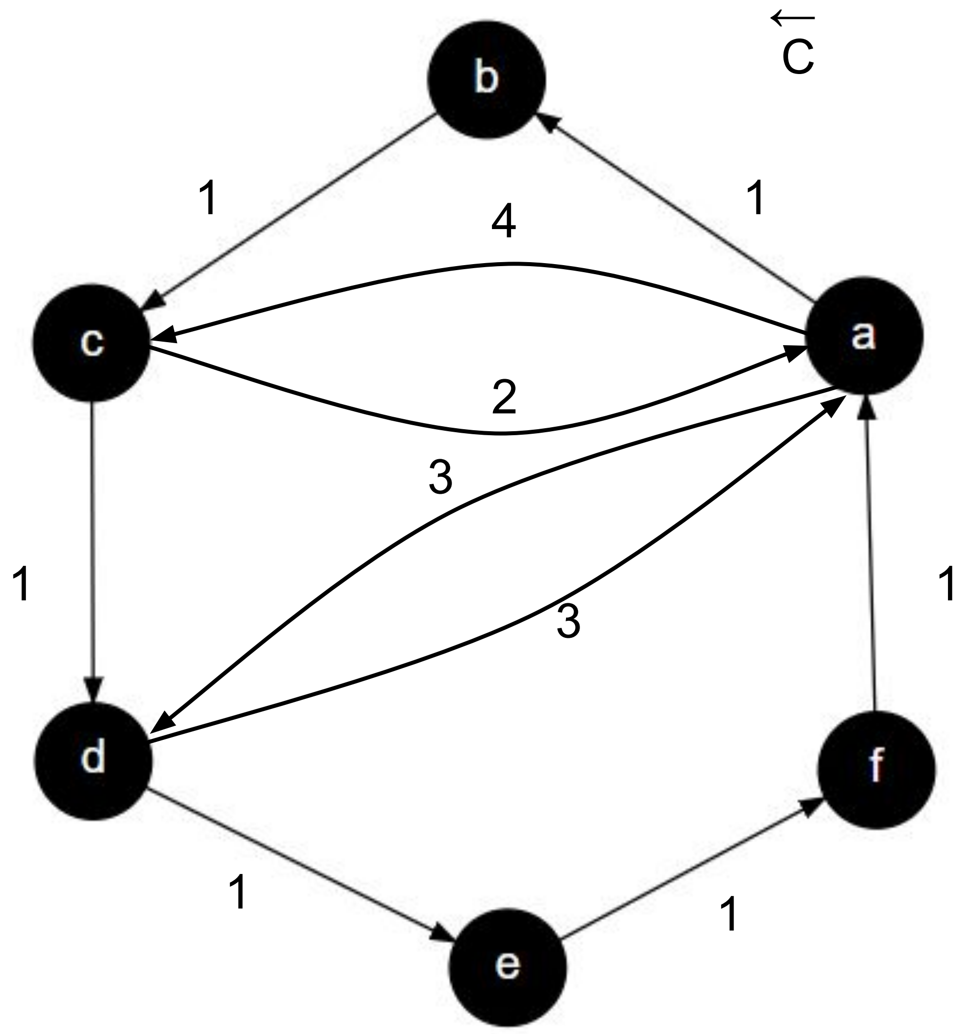




CAT*

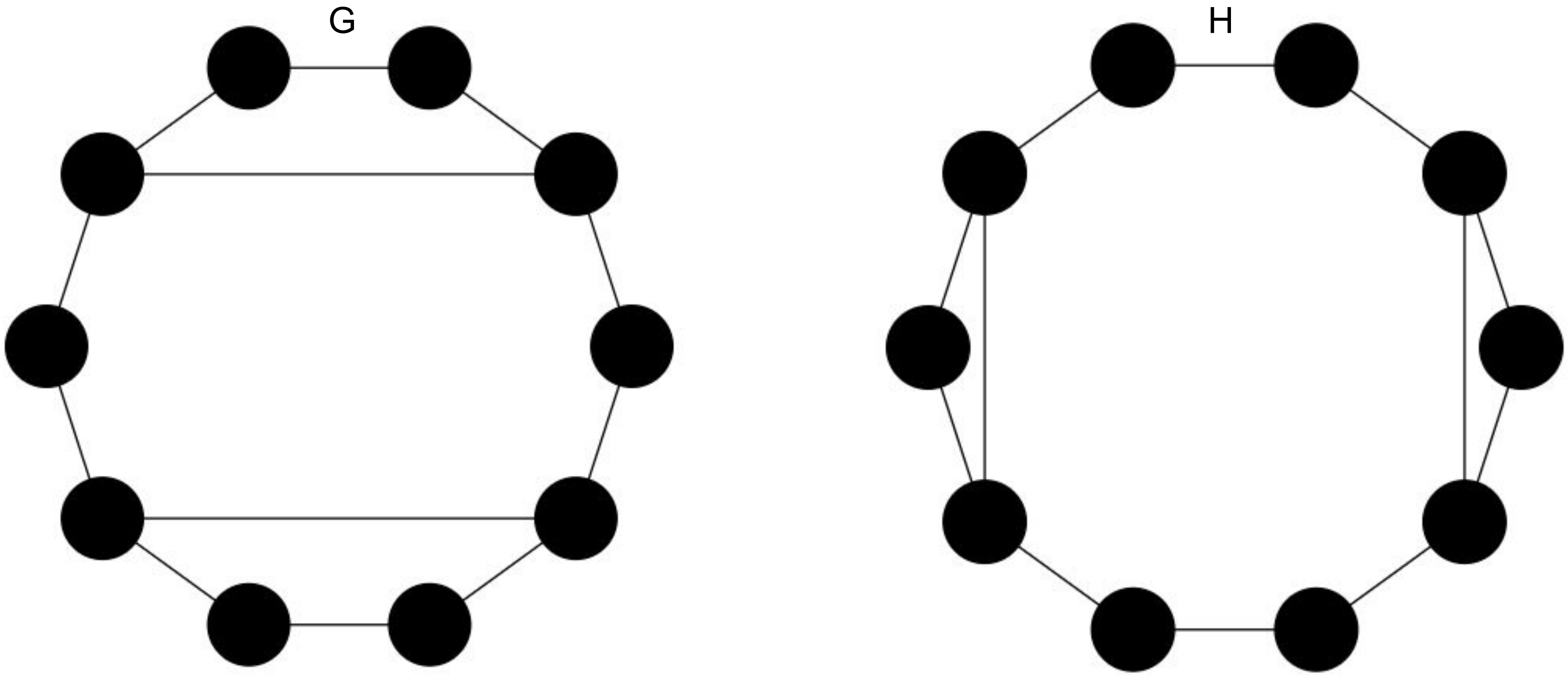
The output of this transformation is 2 connected components





CAT*

Theorem 3: Two biconnected outerplanar graphs G and H are isomorphic, iff WL(CAT*(G)) = WL(CAT*(H))



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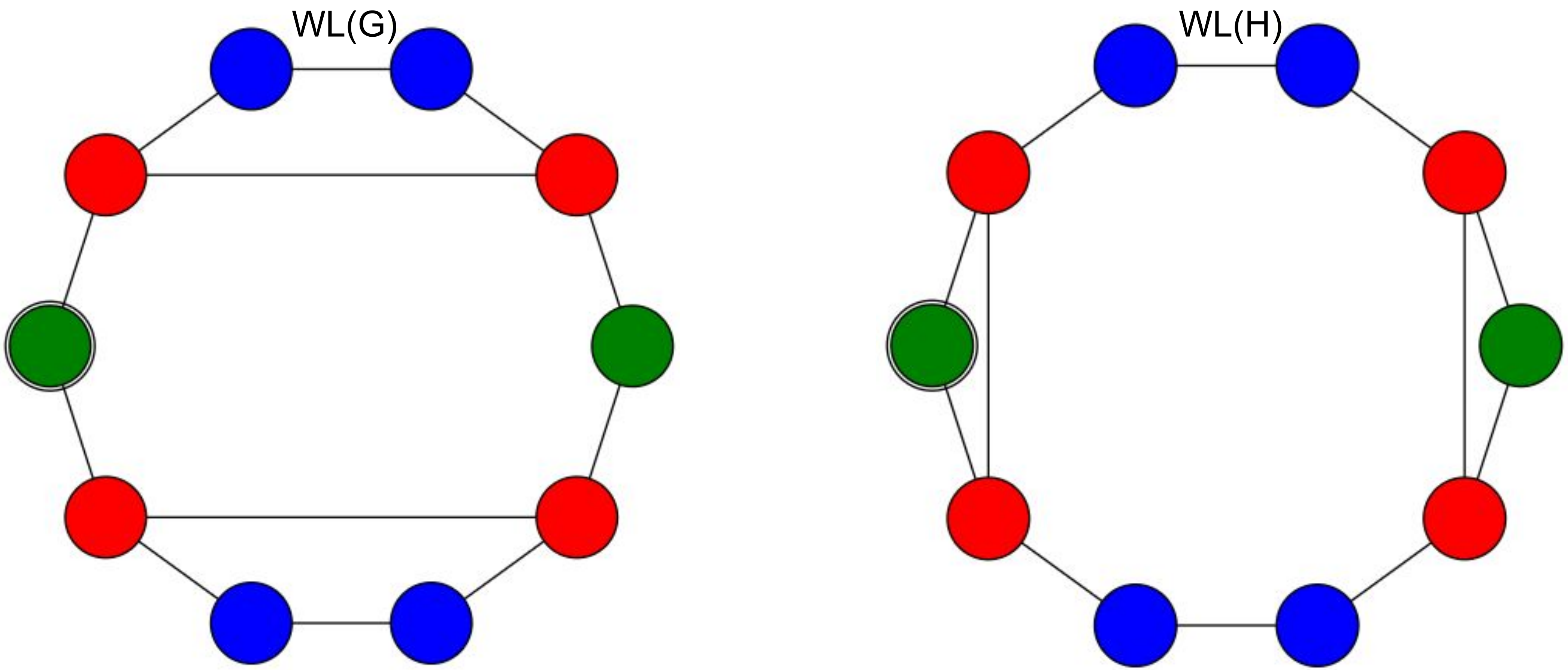

CAT*

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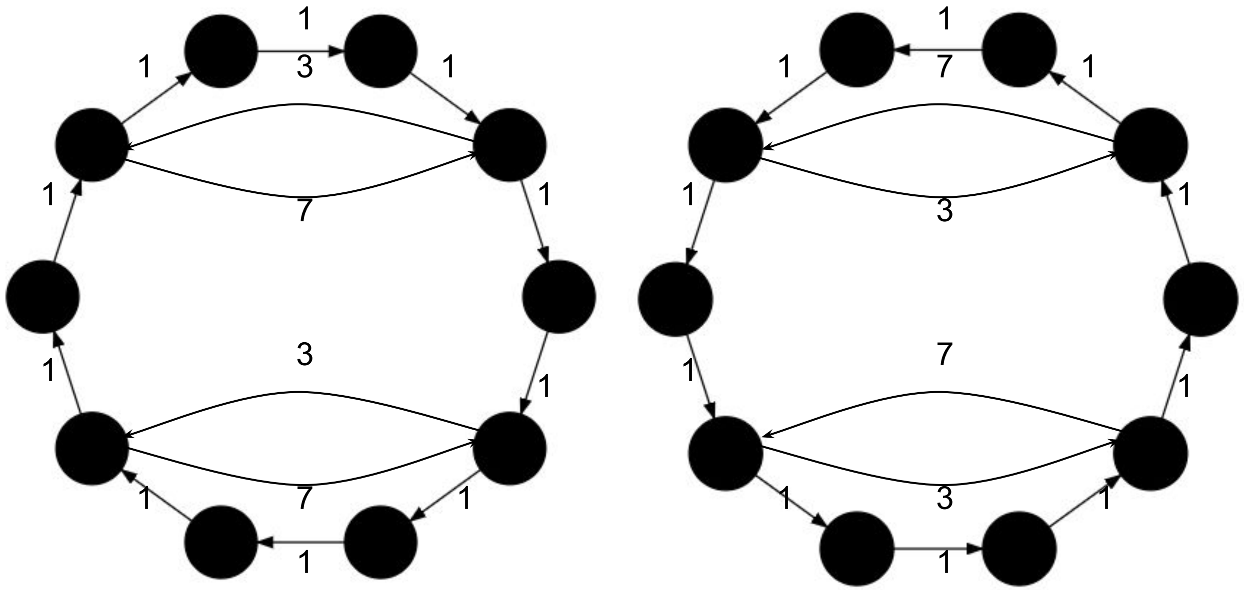
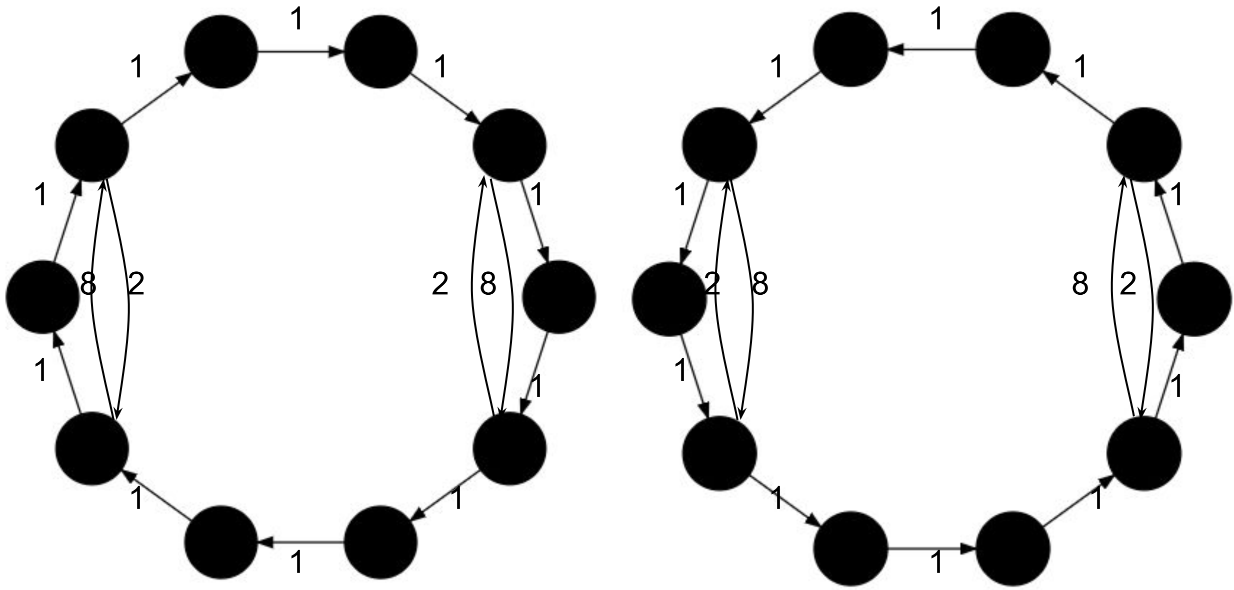
CAT*(G)



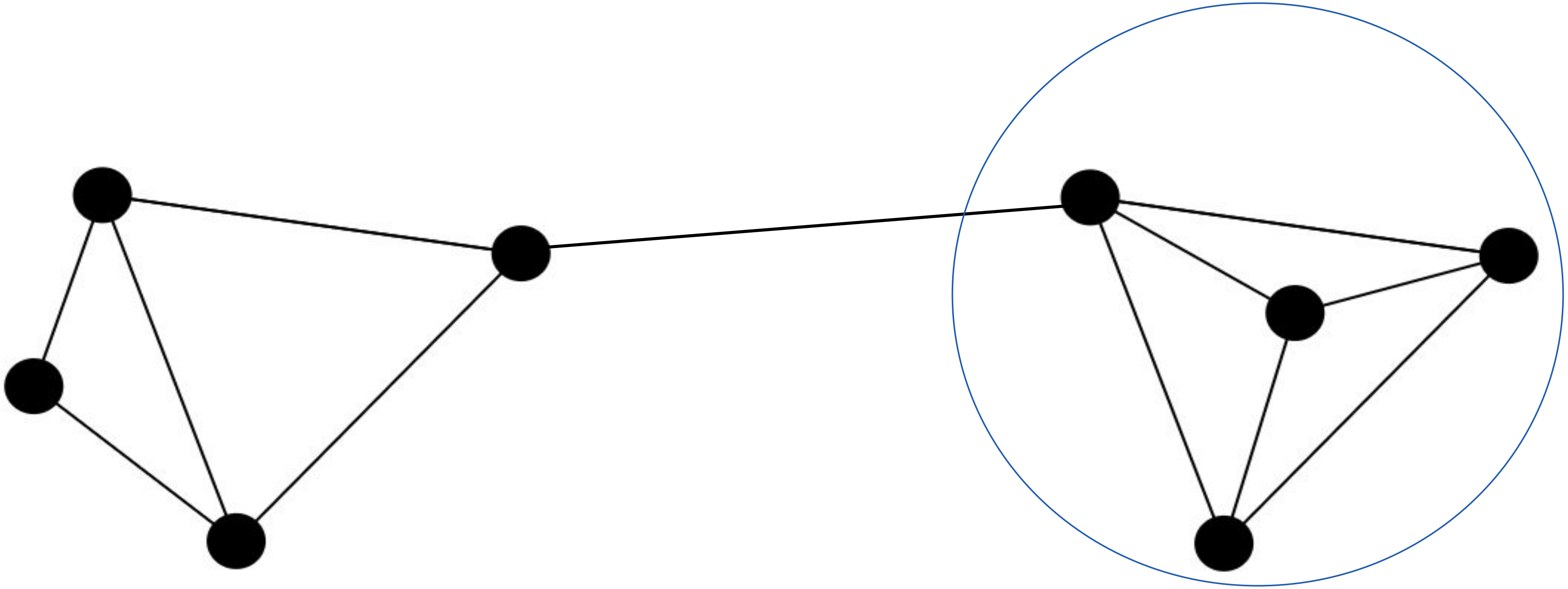
CAT*(H)



Next step:
Let’s extend this to all outerplanar graphs.

Biconnected components and blocks

A biconnected component is a maximal biconnected subgraph (with at least 3 nodes)



Biconnected components and blocks

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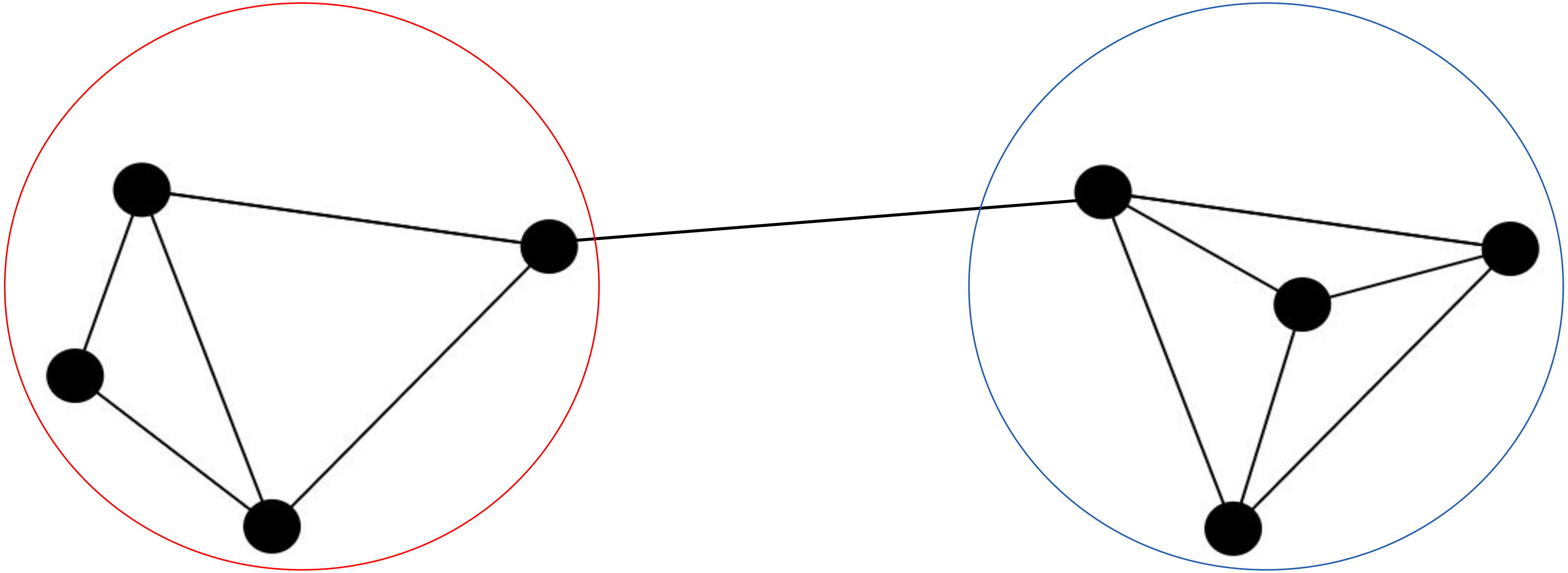
A block is a biconnected outerplanar component



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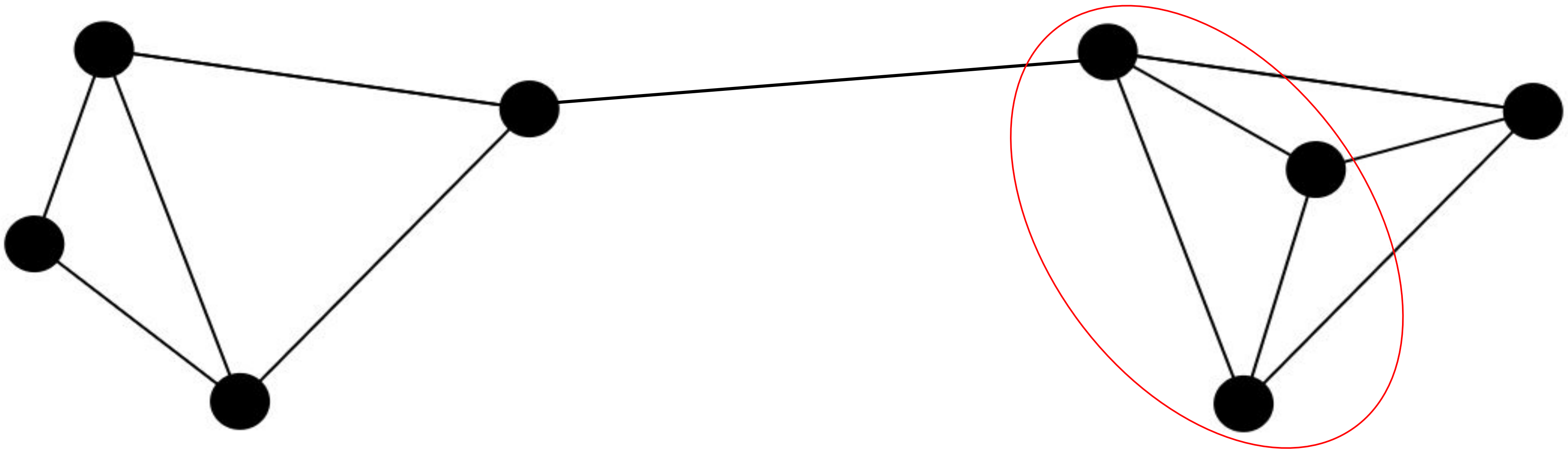

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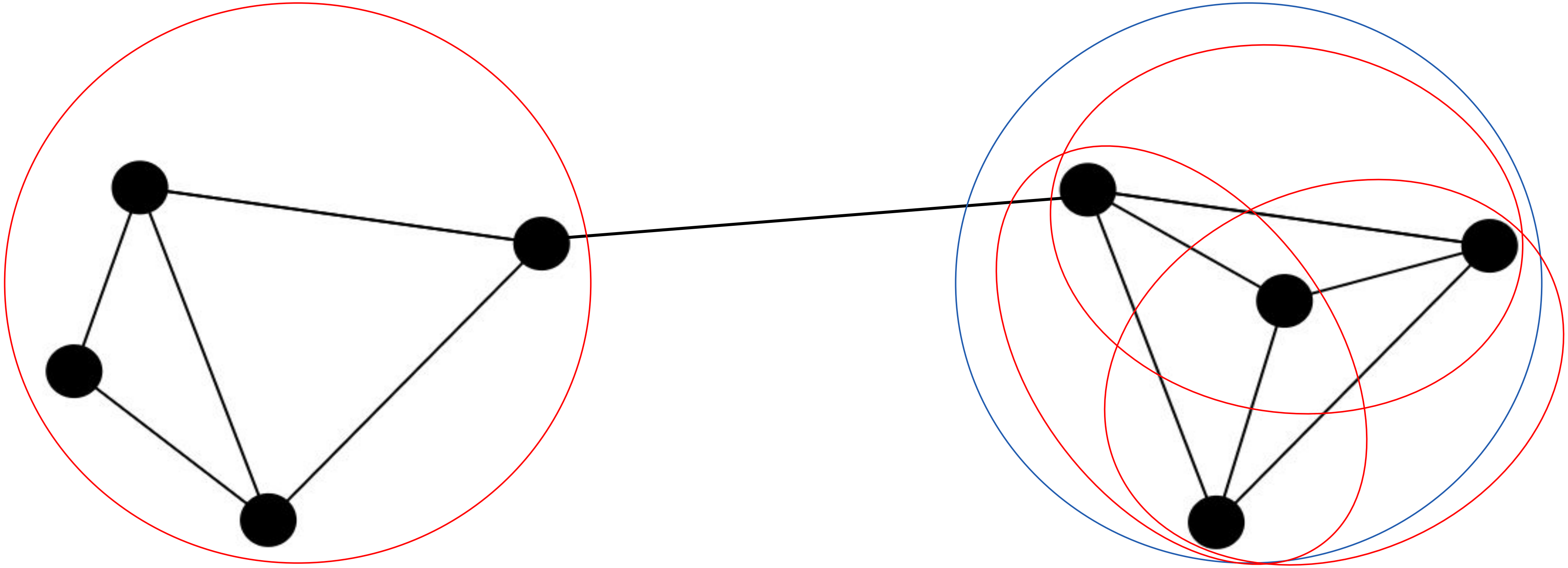

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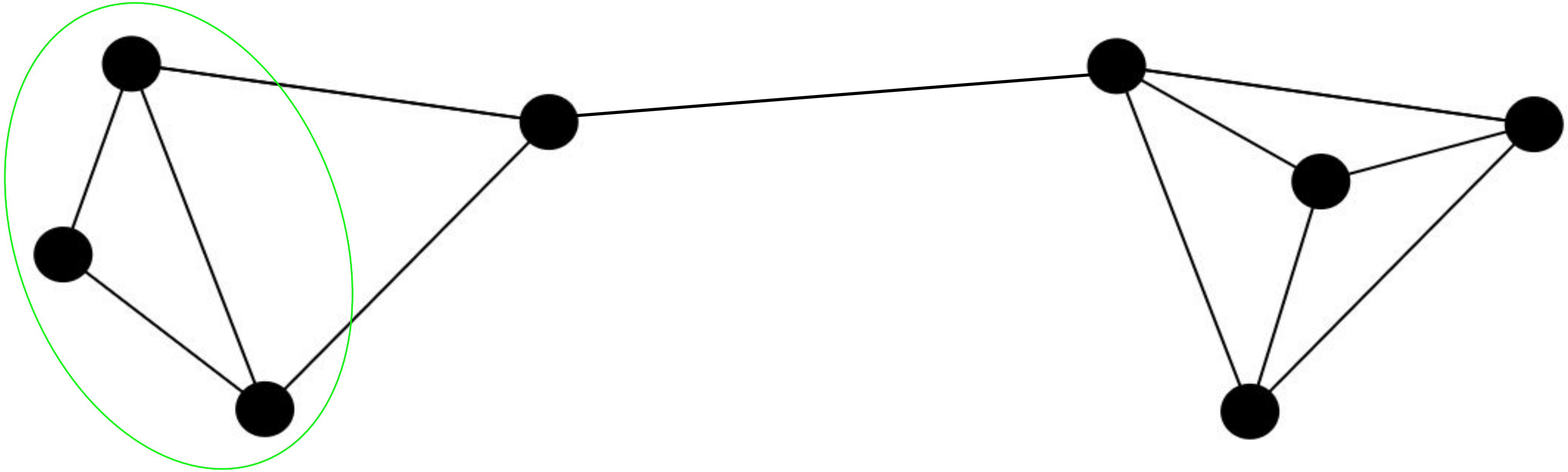
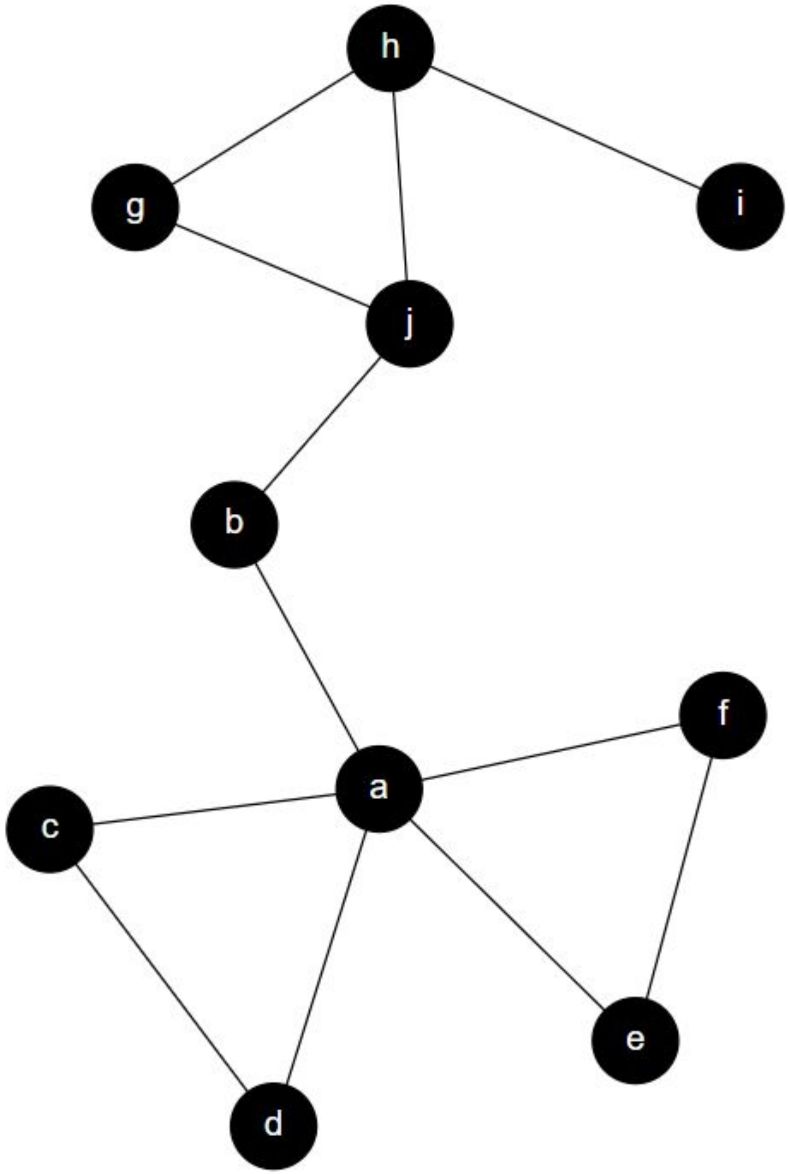
Not maximal

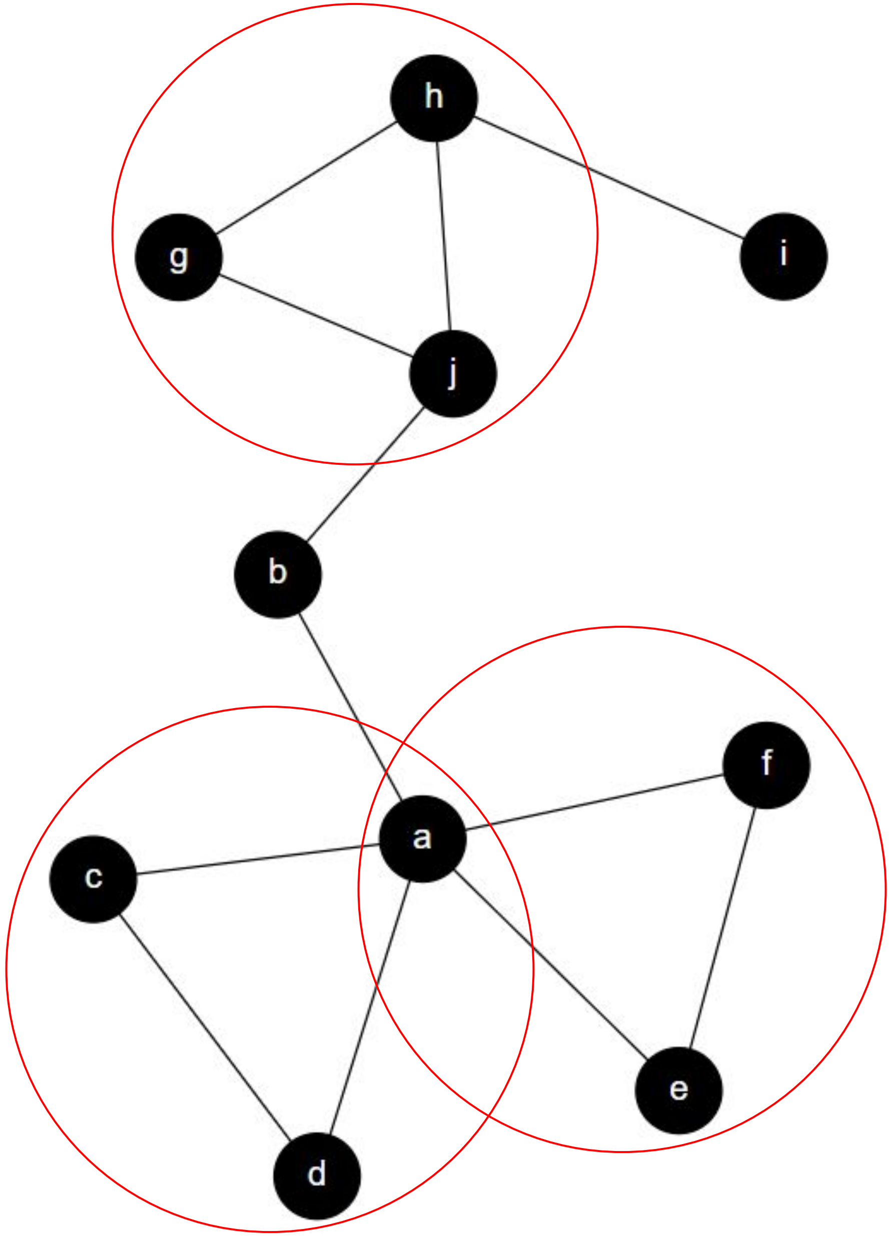


CAT

Transformation of an outerplanar graph

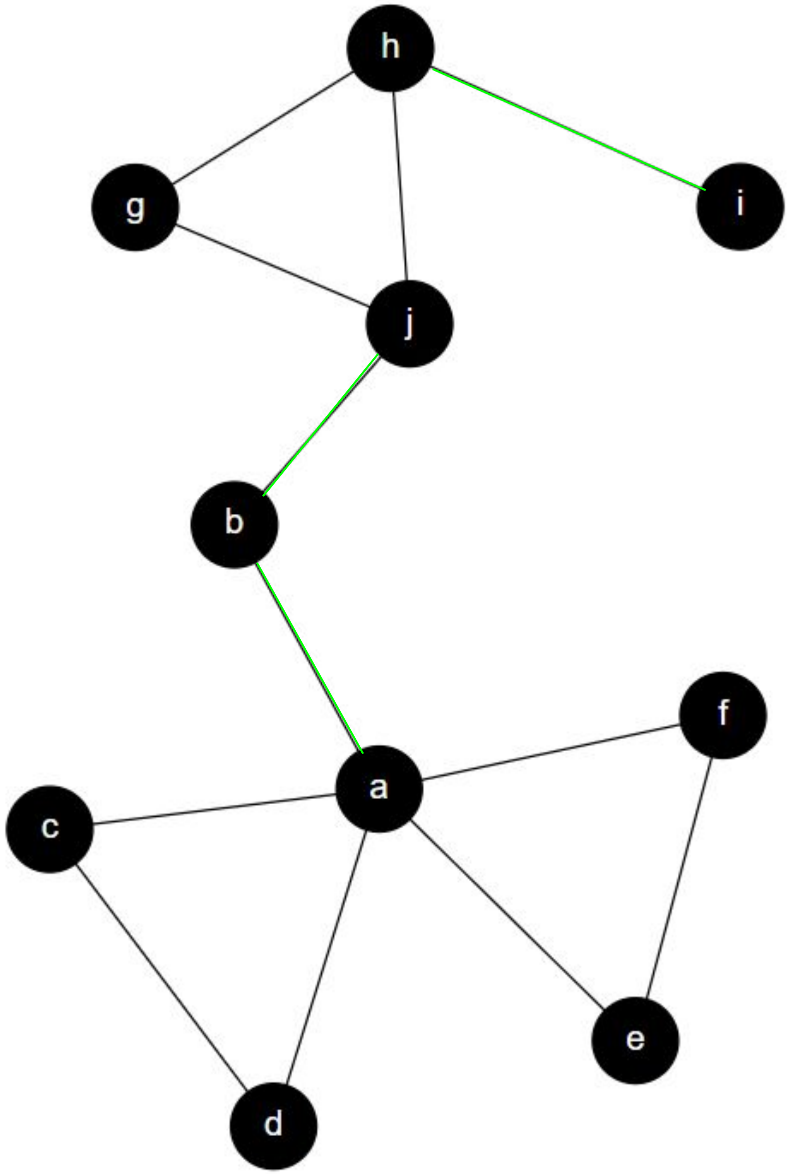


CAT
1. Identify blocks



CAT

2. Let F be the graph induced by the edges that are in none of the blocks



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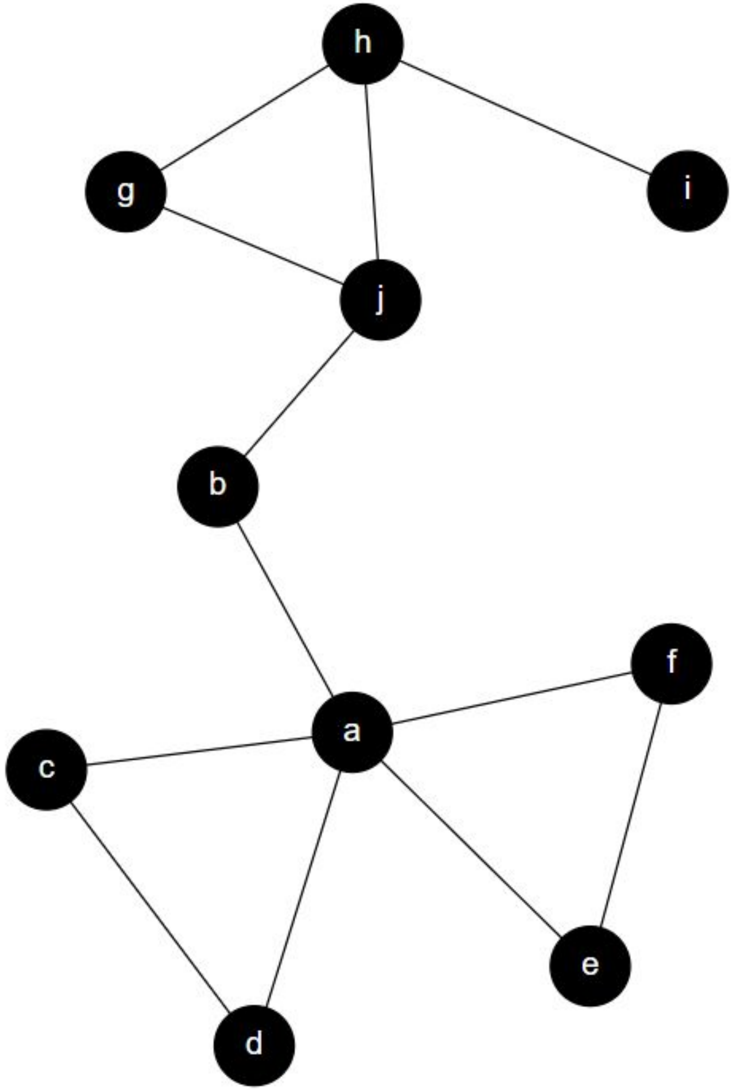
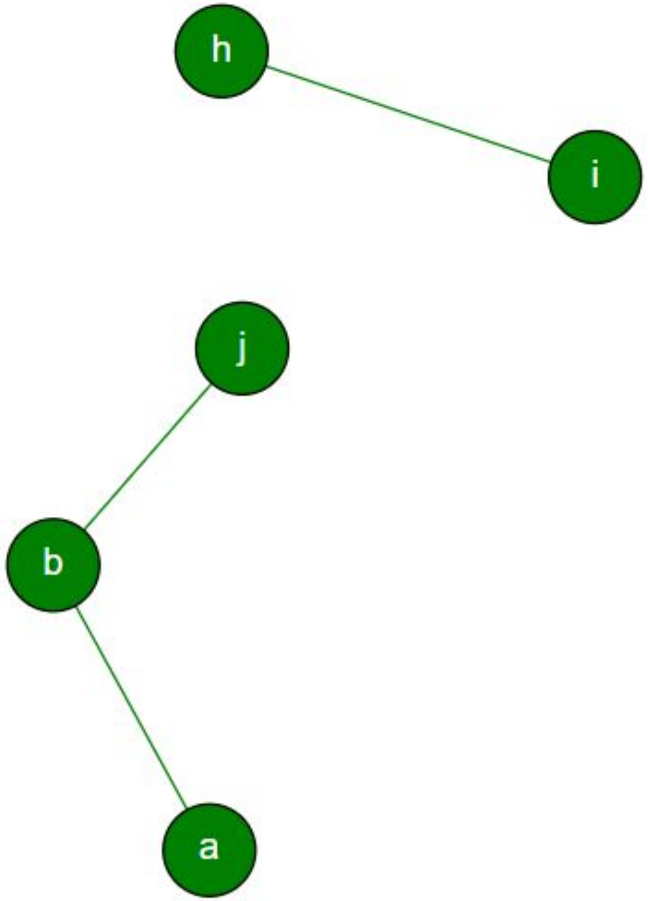
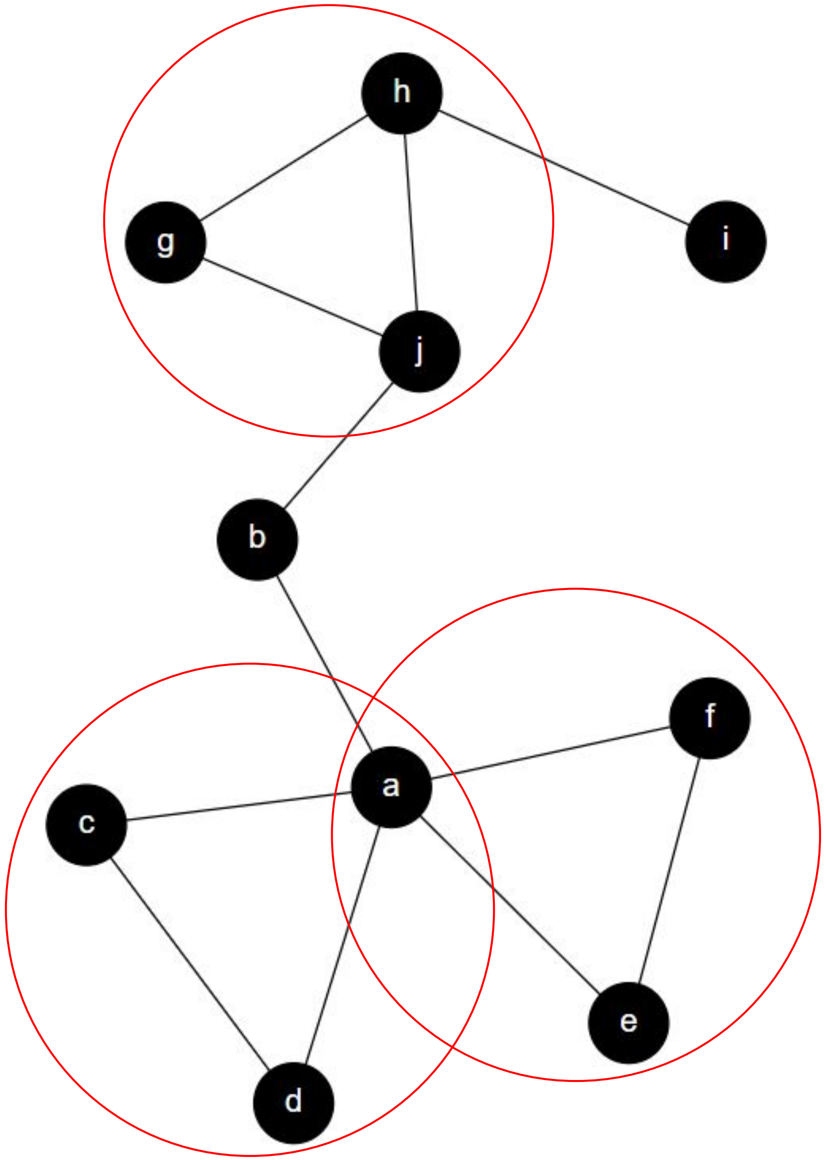
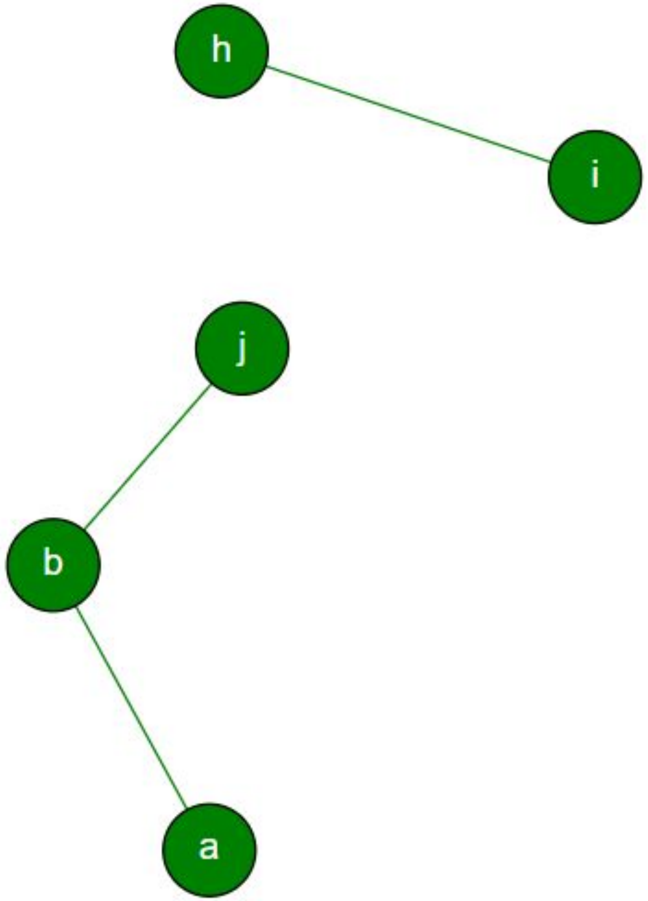




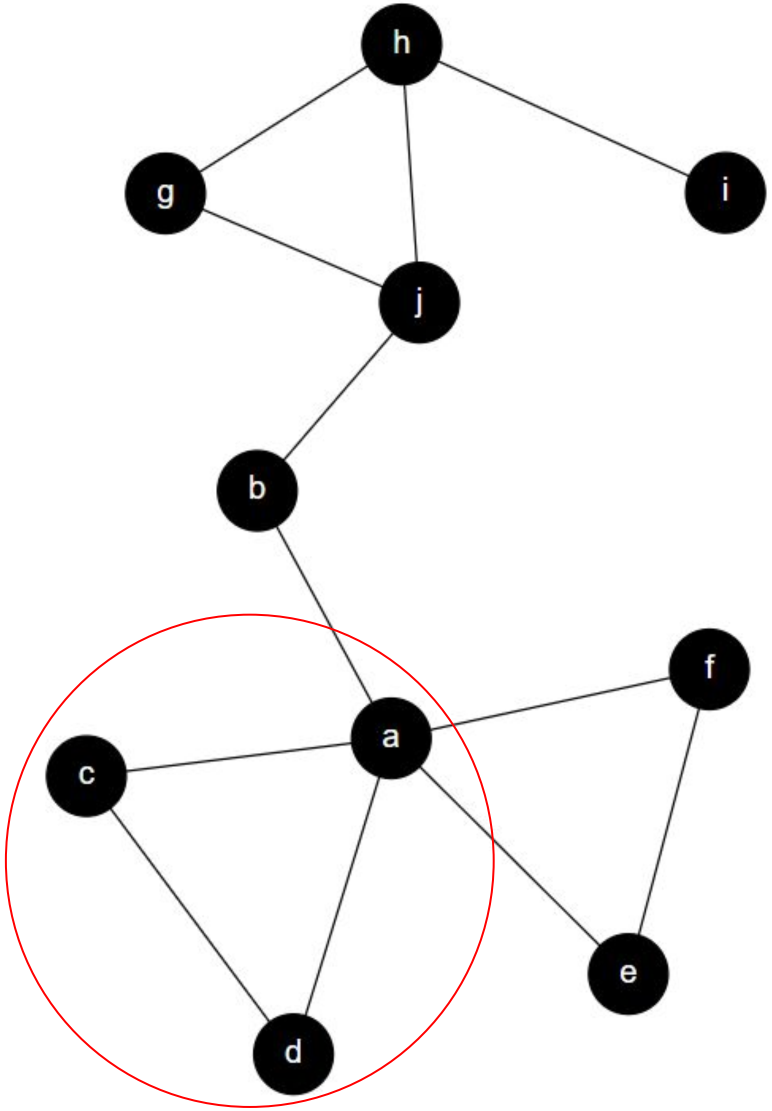
CAT
3. For all blocks B_i

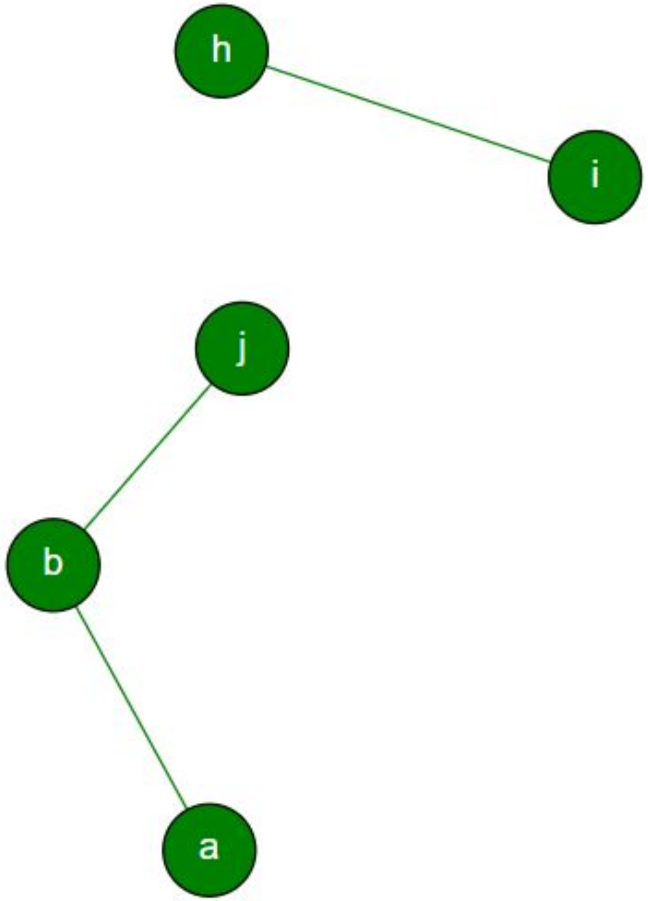




CAT

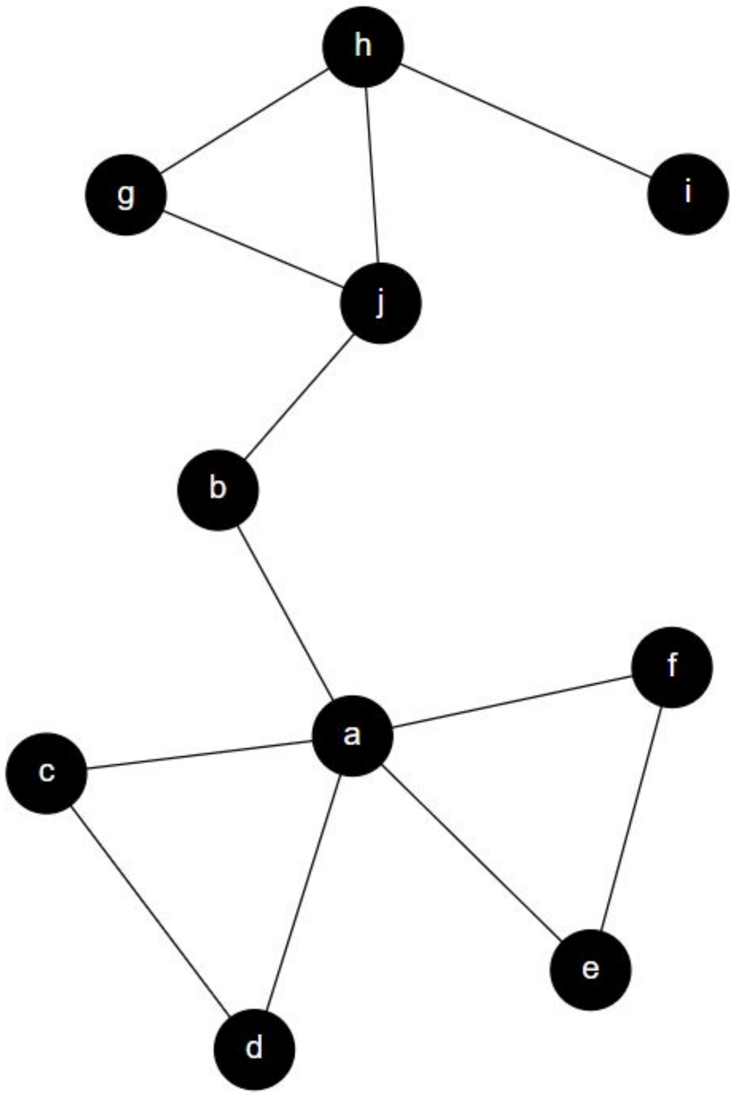
3. Let's start with block B_1

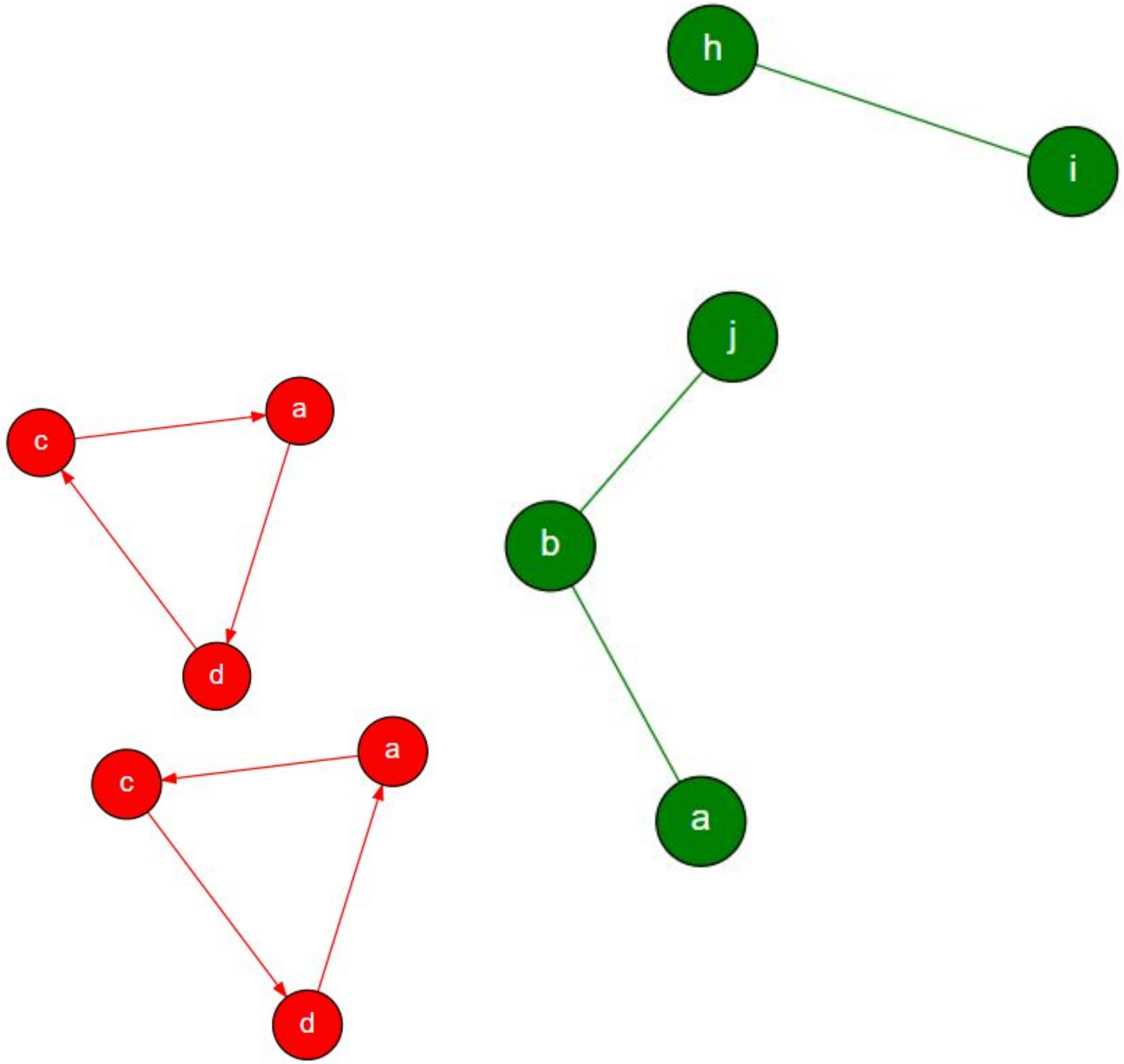




CAT

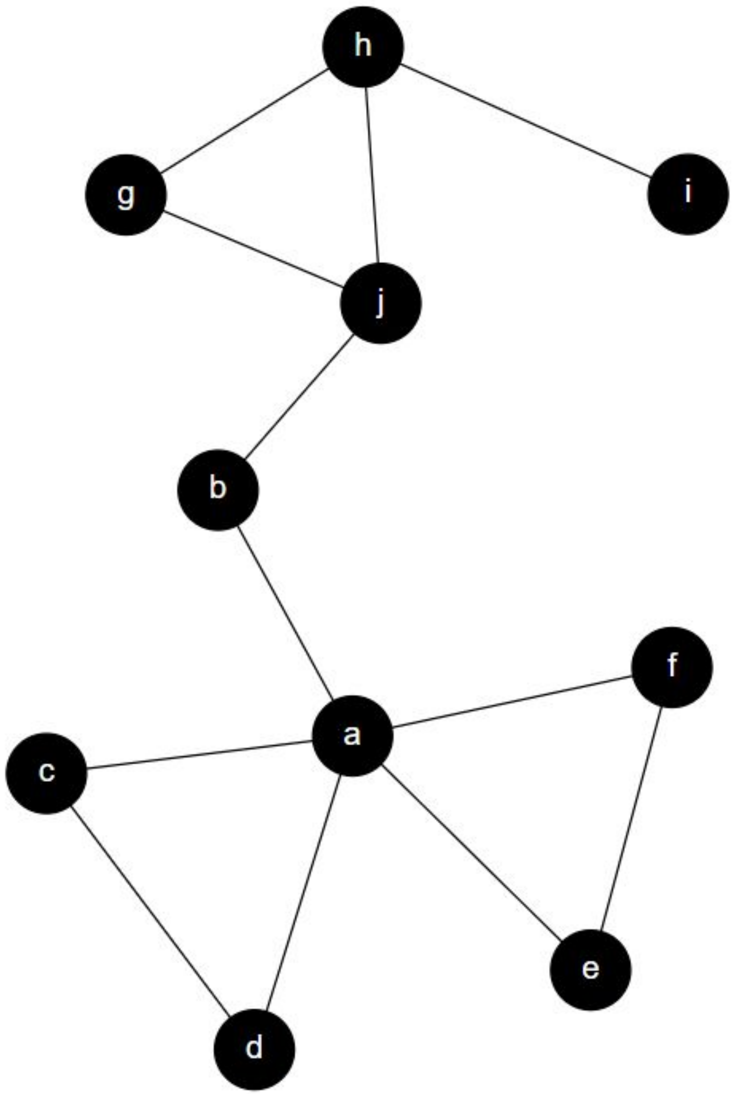
3.1 Add the 2 connected components B'_i, $\overleftarrow{B'}_i$ from CAT*(B_i)

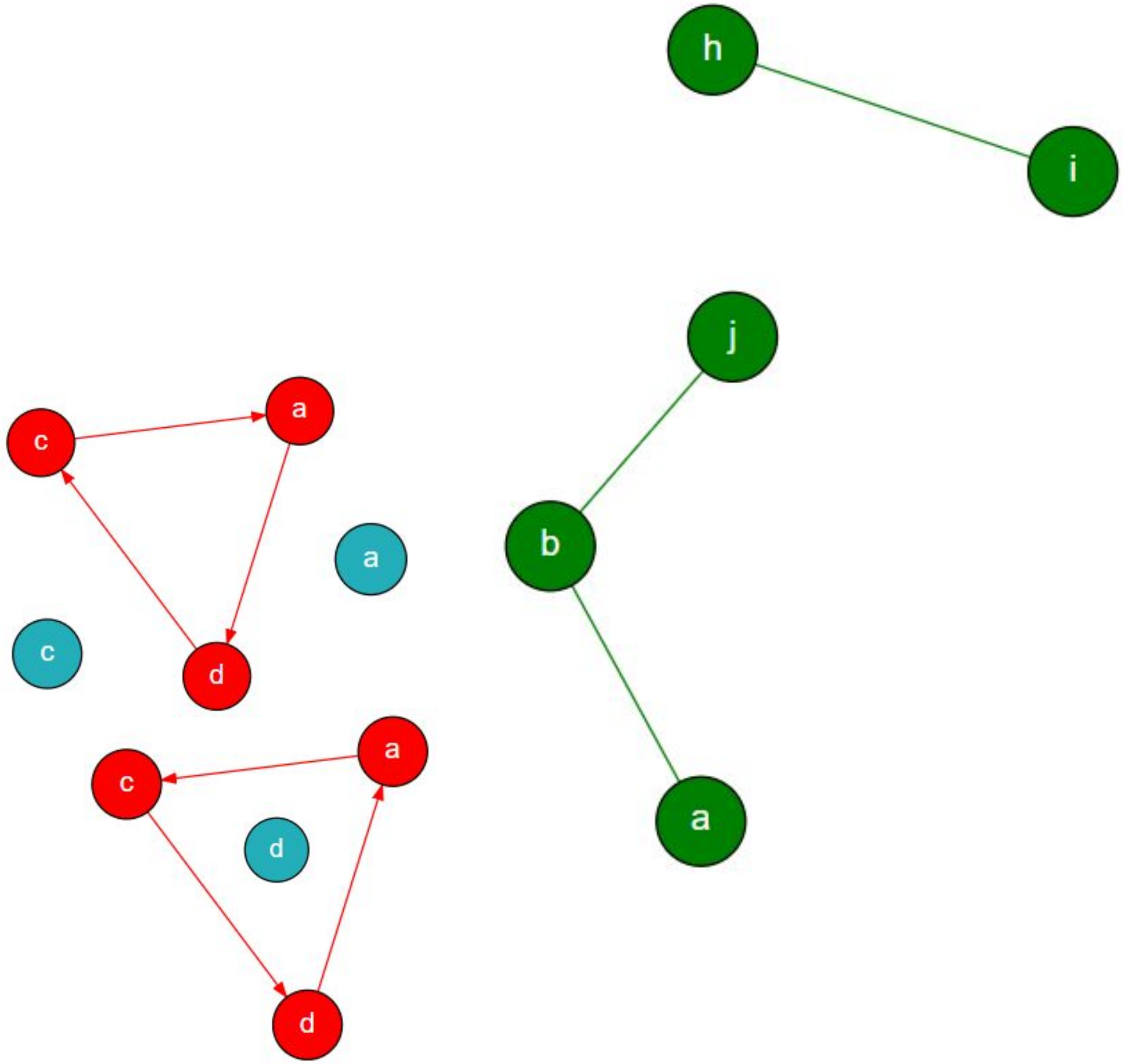




CAT

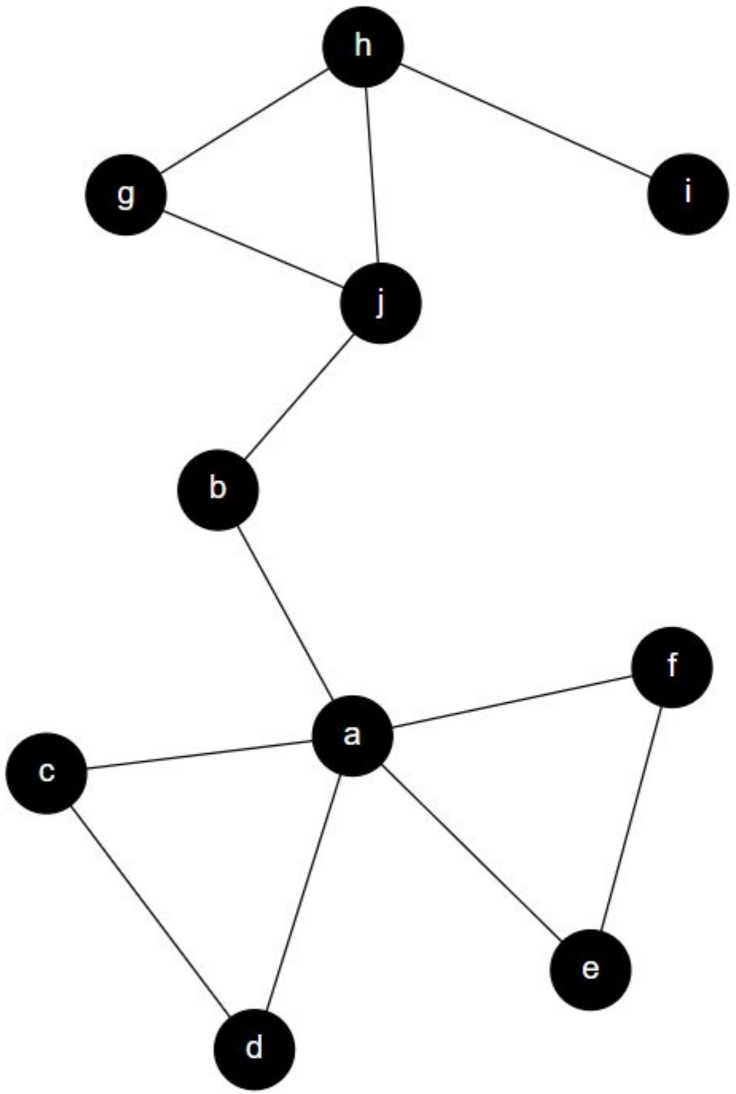
3.4 For all pairs of nodes v, $\overleftarrow{v}$ in B'_i, $\overleftarrow{B'}_i$, add a node p_v

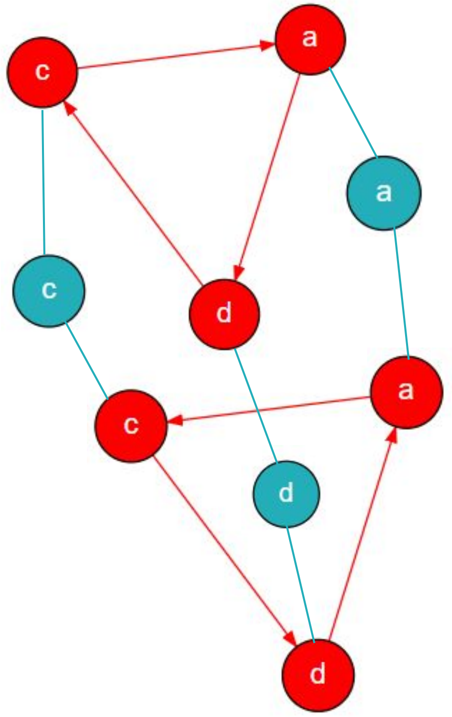


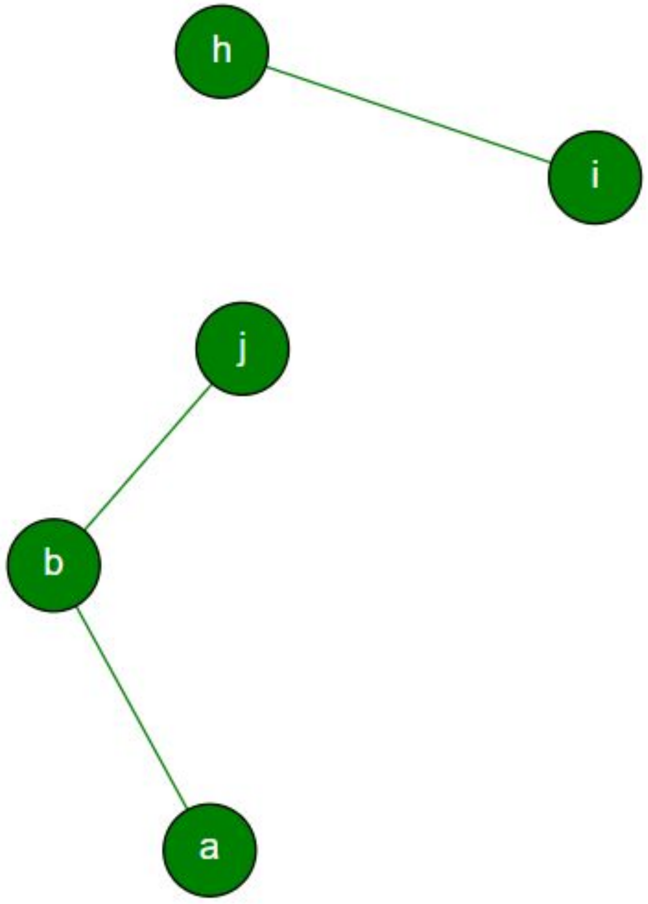


CAT

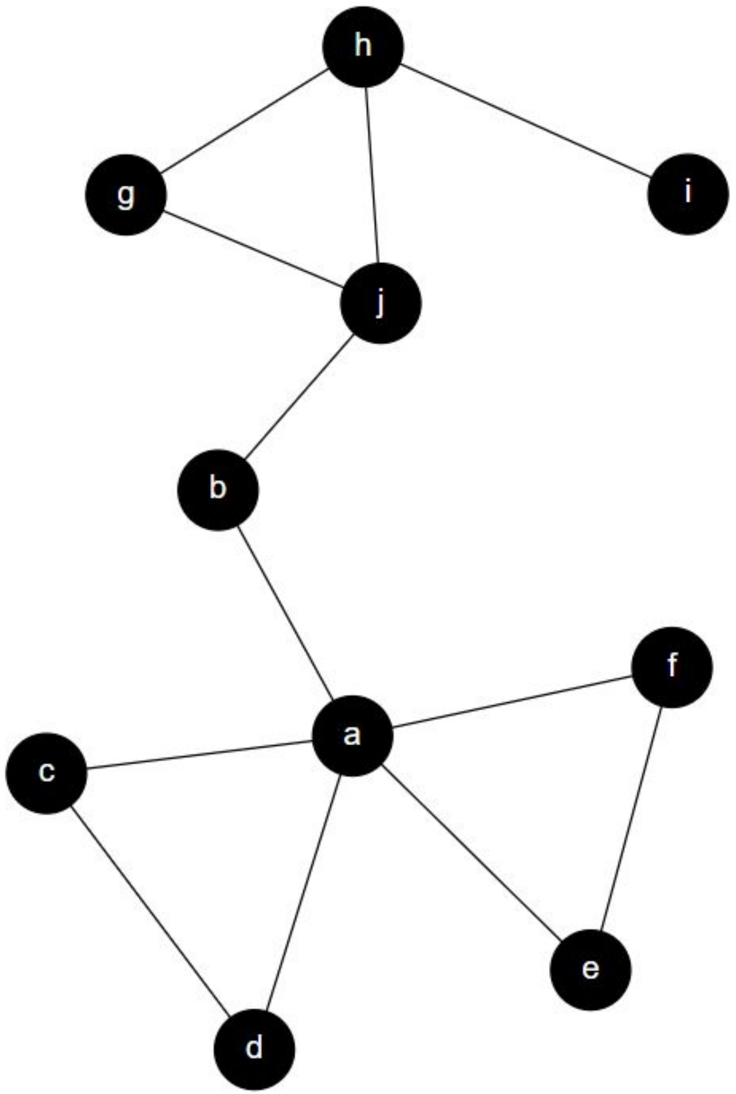
3.4 Add edges edges $\{p_v, v\}$, $\{p_v, \overleftarrow{v}\}$

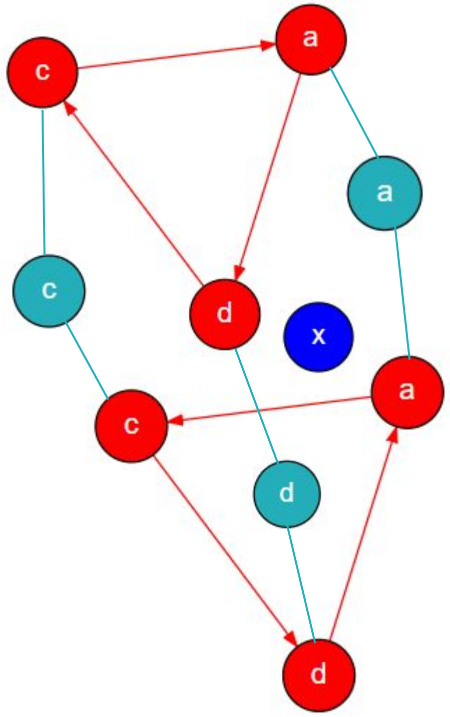


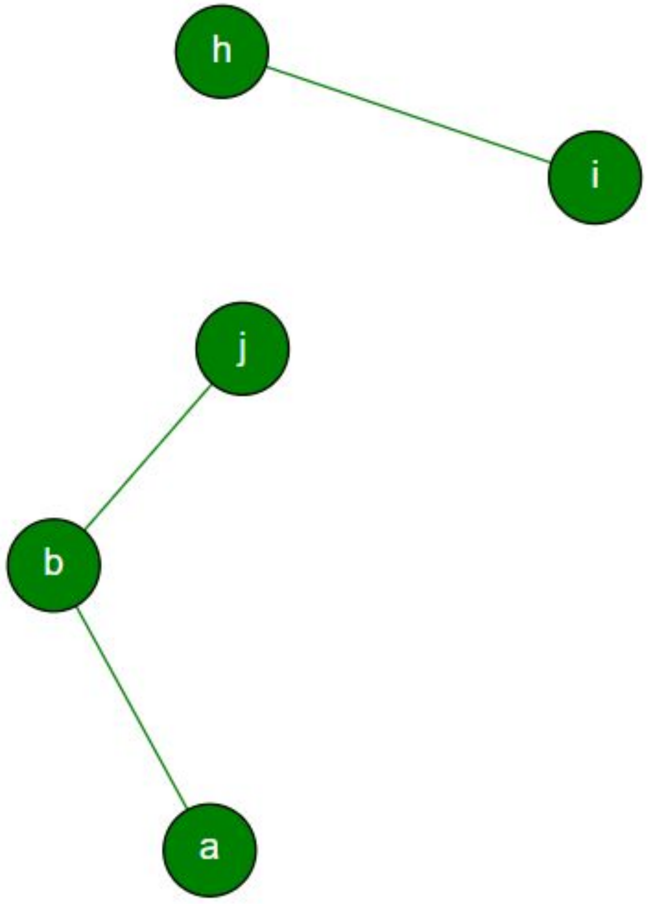




CAT
3.5 Add a node b_i

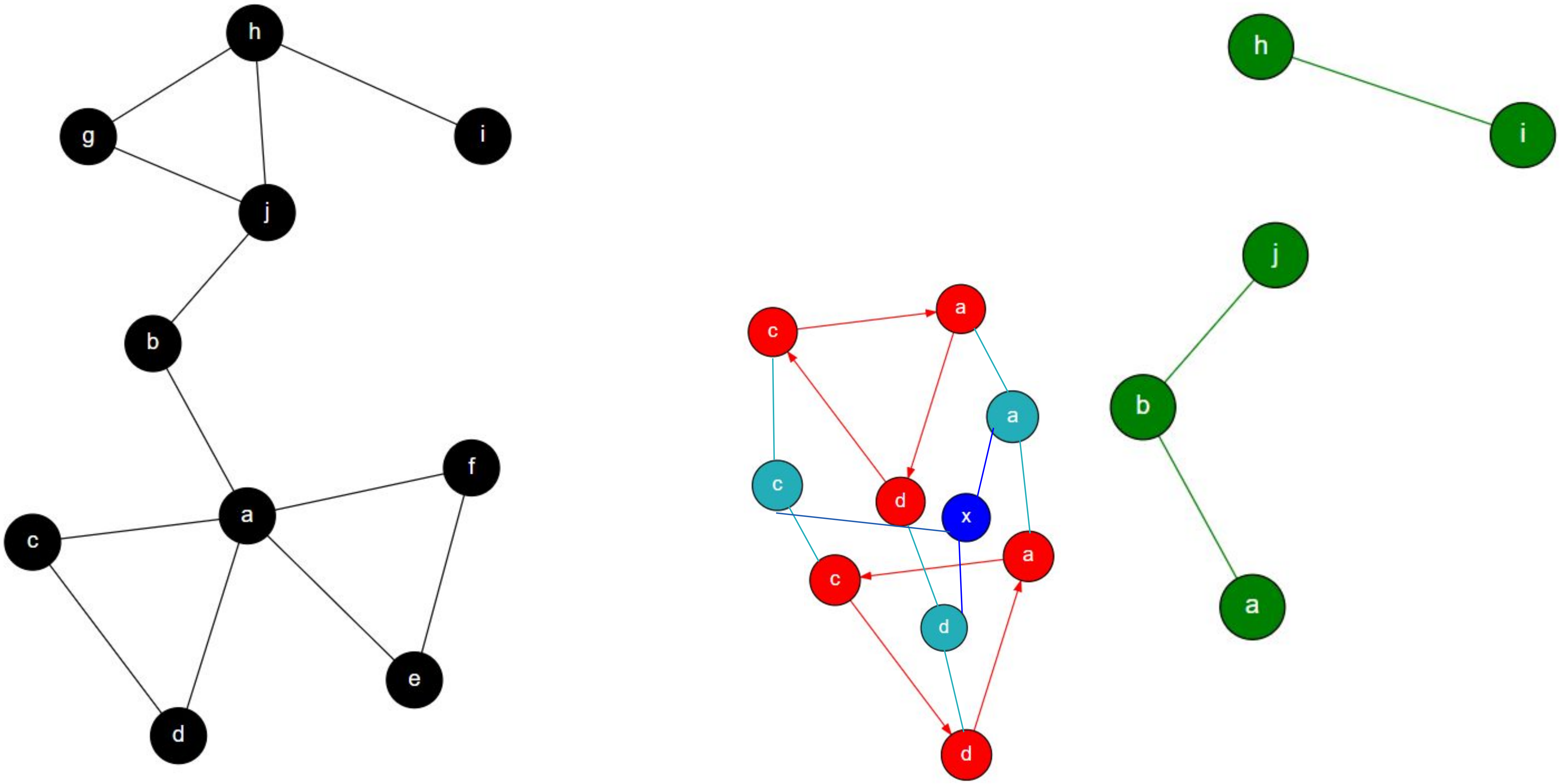






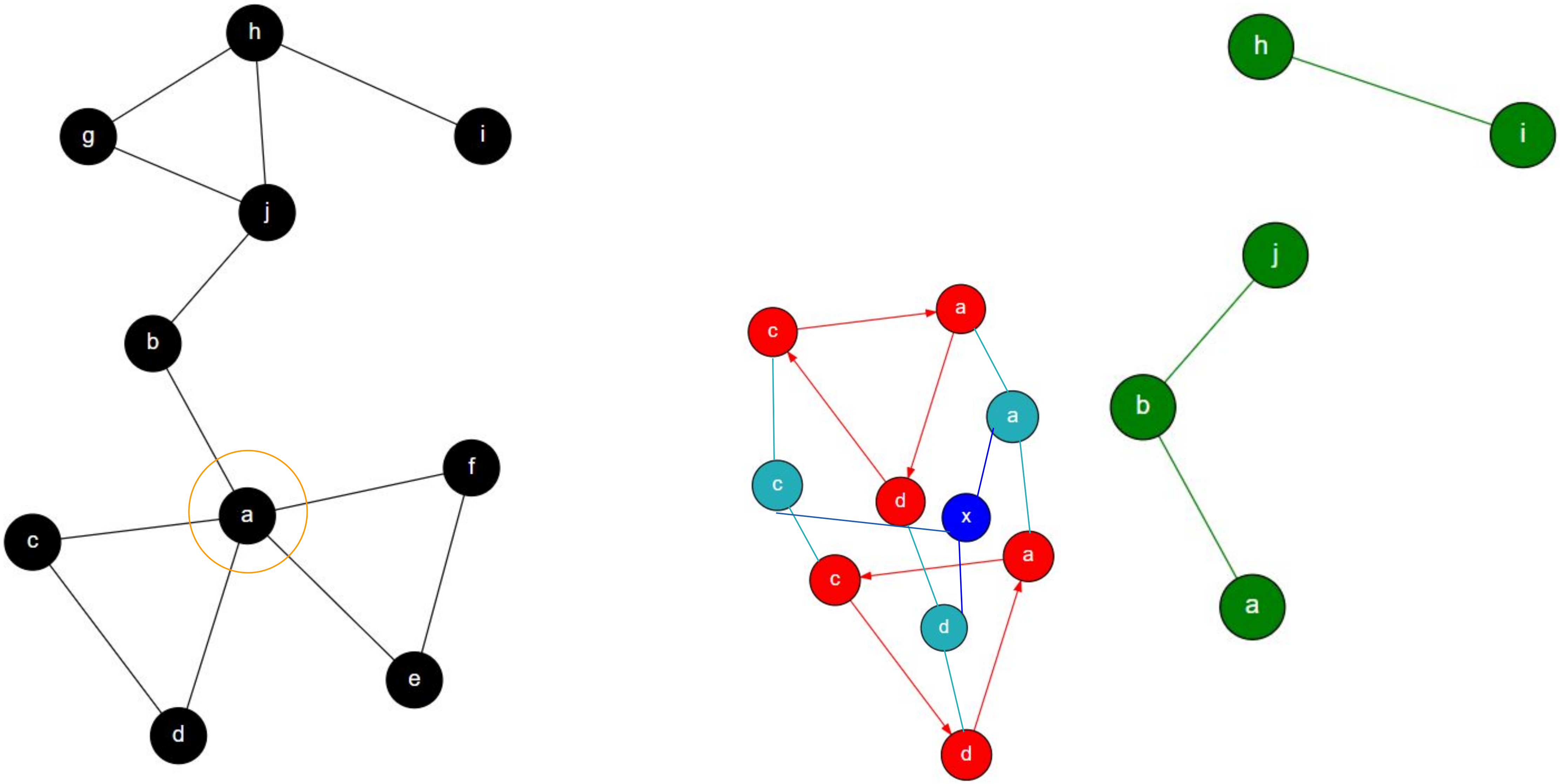
CAT

3.5 Add edges $\{b_i, p_v\}$, $\forall\ v \in V(B_i)$

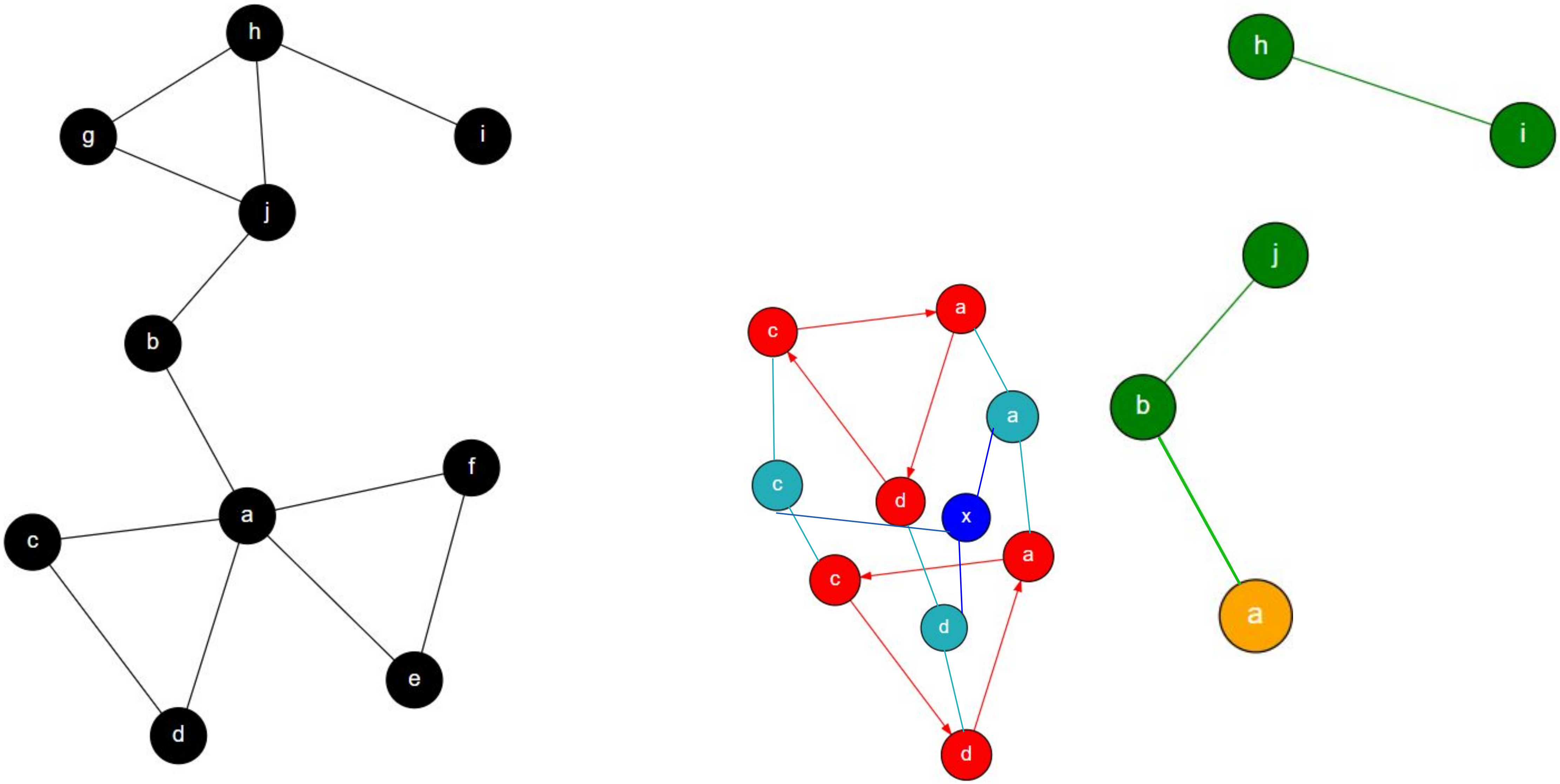


CAT

3.2 Let $A_i := V(B_i) \cap V(F)$

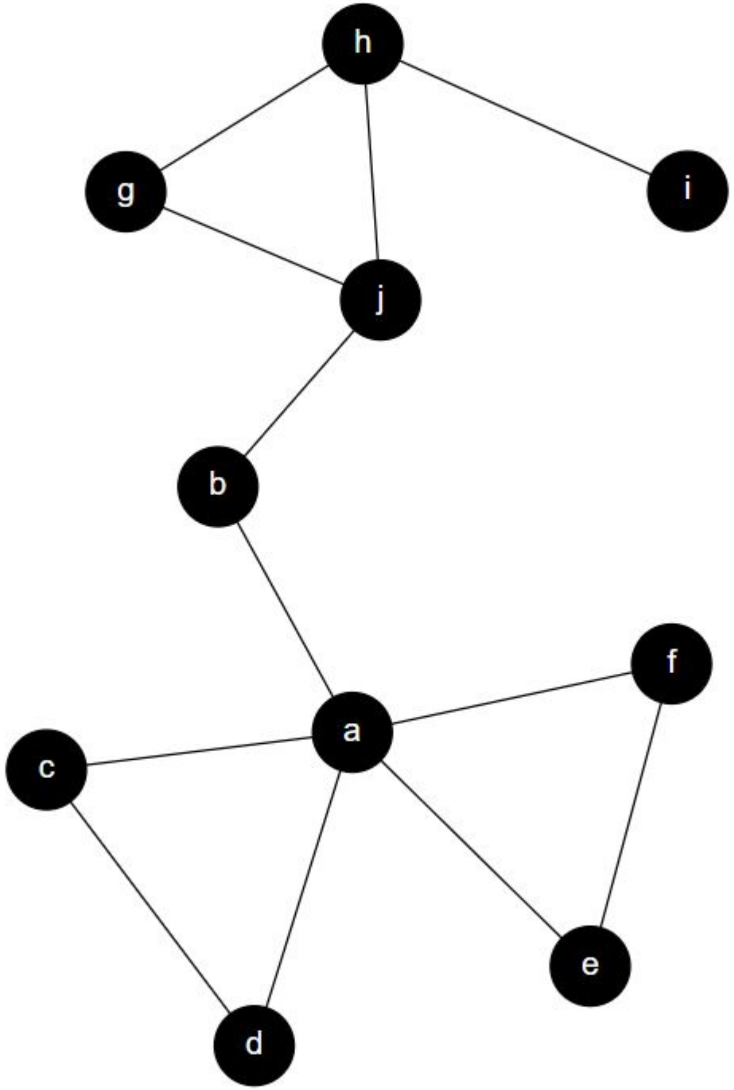


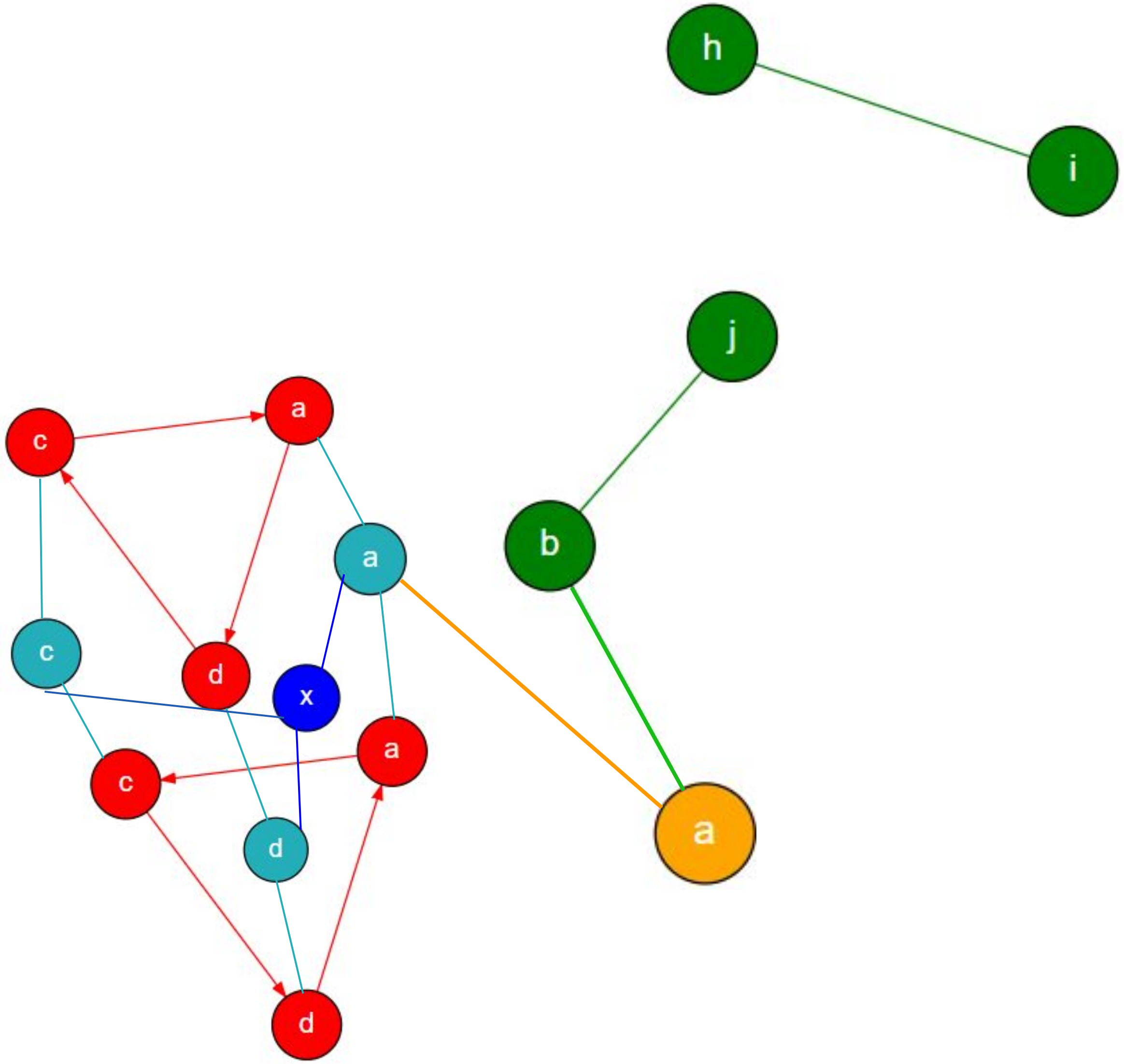
CAT
3.6 Color in orange all green nodes in A



CAT

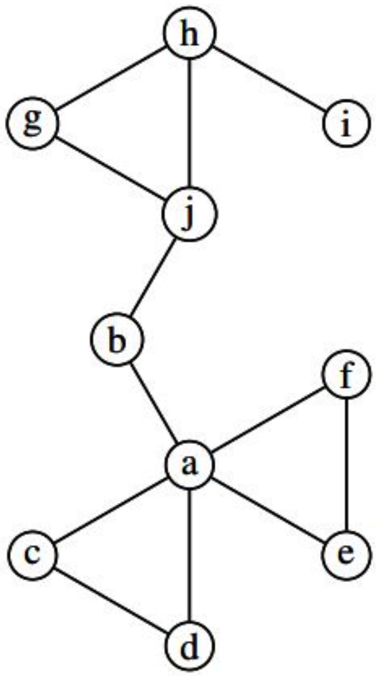
3.6 Connect every node from A to its water green counterpart



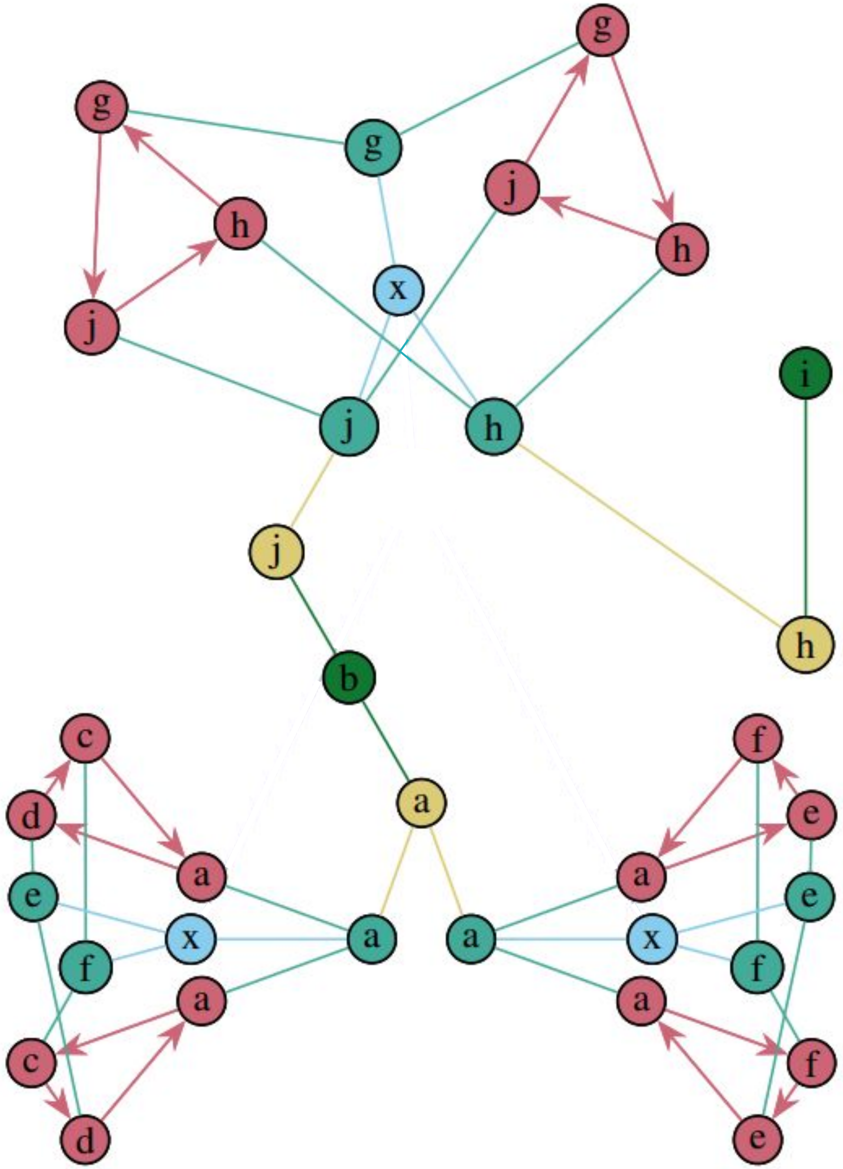


CAT

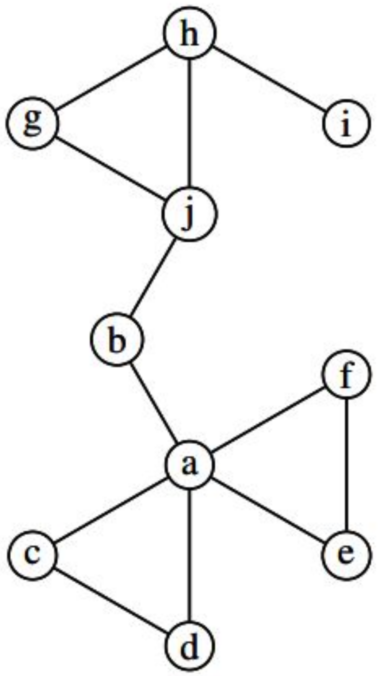
3. Repeat for every block B_i



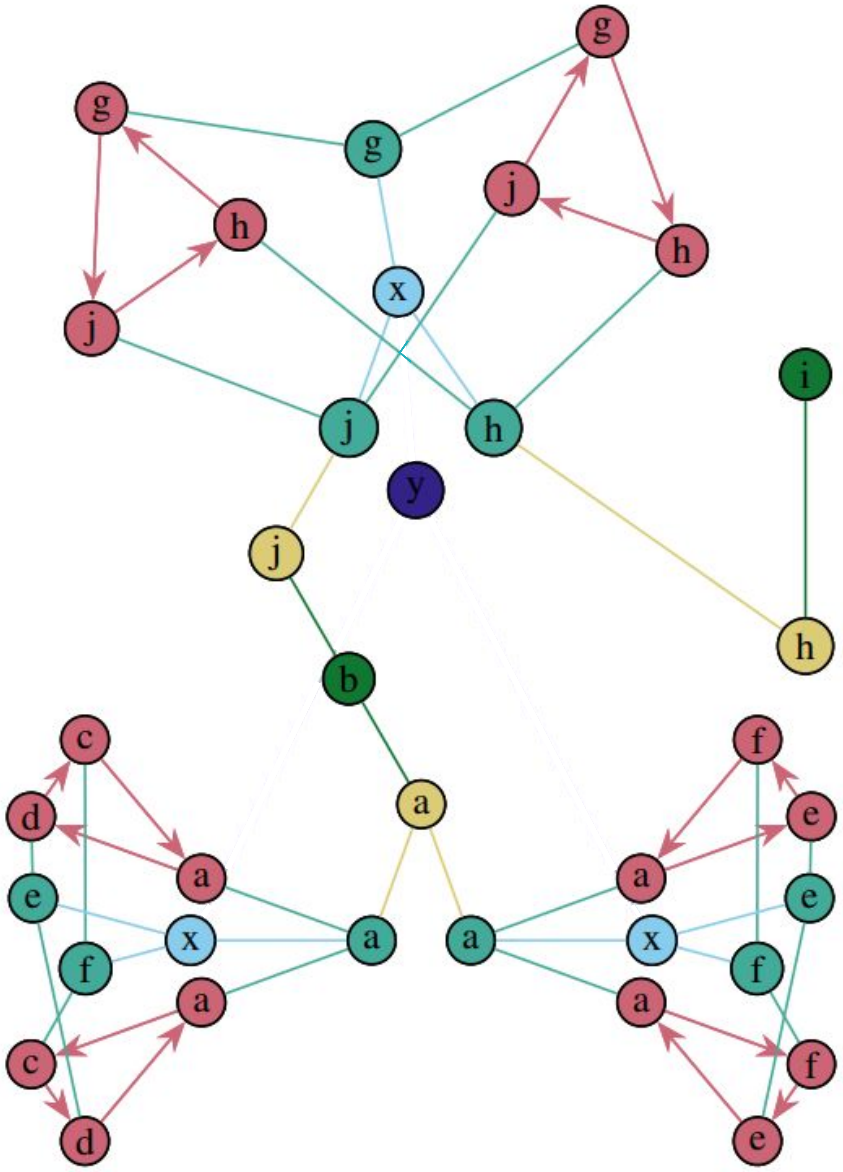
G



CAT
4. Add a node g

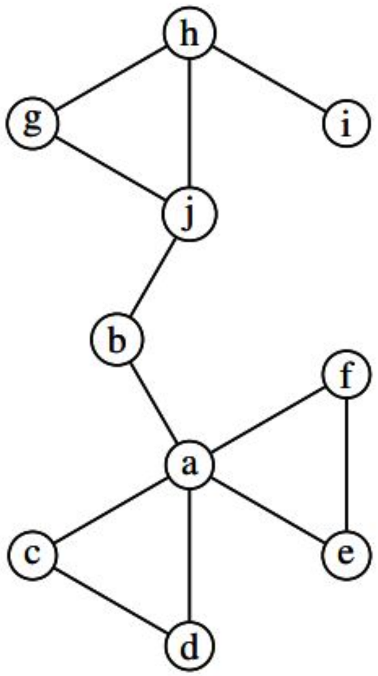


G

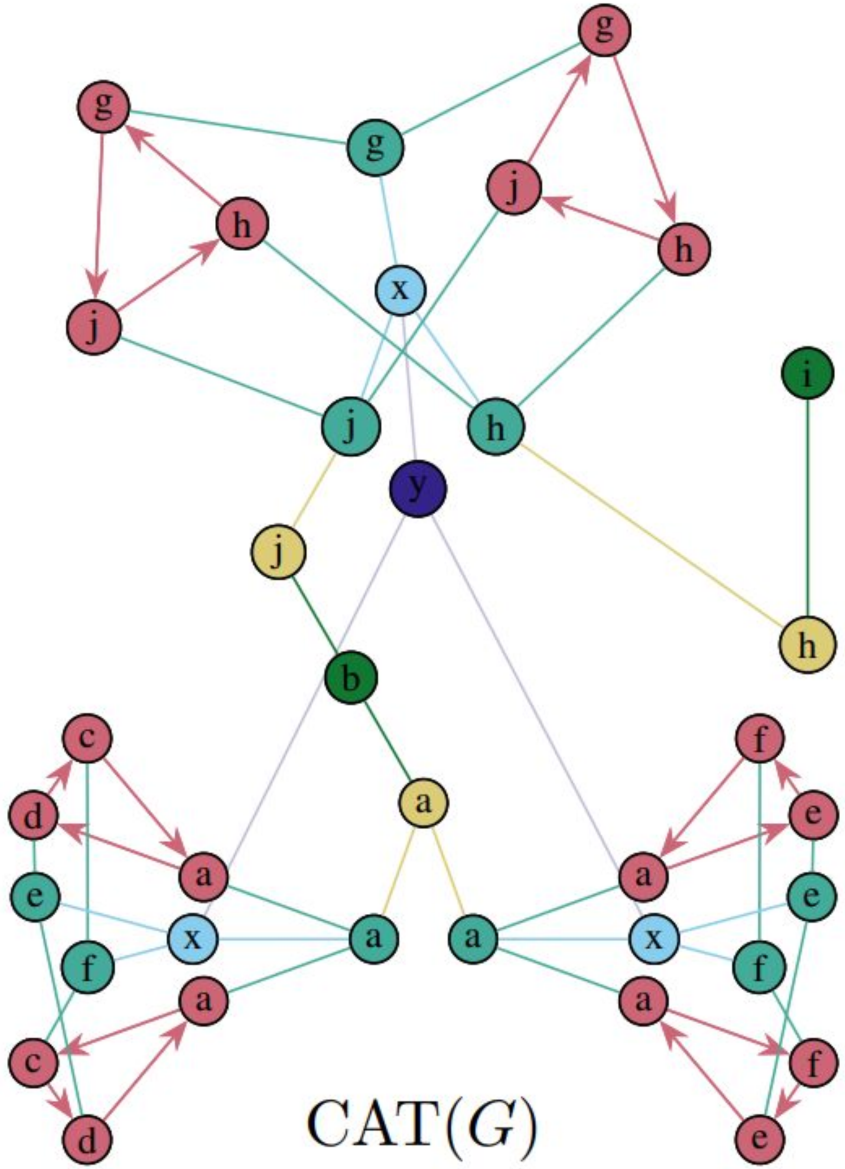


CAT

4. Add edges {g, b_i} for all nodes b_i



G



CAT(*G*)

CAT

Theorem 4: Outerplanar graphs G and H are isomorphic, iff WL(CAT(G)) = WL(CAT(H))

CAT

Linear time complexity:

- Time complexity dominated by computation of blocks and their Hamiltonian cycles (both linear)
- We only add a linear number of nodes and edges. O(|V| + |E|)

Experimental results

Table 4: Predictive performance of MPNNs with and without CAT on different molecular benchmark datasets. Arrows indicate whether smaller (↓) or bigger (↑) results are better. **Bold** entries are an MPNN with CAT that outperforms the same MPNN without CAT.

Dataset → ↓ Model	ZINC MAE ↓	MOLHIV ROC-AUC ↑	MOLBACE ROC-AUC ↑	MOLBBBP ROC-AUC ↑	MOLSIDER ROC-AUC ↑
GIN	0.168 ± 0.007	77.9 ± 1.0	74.6 ± 3.2	66.0 ± 2.1	56.6 ± 1.0
CAT+GIN	**0.101 ± 0.004**	76.7 ± 1.8	**79.5 ± 2.5**	**67.2 ± 1.8**	**58.2 ± 0.9**
GCN	0.184 ± 0.013	76.7 ± 1.4	77.9 ± 1.7	66.1 ± 2.4	56.7 ± 1.5
CAT+GCN	**0.123 ± 0.008**	**77.1 ± 1.6**	**79.2 ± 1.5**	**68.3 ± 1.7**	**57.9 ± 1.8**
GAT	0.375 ± 0.013	76.6 ± 2.0	81.7 ± 2.3	66.2 ± 1.4	58.4 ± 1.0
CAT+GAT	**0.201 ± 0.022**	75.3 ± 1.6	79.3 ± 1.6	66.0 ± 1.9	58.3 ± 1.3
Dataset → ↓ Model	MOLESOL RMSE ↓	MOLTOXCAST ROC-AUC ↑	MOLLIPO RMSE ↓	MOLTOX21 ROC-AUC ↑	
GIN	1.105 ± 0.077	65.3 ± 0.6	0.717 ± 0.016	75.8 ± 0.7	
CAT+GIN	**0.985 ± 0.055**	**65.6 ± 0.5**	0.798 ± 0.031	74.8 ± 1.0	
GCN	1.053 ± 0.087	64.4 ± 0.4	0.748 ± 0.018	76.4 ± 0.3	
CAT+GCN	**1.006 ± 0.036**	**66.2 ± 0.8**	0.771 ± 0.023	74.9 ± 0.8	
GAT	1.037 ± 0.063	63.8 ± 0.8	0.728 ± 0.024	76.3 ± 0.6	
CAT+GAT	1.09 ± 0.048	**64.5 ± 0.8**	0.754 ± 0.021	75.4 ± 0.7	

Strengths

- Better time complexity than other maximally expressive architecture for outerplanar graphs:
  - 3-GNN (linear vs cubic)
  - PlanE (linear vs quadratic)
- Very strong results in some datasets
- CAT can be applied to non-outerplanar graphs in linear time (without same guarantees)
- Recent work indicates CAT increases connectivity on the graph
- Most pharmaceutical molecules can be represented as outerplanar graphs.

Weaknesses

- Experimental results not consistent: sometimes is even outperformed by base model on G (especially common for GAT). Considerations:
    - CAT transformation introduces new “virtual” nodes and edges, so we have:
        - longer dependencies
        - GNN has to learn different representation for “virtual” nodes and edges
    - No SOTA models implemented
- Guarantees restricted to outerplanar graphs (not very impactful)
    - Would be good to generalize it to planar graphs (isomorphism still verifiable in polynomial time) like PlanE.

QUESTIONS?

References

- Franka Bause, Fabian Jogl, Pascal Welke, & Maximilian Thiessen (2023). Maximally Expressive GNNs for Outerplanar Graphs. In The Second Learning on Graphs Conference.
- Franka Bause, Fabian Jogl, Patrick Indri, Tamara Drucks, David Penz, Nils Morten Kriege, Thomas Gärtner, Pascal Welke, & Maximilian Thiessen. (2024). Maximally Expressive GNNs for Outerplanar Graphs
- Xu, K., Hu, W., Leskovec, J., & Jegelka, S. (2019). How Powerful are Graph Neural Networks? In *International Conference on Learning Representations*.
- Radoslav Dimitrov, Zeyang Zhao, Ralph Abboud, & İsmail İlkan Ceylan. (2023). PlanE: Representation Learning over Planar Graphs.
- Hopcroft John E. and Tarjan Robert Endre. 1972. Isomorphism of planar graphs. In Complexity of Computer Computations (The IBM Research Symposia Series). Plenum Press, New York, 131–152.
- Hopcroft John E. and Wong J. K.. 1974. Linear time algorithm for isomorphism of planar graphs (preliminary report). In 6th ACM Symposium on Theory of Computing (STOC). ACM Press, 172–184.
- Grötschla Florian
- https://www.wikipedia.org/
- https://csacademy.com/app/graph_editor
- https://edgitor.chunlaw.io/

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