# Subgraphs Mining

Prof. O-Joun Lee

Dept. of Artificial Intelligence,
The Catholic University of Korea
*ojlee@catholic.ac.kr*

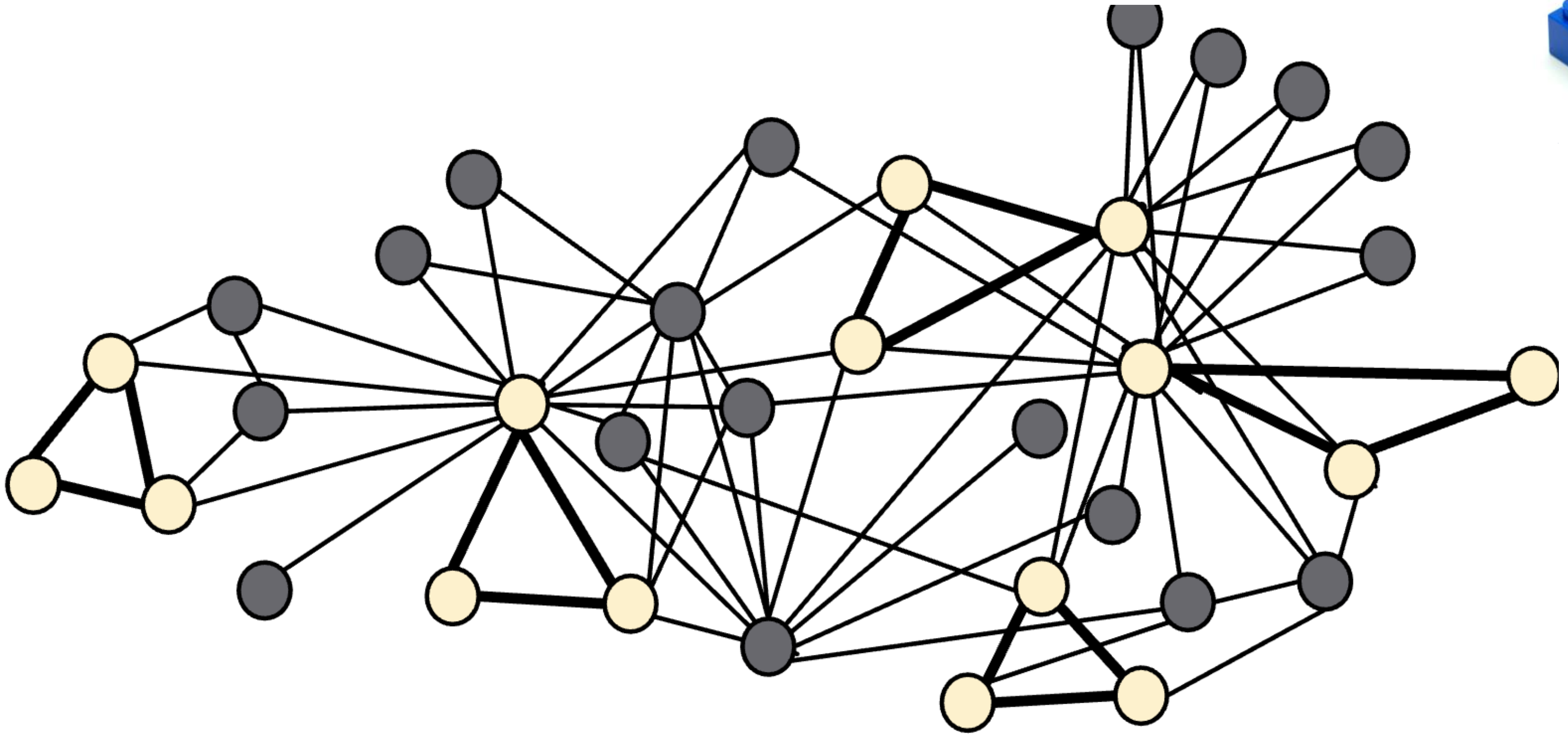
네트워크 과학 연구실 NETWORK SCIENCE LAB

가톨릭대학교 THE CATHOLIC UNIVERSITY OF KOREA

# Contents

# What is Subgraph?

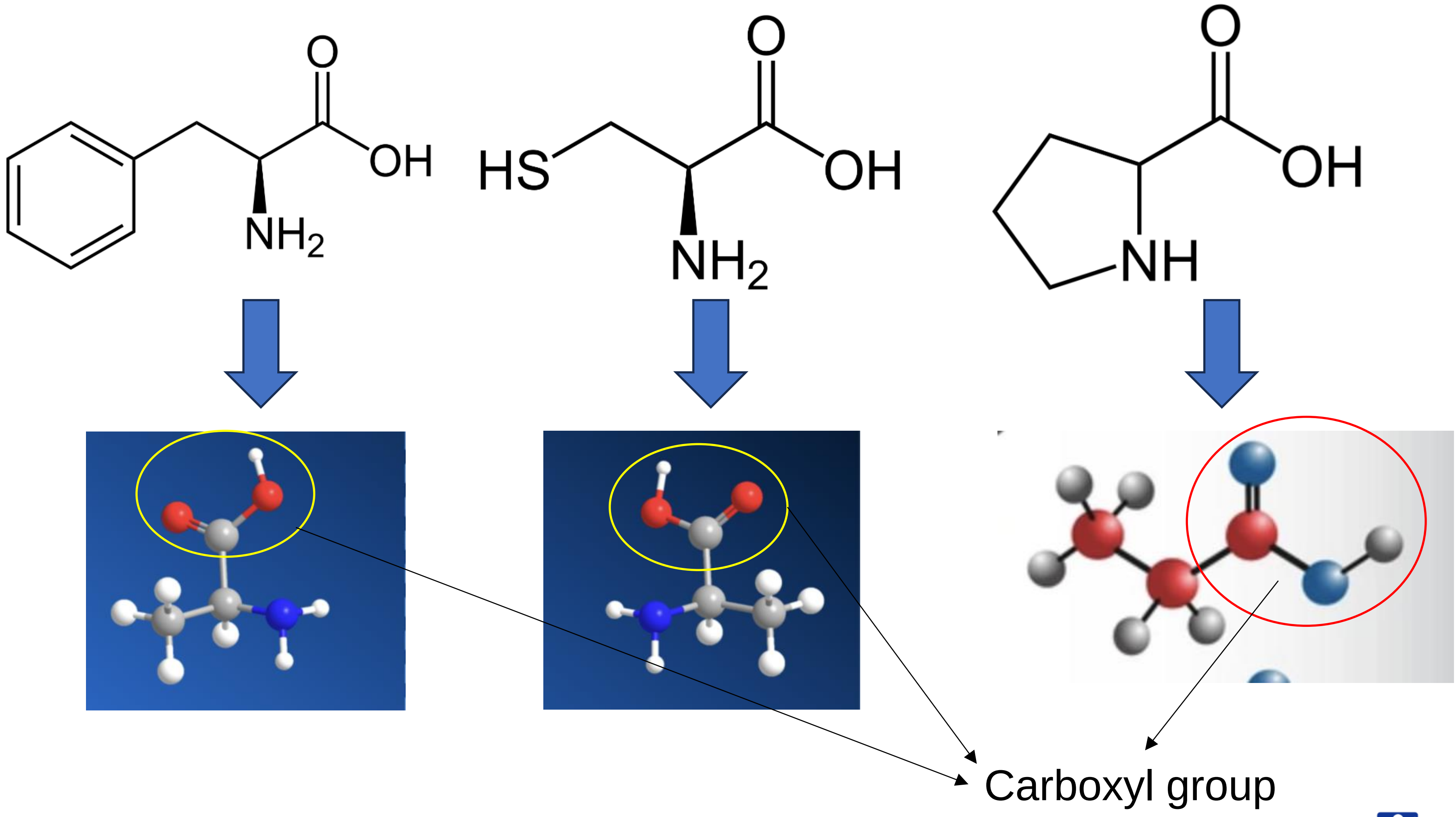
- **Subgraph**: are the building blocks of networks



- They have the power to characterize and discriminate networks

Source: Lego

- In many domains, recurring structural components determine the function or behaviour of the graph



- Given a graph $G = (V, E)$
- Two ways to formalize "network building blocks”:
  - Node-induced subgraph
  - Edge-induced subgraph

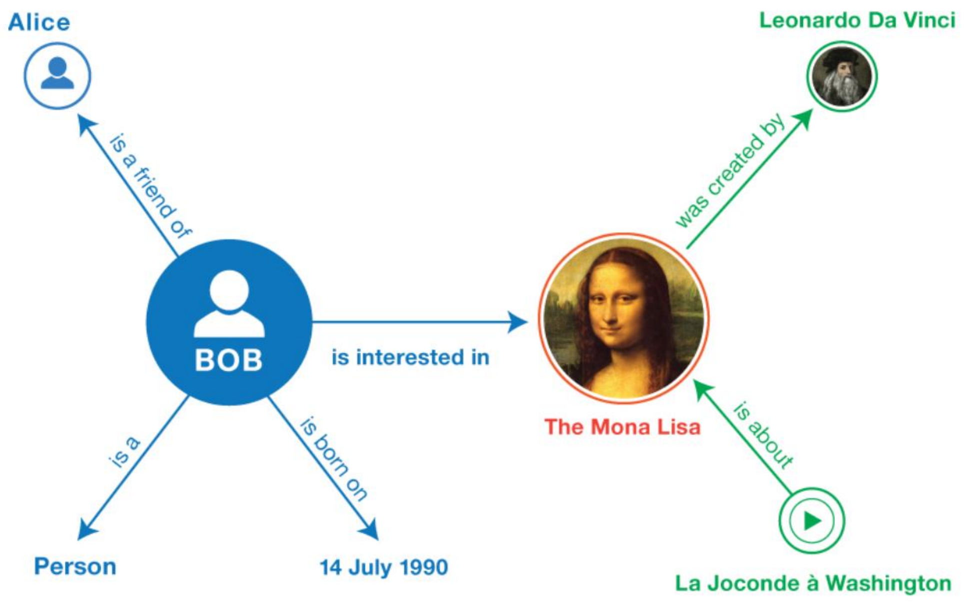
- **Node-induced subgraph**: Take subset of the nodes and all edges induced by the nodes:
  - $G' = (V', E')$ is a node-induced subgraph iff (if and only if)
    - $V' \subseteq V$
    - $E' = \{(u, v) \in E | u, v \in V'\}$
    - $G'$ is the subgraph of $G$ induced by $V'$

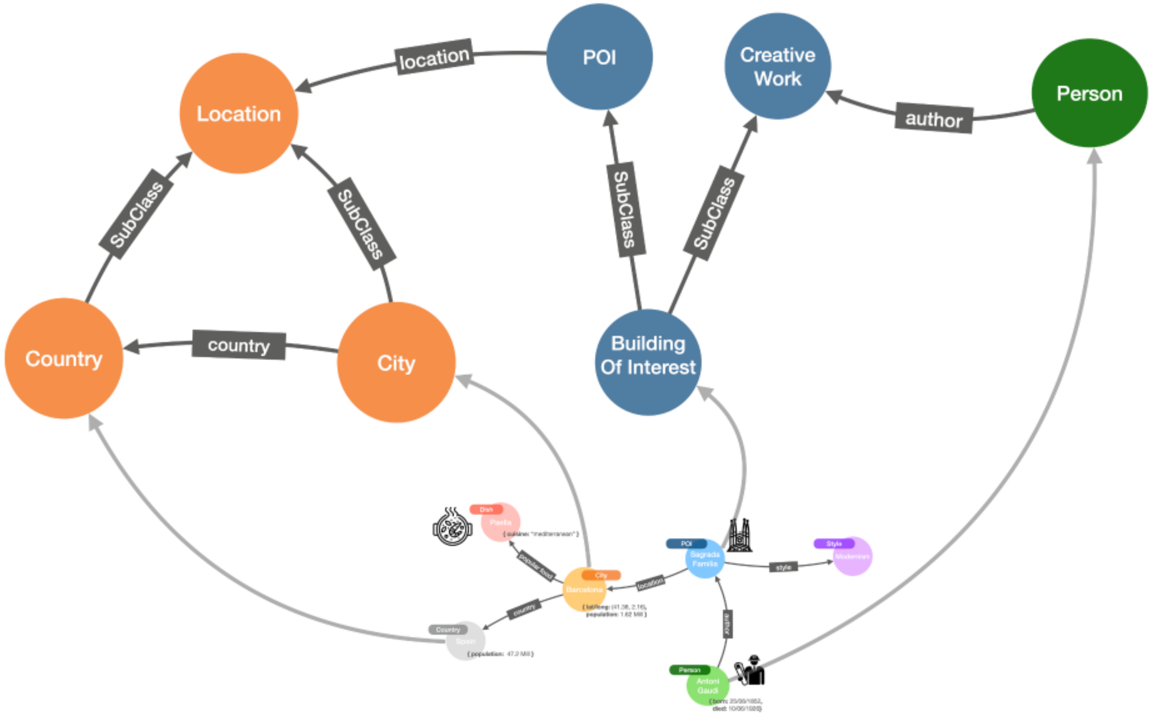
# Subgraph Definition



- **Edge-induced subgraph:** Take subset of the edges and all corresponding nodes:
  - $G' = (V', E')$ is an edge-induced subgraph iff
    - $E' \subseteq E$
    - $V' = \{v \in V | (v, u) \in E'$ for some $u\}$

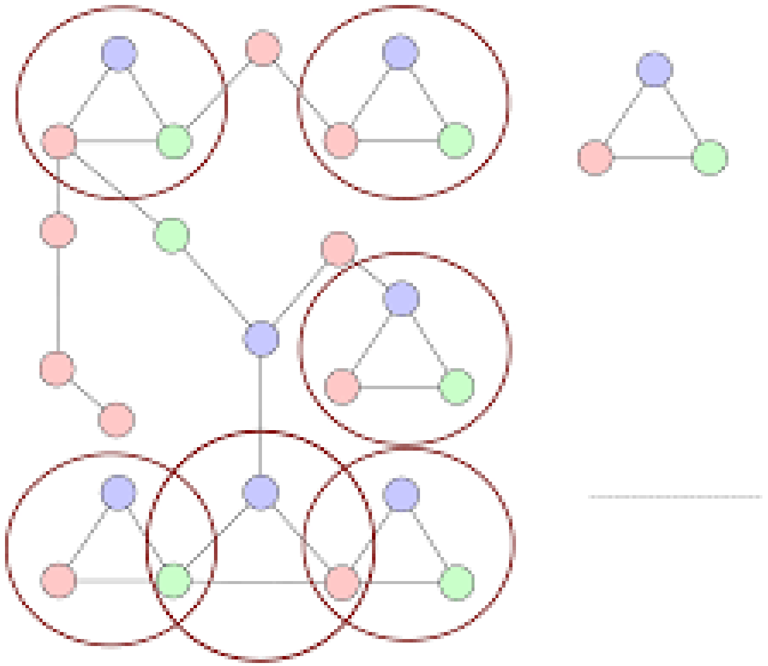
- **Chemistry:** Node-induced (functional groups)
- **Knowledge graphs:** Often edge-induced (focus is on edges representing logical relations)



# Why Frequent Patterns?

- Frequent pattern: a structure (a set of items, subsequence, substructures, etc.) that occurs frequently in a data set
- Motivation: Finding inherent regularities in data
  - What products were often purchased together?
  - What are the subsequent purchases after buying a PC?
  - What sequences of DNA are sensitive to this new drug?
  - Which topics are in a collection of documents?



- Frequent subgraphs:
  - A (sub)graph is **frequent** if its support (occurrence frequency) in each dataset is no less than a minimum support threshold
- Applications of graph pattern mining:
  - Mining biochemical structures
  - Program control flow analysis
  - Mining XML structures or Web communities
  - Building blocks for graph classification, clustering, compression, comparison, and correlation analysis

# The Apriori Principle



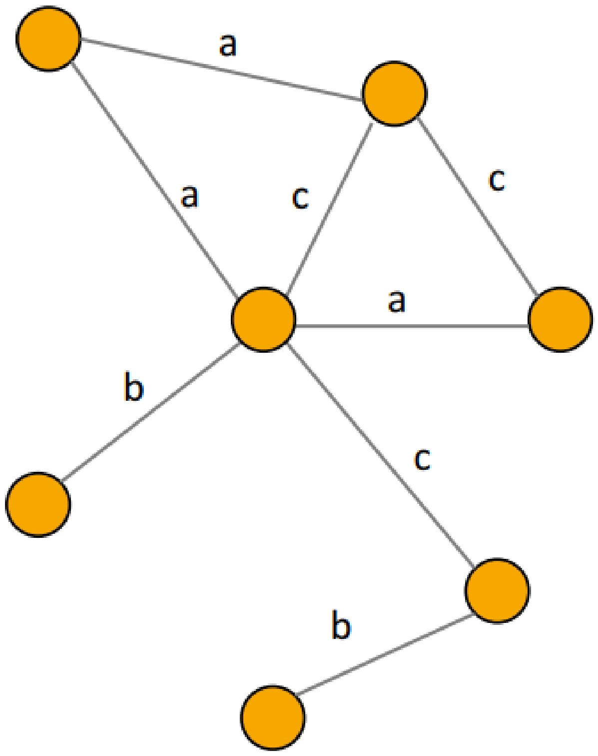
- Also called Downward closure Property
- All subsets of a frequent pattern must also be frequent
  - Because any item that contains X must also contains subset of X

If we have already verified that X is infrequent, there is no need to count X's supersets because they MUST be infrequent too

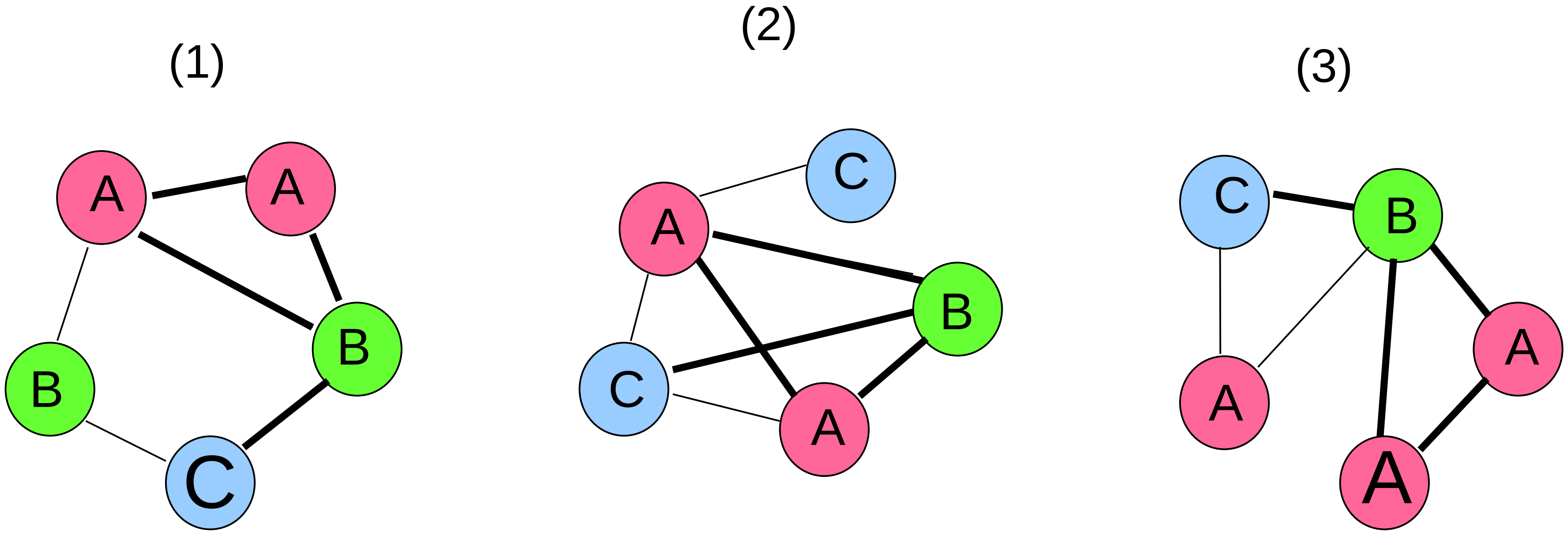
- Problem: Find all subgraphs of G that appear at least t times

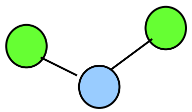
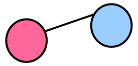
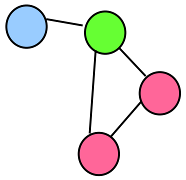
- Suppose t = 2, the frequent subgraphs are (only edge labels)
  - a, b, c
  - a-a, a-c, b-c, c-c
  - a-c-a …

- Exponential number of patterns!



# Frequent Subgraph Example




| Support | 1 | 3 | 3 |
|---|---|---|---|
| Subgraph |  |  |  |

# How to Mine Frequent Subgraphs?

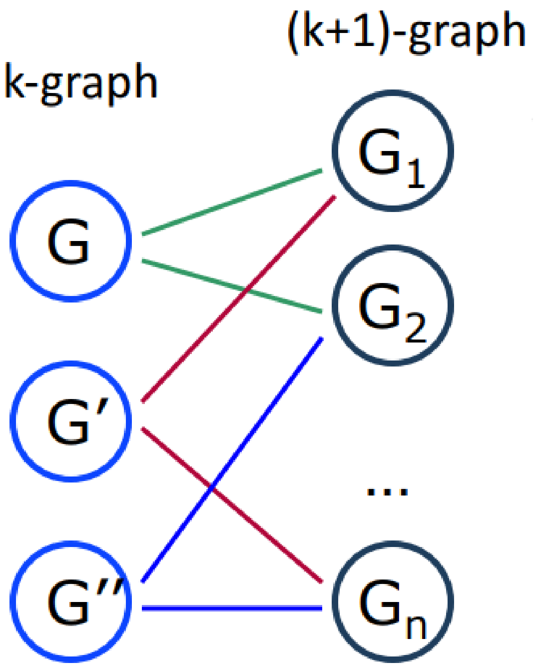


- Apriori-based approaches:
  - Start with small-size subgraphs and proceeds in a bottom-up manner
  - Join two patterns to create bigger size patterns (through Apriori principle)
  - Several approaches:
    - FSG.
    - PATH#
- Pattern-growth approaches:
  - Extends existing frequent graphs by adding one edge
  - Several approaches:
    - gSpan, MoFa
    - Gaston FFSM, SPIN
- Greedy approaches:
  - Subdue

# Apriori-Based Approaches



- Start with small-size subgraphs and proceeds in a bottom-up manner
- Join two patterns to create bigger size patterns (through Apriori principle)

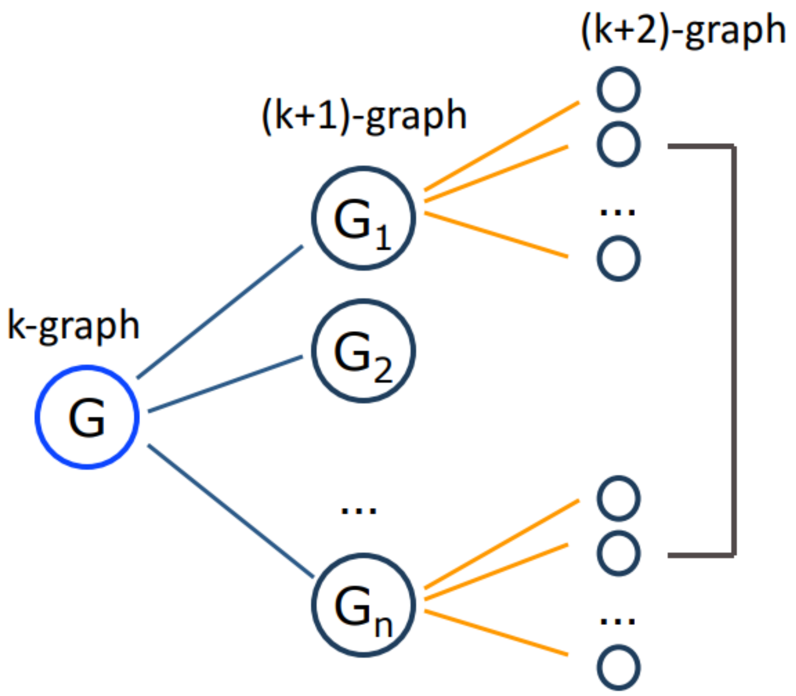



- Problem:
  - Join operation among graphs is extremely expensive

# Pattern Growth Method



- Generate patterns expanding existing ones
- Extends existing frequent graphs by adding one edge

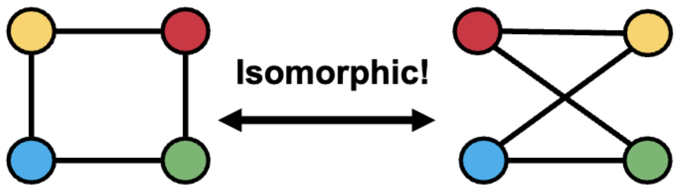


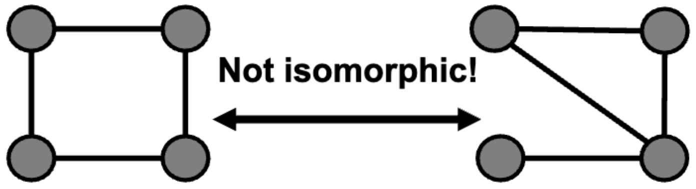

- Problems:
  - Duplicate graphs

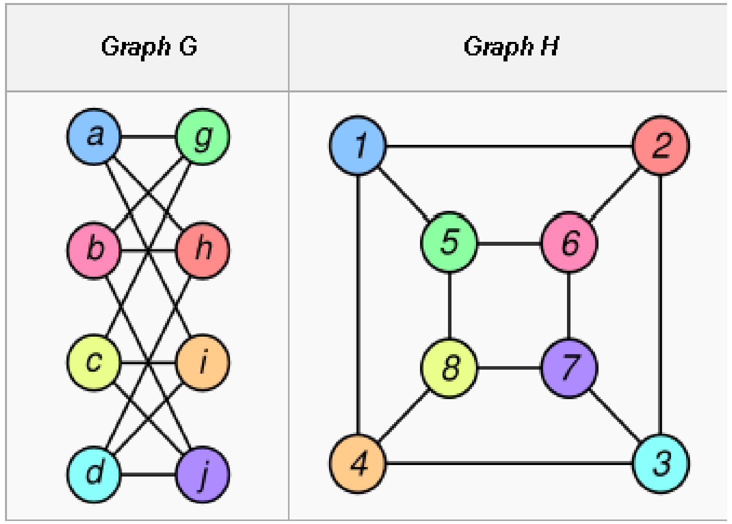
# Key Challenges in Subgraph Mining



- **Graph isomorphism:**
  - To detect if two graphs are identical in structure
  - $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ are isomorphic if there exists a bijection $f: V_1 \rightarrow V_2$ such that $(u, v) \in E_1$ if $\big(f(u), f(v)\big) \in E_2$
    - $f$ is called the **isomorphism**:

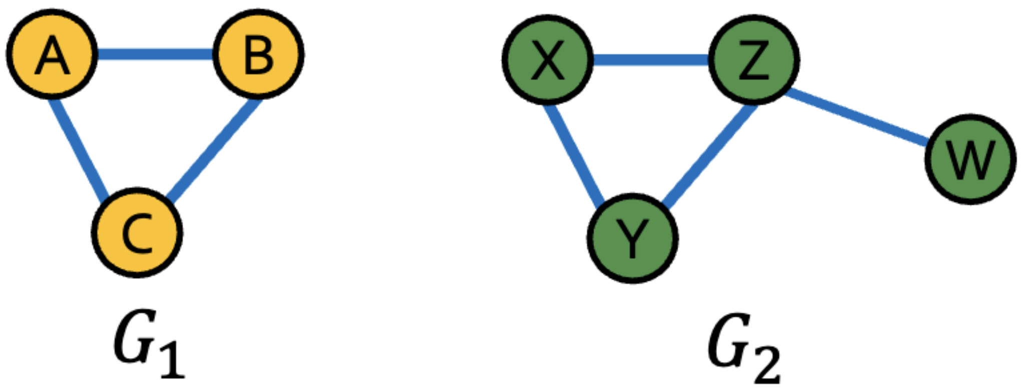



- Graph representation (Canonical Labeling)
  - A canonical label is a unique code of a given graph
  - Canonical label should be the same no matter how graphs are represented, as long as graphs have the same topological structure and the same labeling of edges and nodes

- $G_2$ is **subgraph-isomorphic** to $G_1$ if some subgraph of $G_2$ is isomorphic to $G_1$
  - We also commonly say $G_1$ is a subgraph of $G_2$
  - We can use either the node-induced or edge-induced definition of subgraph.
  - This is NP-hard problem




$f$:

| $V_1$ | $V_2$ |
|---|---|
| A | X |
| B | Y |
| C | Z |

A-B-C matches with X-Y-Z: There is a subgraph isomorphism between $G_1$ and $G_2$

# Graph Isomorphism: Sample code



- Returns True if the graphs G1 and G2 are isomorphic and False otherwise.

  (The two graphs G1 and G2 must be the same type)

```
#Import networkx, isomorphism
import networkx as nx
import networkx.algorithms.isomorphism as iso

#create graph 1
G1 = nx.Graph()

G1.add_nodes_from(['A','B','C','D','E','F'])

G1.add_edges_from([('A','B'),('A','C'),('A','D'),('A','E'),('A','F')])


#create graph 2
G2 = nx.star_graph(5)
```

## Testing if two graphs are isomorphic

```
nx.is_isomorphic(G1, G2)
```

```
True
```

# Graph Isomorphism: Sample code



- How to find edge mapping

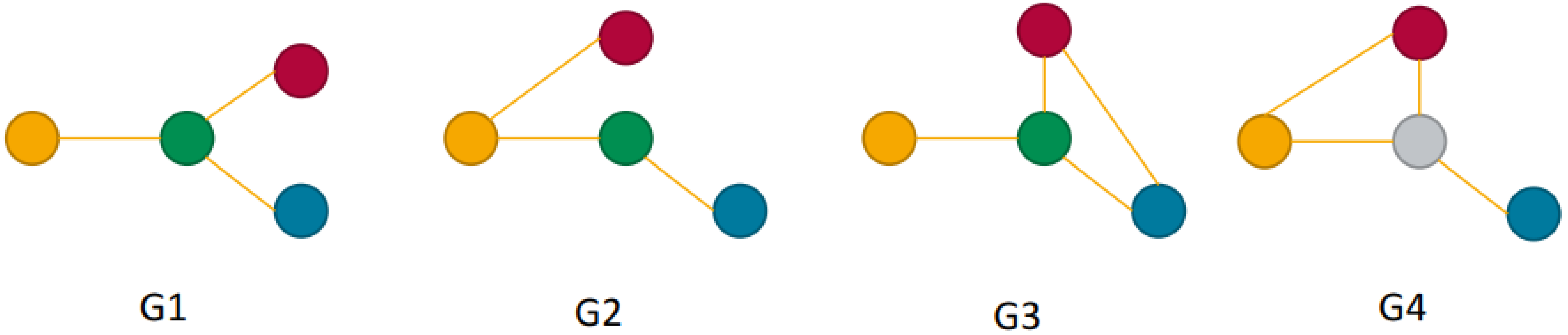
```
import networkx as nx
G1 = nx.Graph()
G1.add_weighted_edges_from([(0,1,0), (0,2,1), (0,3,2)], weight = 'aardvark')
G2 = nx.Graph()
G2.add_weighted_edges_from([(0,1,0), (0,2,2), (0,3,1)], weight = 'baboon')
G3 = nx.Graph()
G3.add_weighted_edges_from([(0,1,0), (0,2,2), (0,3,2)], weight = 'baboon')

def comparison(D1, D2):
    #for an edge u,v in first graph and x,y in second graph
    #this tests if the attribute 'aardvark' of edge u,v is the
    #same as the attribute 'baboon' of edge x,y.

    return D1['aardvark'] == D2['baboon']

nx.is_isomorphic(G1, G2, edge_match = comparison)
```

```
True
```

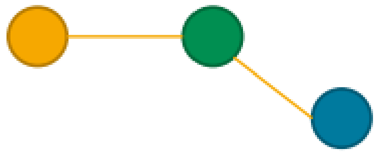
```
nx.is_isomorphic(G1, G3, edge_match = comparison)
```

```
False
```

- Given a set of 4 graphs:




- Support: frequency of a subgraph appearing in a set of graphs
- Frequent subgraph Min support = 3/4



Apriori principle (for graphs): If a graph is frequent, all of its subgraphs are frequent

# Labeled Graph



- We define a labeled graph $G$ as a five-element tuple $G = \{V, E, \Sigma_V, \Sigma_E, \delta\}$

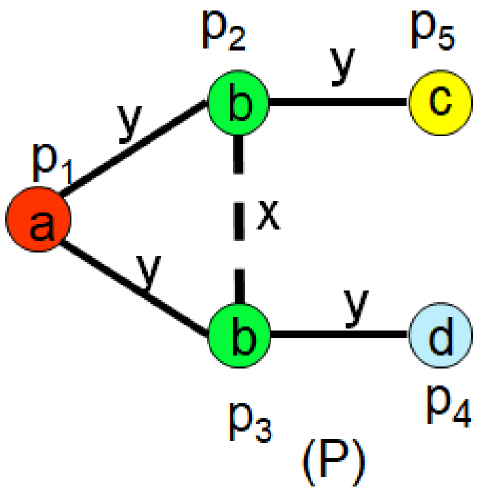
  Where:

  $V$ is the set of vertices of $G$,

  $E \subseteq V \times V$ is a set of undirected edges of $G$,

  $\Sigma_V$ ($\Sigma_E$) are set of vertex (edge) labels,

  $\delta$ is the labeling function: $V \subseteq \Sigma_V$ and $E \rightarrow \Sigma_E$ that maps vertices and edges to their labels



# Subgraph Mining Problem



- Support: Given a set of labelled graphs:
  - $D = \{G_1, G_2, \ldots, G_n\}, G_i =< V_i, E_i, l_i >$
  - A subgraph $G$
- The supporting set of $G$ is: $D = \{G_i | G \sqsubseteq G_i, G_i \in D\}$

  Where $G \sqsubseteq G_i$ indicates that $G$ is subgraph isomorphic to $G_i$

- The support is defined as:

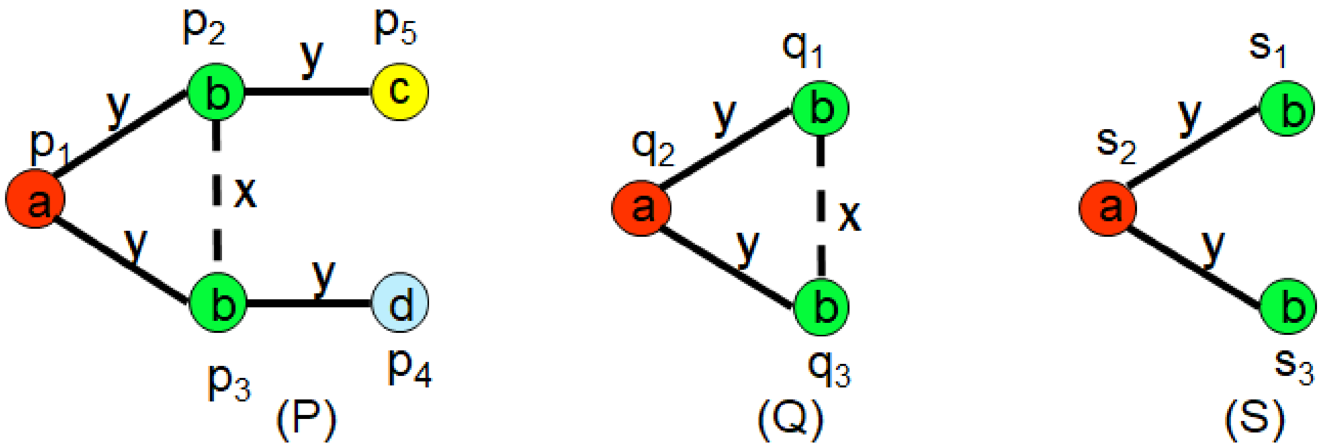
$$\sigma(G) = \frac{|D_G|}{|D|}$$

# Frequent Subgraph Mining

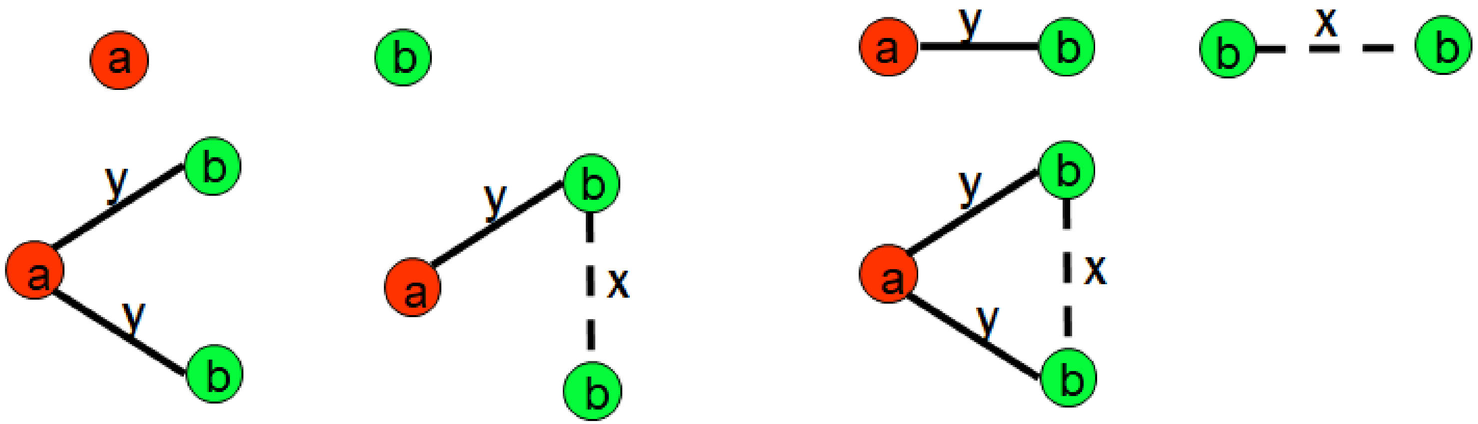


- Input: A set Graph data of labeled undirected graphs

$\sigma = 2/3$




- All frequent subgraphs (w. r. t. $\sigma$) from *Graph data*



# Subgraph Mining Problem: Input and Output



- Input:
  - Set of labeled-graphs $D = \{G_1, G_2, \dots, G_n\}, G_i = \langle V_i, E_i, \ell_i \rangle$
  - Minimum support min_sup
- Output:
  - A subgraph G is frequent if $\sigma(G) \geq \text{min\_}sup$
  - Each subgraph is connected

# Mining approaches



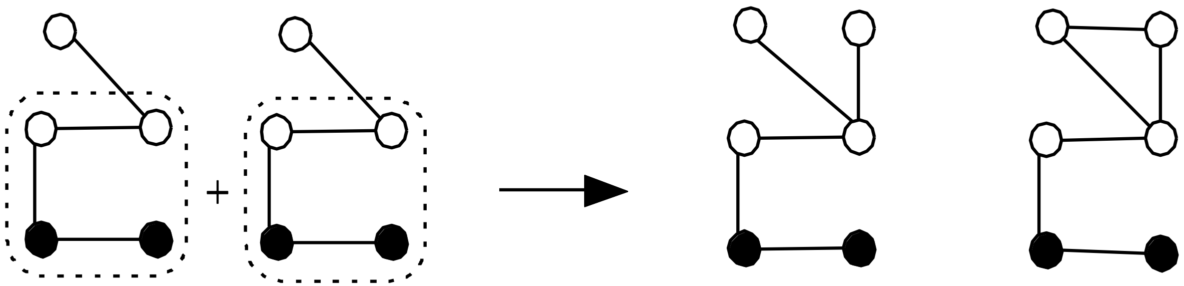
- Apriori-based approaches:
  - FSG
- Pattern-growth approaches:
  - gSpan
- Greedy approach:
  - Subdue

# Apriori-Based, Breadth-First Search

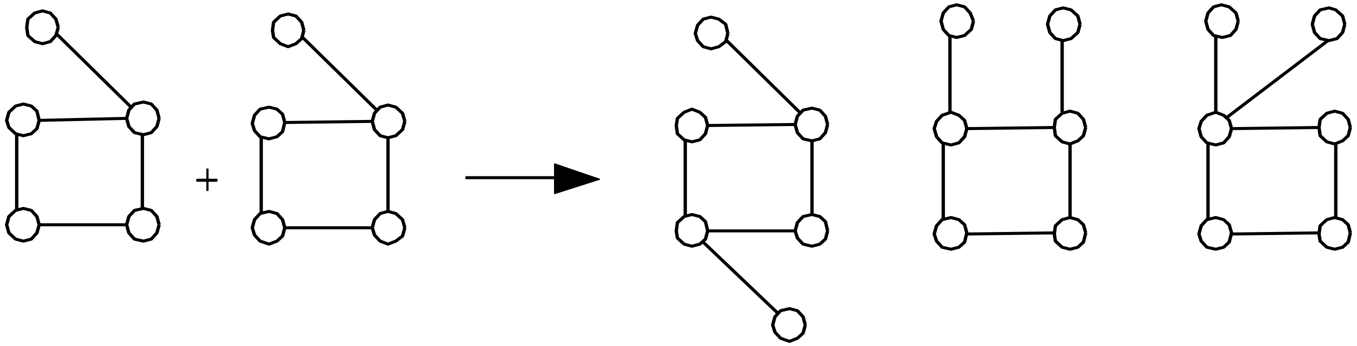


- Methodology: breadth-search, joining two graphs

1. Generates new graphs with one more node



2. Generates new graphs with one more edge



# FSG Algorithm



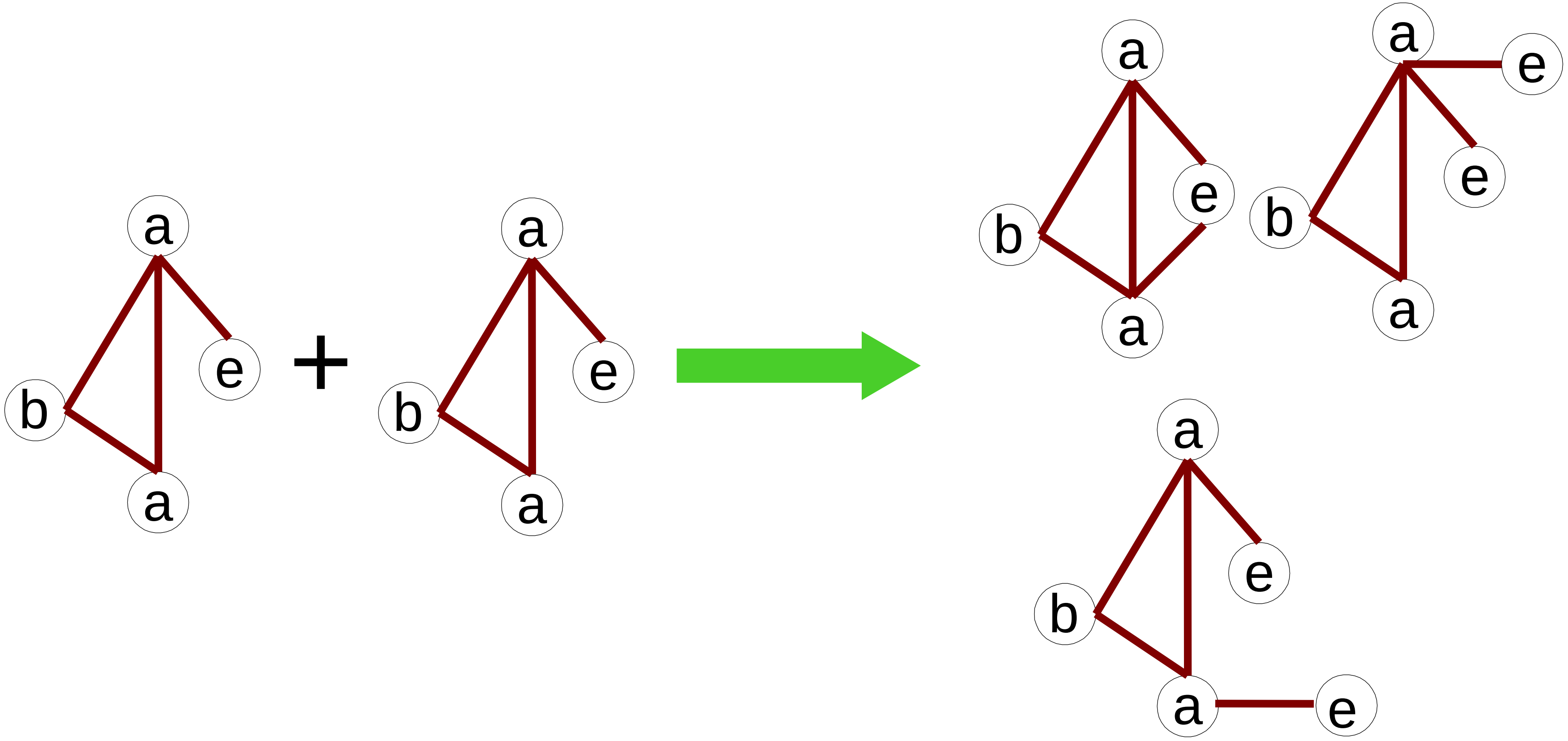
- $K = 1$
- $F_1$ = all frequent edges
- Repeat
  - $K = K + 1;$
  - $C_K$ = join($F_{K-1}$)
  - $F_K$ = frequent patterns in $C_K$
  - Until $F_K$ is empty

# Join: Key Operation

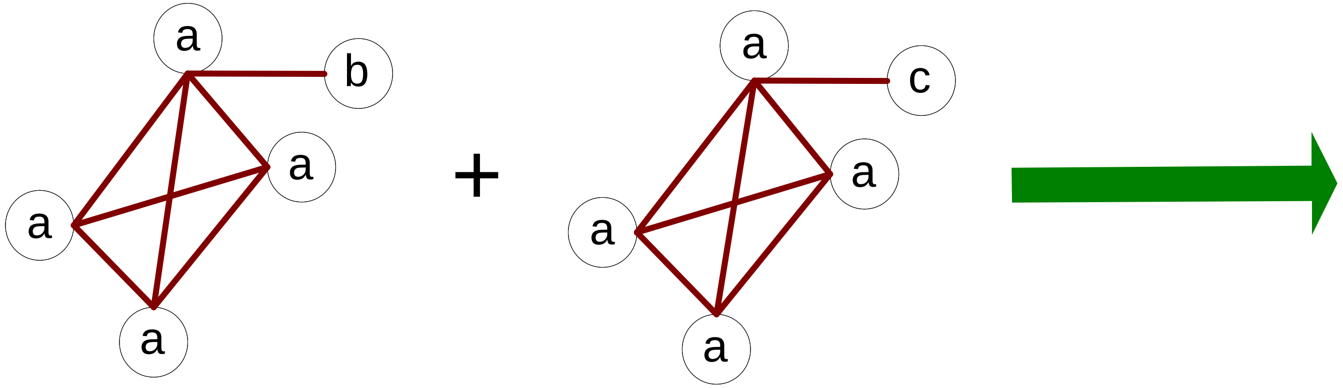
- Join(L) = $\cup$ join(P, Q) for all P, Q $\in$ L
- Join(P, Q) = {G | P, Q, $\subset$ G, |G| = |P| + 1, |P| = |Q|}
- Two graphs P and Q are ***joinable*** if the join of the two graphs produces a non-empty set
- Theorem: two graphs P and Q are joinable if P ∩ Q is a graph with size |P| -1 or share a common "core" with size P-1

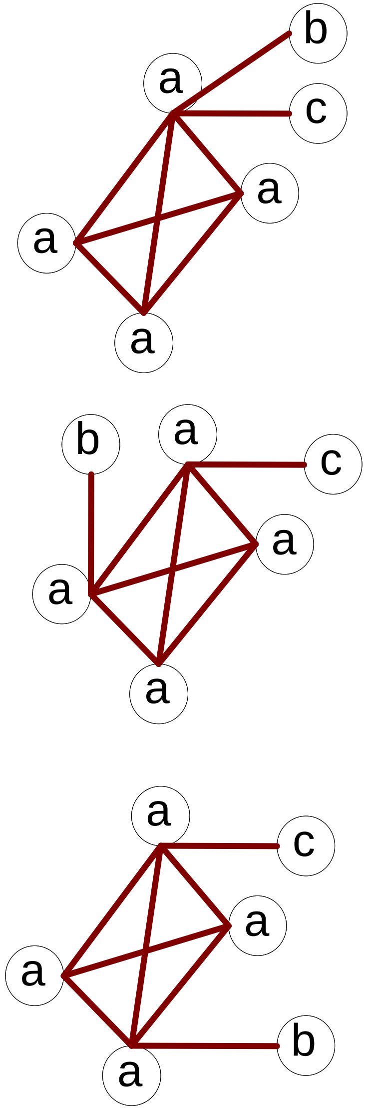
# Multiplicity of Candidates

- Case 1: Identical node labels



- Case 2: Core contains identical labels

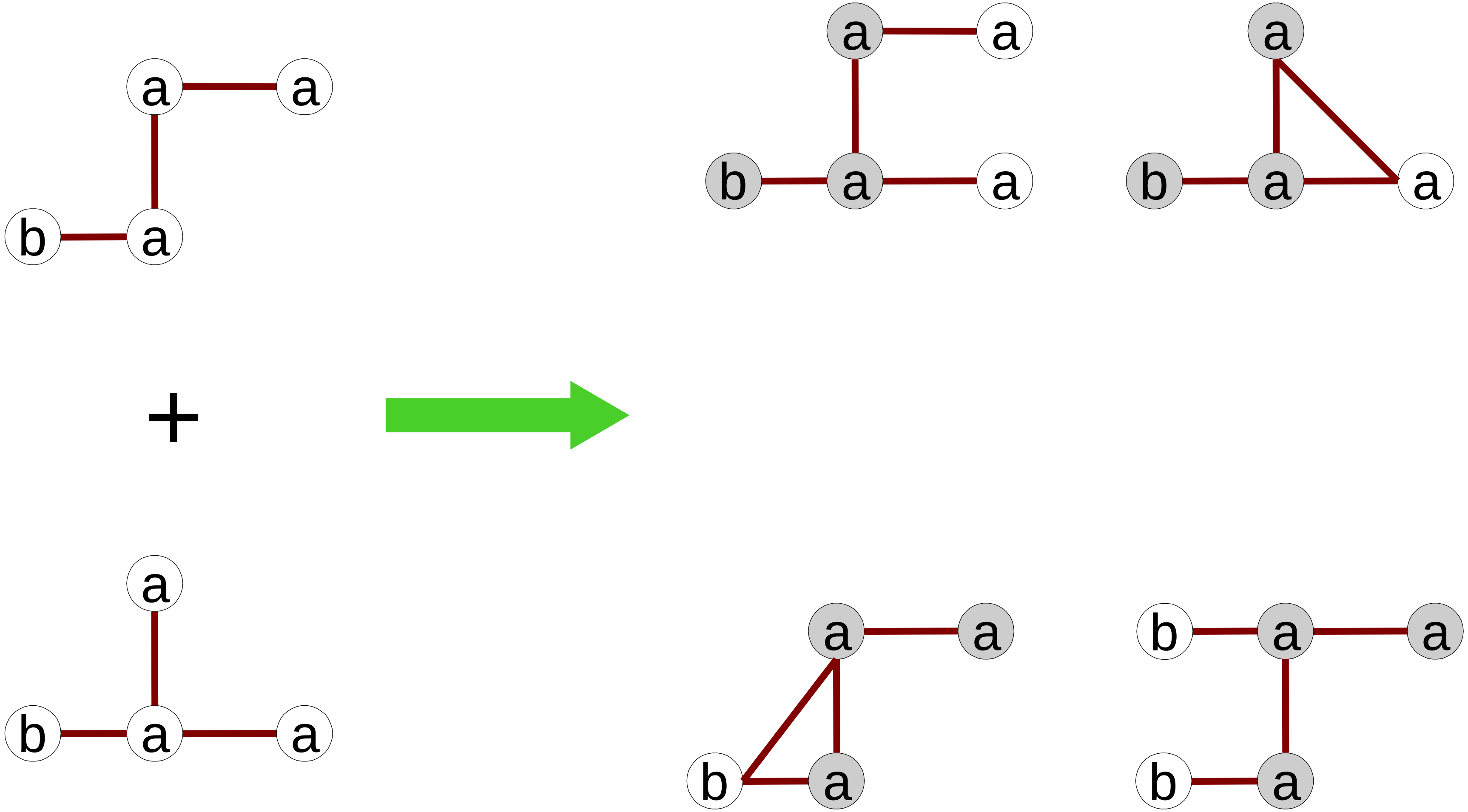



Core: The (k-1) subgraph that is common between the joint graphs

# Multiplicity of Candidates

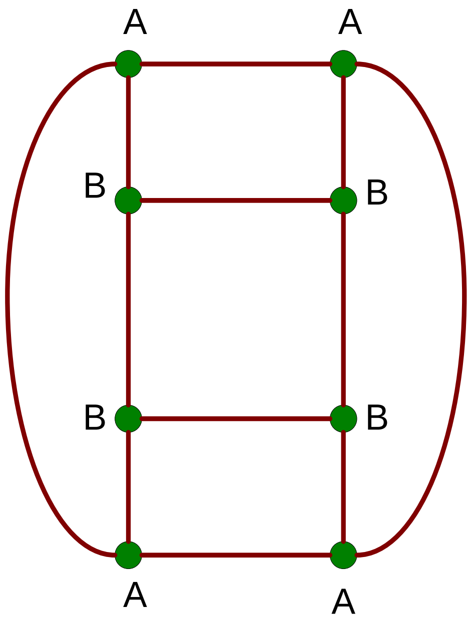
- Case 3: Core multiplicity

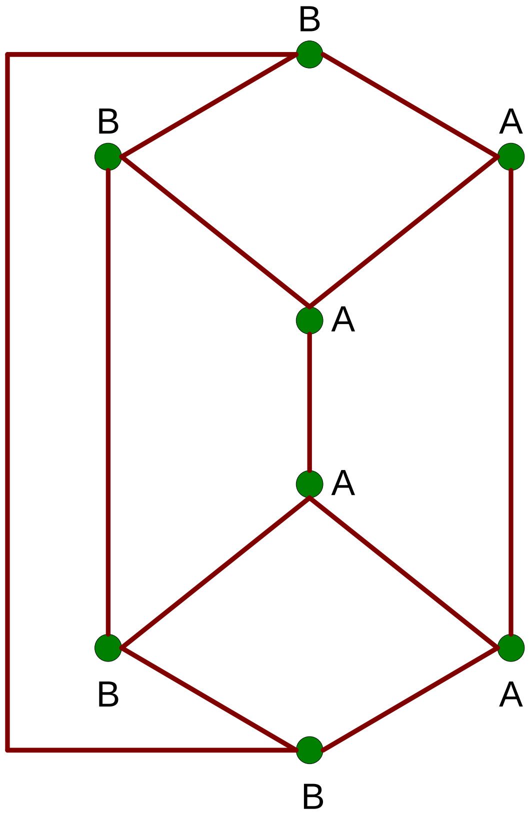


# Challenges

- Graph isomorphism
  - Two graphs may have the same topology though their layouts are different
- Computational complexity: computing a generating set for the automorphism group of a graph have the same complexity
  - NP-hard problem
- Subgraph isomorphism
  - How to compute the support value of a pattern
- Neural subgraph matching uses a machine learning-based approach to learn the NP-hard problem of subgraph isomorphism

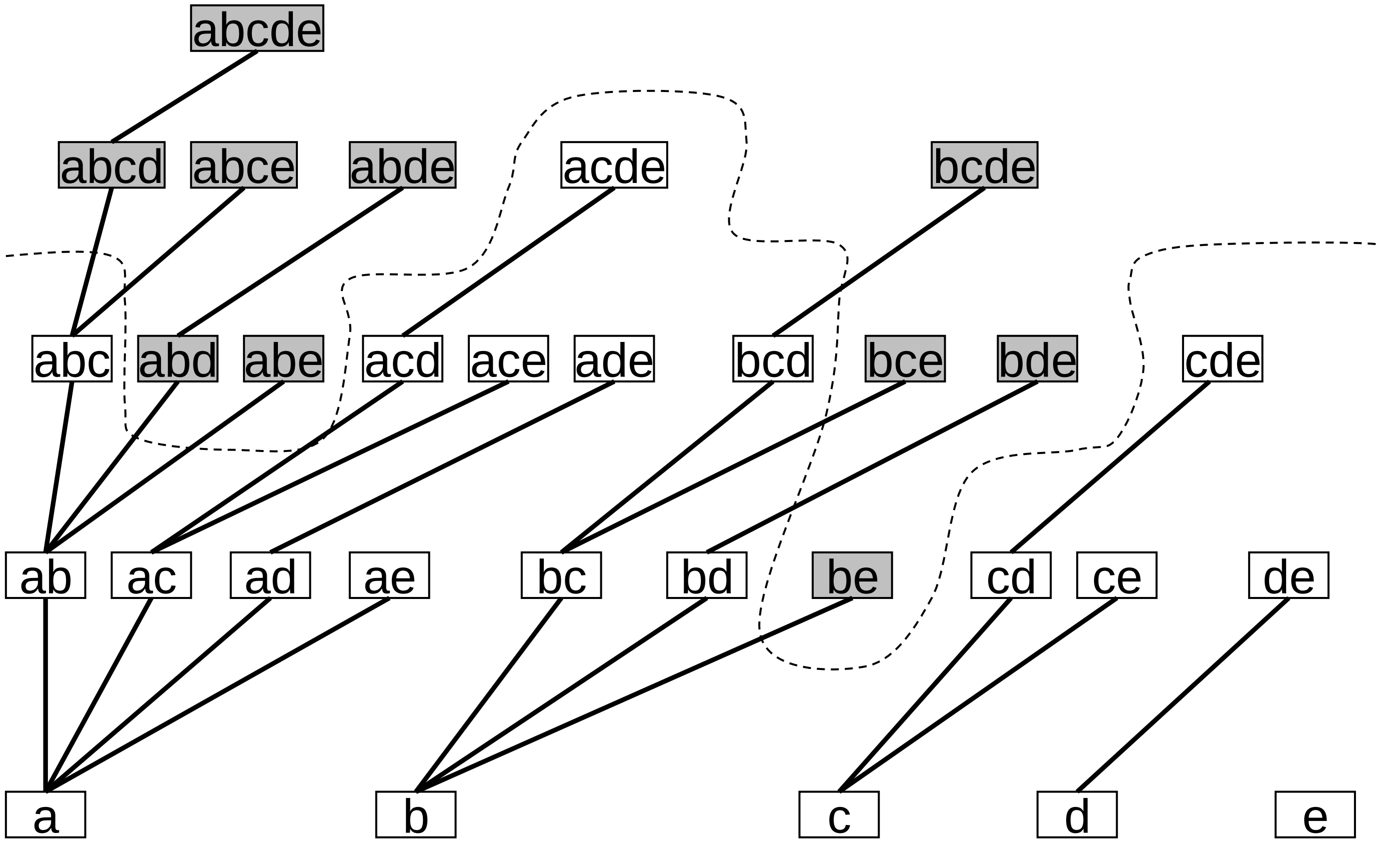
- A graph is isomorphic if it is topologically equivalent to another graph



# gSpan Motivation: DFS exploration wrt. itemsets

- Itemset search space – prefix based



# Motivation for Tree Search

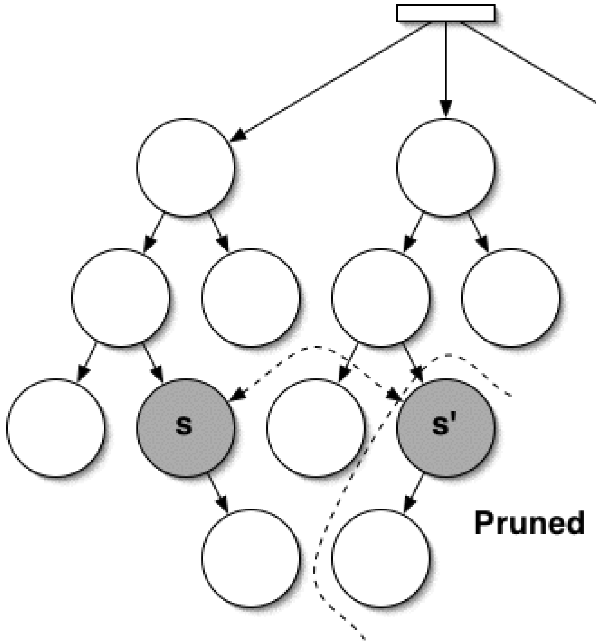


- Canonical representation of itemset is obtained by a complete order over the items
- Each possible itemset appear in TSS exactly once - no duplications or omissions

- Properties of Tree search space
  - For each k-label, its parent is the k-1 prefix of the given k-label
  - The relation among siblings is in ascending lexicographic order

# DFS Code Trees

- Organize DFS code nodes as parent-child
- Pre-order traversal follows DFS lexicographic order
- If s and s’ are the same graph with different DFS codes, s’ is not the min imum and can be pruned



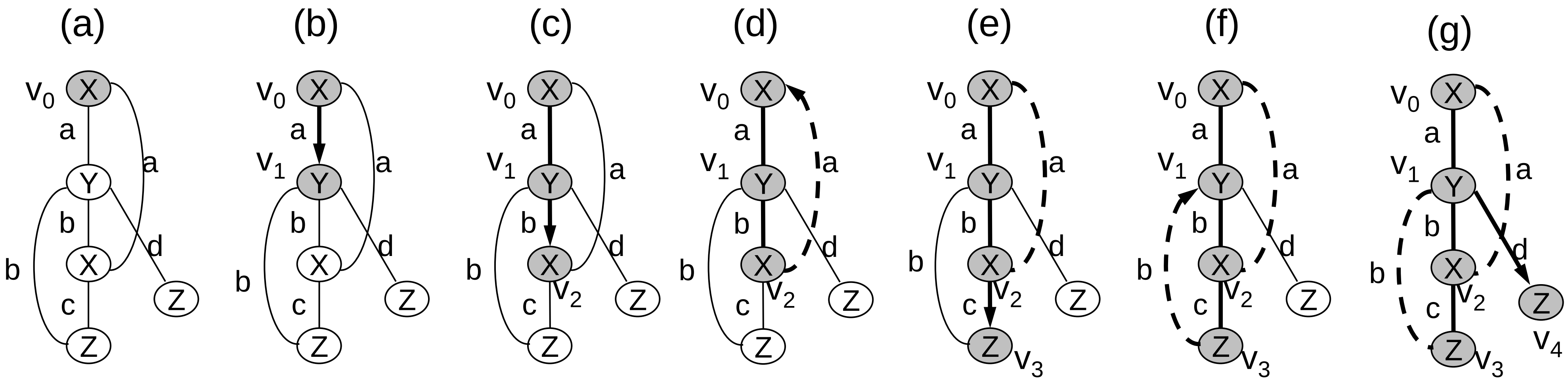
# DFS Code Construction: Tree Search Space



- Map each graph (2-Dim) to a sequential DFS Code (1-Dim)
- Lexicographically order the codes
- Construct Tree Search Space based on the lexicographic order

# DFS Code Construction

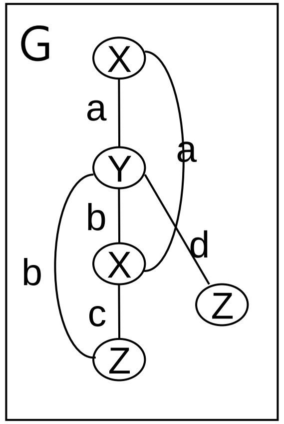
- Given a graph G. for each Depth First Search over graph G, construct the corresponding DFS-Code

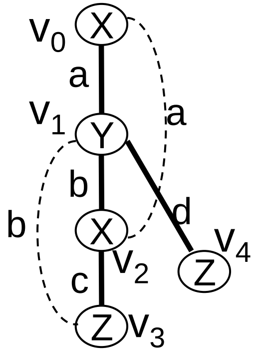



| | | | | | | |
|---|---|---|---|---|---|---|
| | (0,1,X,a,Y) | (1,2,Y,b,X) | (2,0,X,a,X) | (2,3,X,c,Z) | (3,1,Z,b,Y) | (1,4,Y,d,Z) |

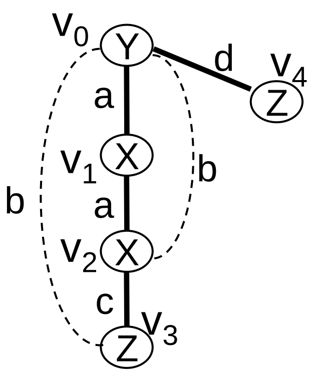
# Single Graph, several DFS-Codes

| | (a) | (b) | (c) |
|---|---|---|---|
| 1 | (0, 1, X, a, Y) | (0, 1, Y, a, X) | (0, 1, X, a, X) |
| 2 | (1, 2, Y, b, X) | (1, 2, X, a, X) | (1, 2, X, a, Y) |
| 3 | (2, 0, X, a, X) | (2, 0, X, b, Y) | (2, 0, Y, b, X) |
| 4 | (2, 3, X, c, Z) | (2, 3, X, c, Z) | (2, 3, Y, b, Z) |
| 5 | (3, 1, Z, b, Y) | (3, 0, Z, b, Y) | (3, 0, Z, c, X) |
| 6 | (1, 4, Y, d, Z) | (0, 4, Y, d, Z) | (2, 4, Y, d, Z) |

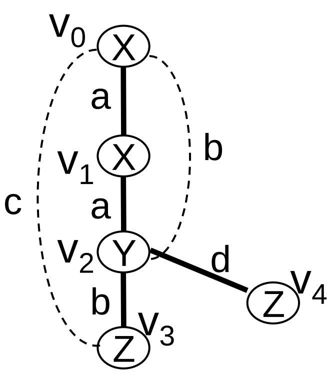



(a)




(b)



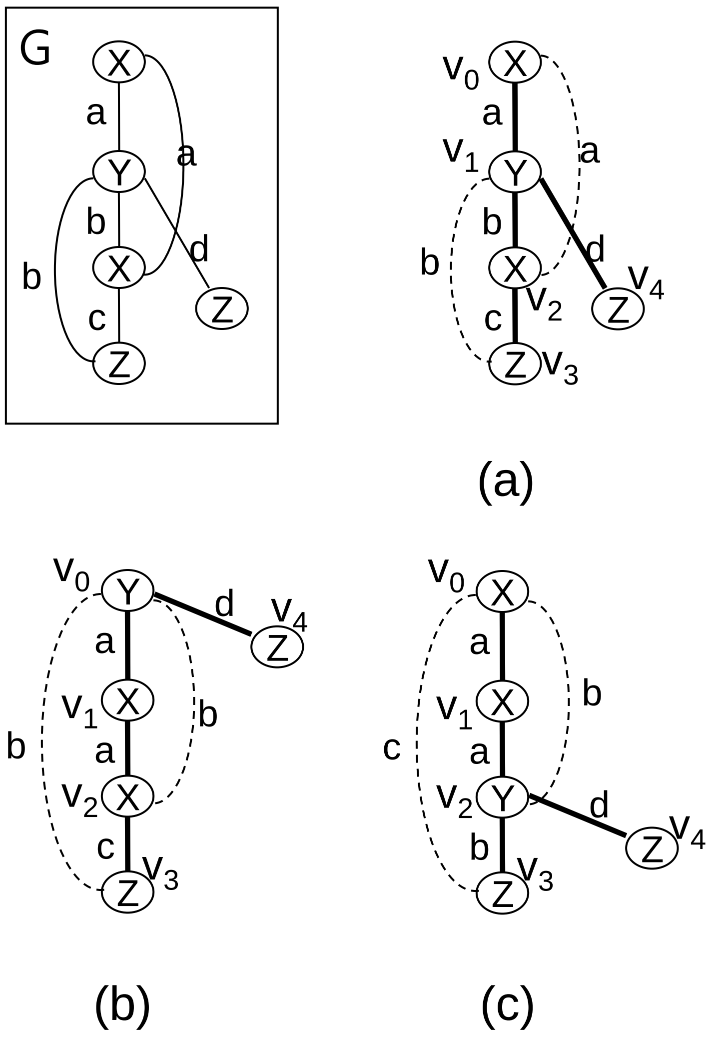

(c)

# Single Graph - Single Min DFS-Code



Min DFS-Code

| | (a) | (b) | (c) |
|---|---|---|---|
| 1 | (0, 1, X, a, Y) | (0, 1, Y, a, X) | **(0, 1, X, a, X)** |
| 2 | (1, 2, Y, b, X) | (1, 2, X, a, X) | **(1, 2, X, a, Y)** |
| 3 | (2, 0, X, a, X) | (2, 0, X, b, Y) | **(2, 0, Y, b, X)** |
| 4 | (2, 3, X, c, Z) | (2, 3, X, c, Z) | **(2, 3, Y, b, Z)** |
| 5 | (3, 1, Z, b, Y) | (3, 0, Z, b, Y) | **(3, 0, Z, c, X)** |
| 6 | (1, 4, Y, d, Z) | (0, 4, Y, d, Z) | **(2, 4, Y, d, Z)** |



# Minimum DFS-Code

- The minimum DFS code *min(G)*, in DFS lexicographic order, is a canonical representation of graph *G*

- Graphs *A* and *B* are isomorphic iff:

$$min(A) = min(B)$$

# DFS-Code Tree: parent-child relation

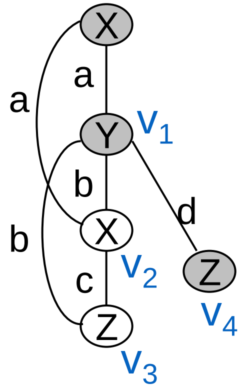


- If $min(G_1) = \{ a_0, a_1, \ldots.., a_n\}$ and $min(G_2) = \{ a_0, a_1, \ldots.., a_n, b\}$
  - $G_1$ is parent of $G_2$
  - $G_2$ is child of $G_1$
- A valid DFS code requires that **b** grows from a node on the rightmost path (inherited property from the DFS search)

# DFS-Code Tree: Parent-Child Relation



Graph $G_1$:

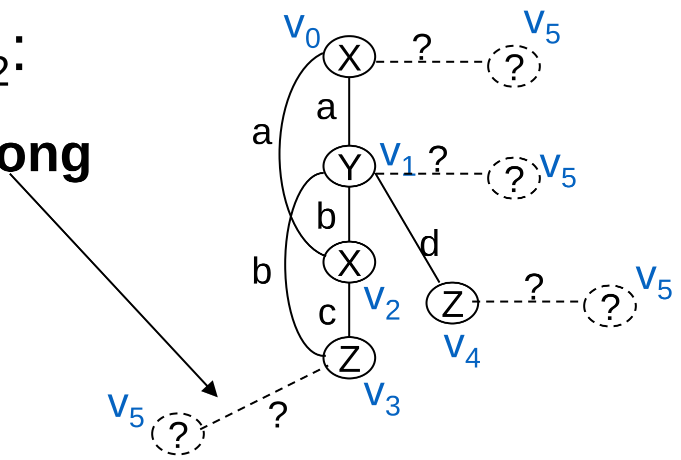



Min(g) = (0,1,X,a,Y) (1,2,Y,b,X) (2,0,X,a,X) (2,3,X,c,Z) (3,1,Z,b,Y) (1,4,Y,d,Z)

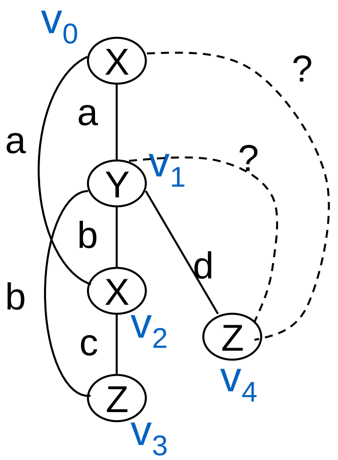
A child of graph $G_1$ *must grow edge from rightmost path of* $G_1$ (necessary condition)

Graph $G_2$:

**wrong**




Forward edge




Backward edge

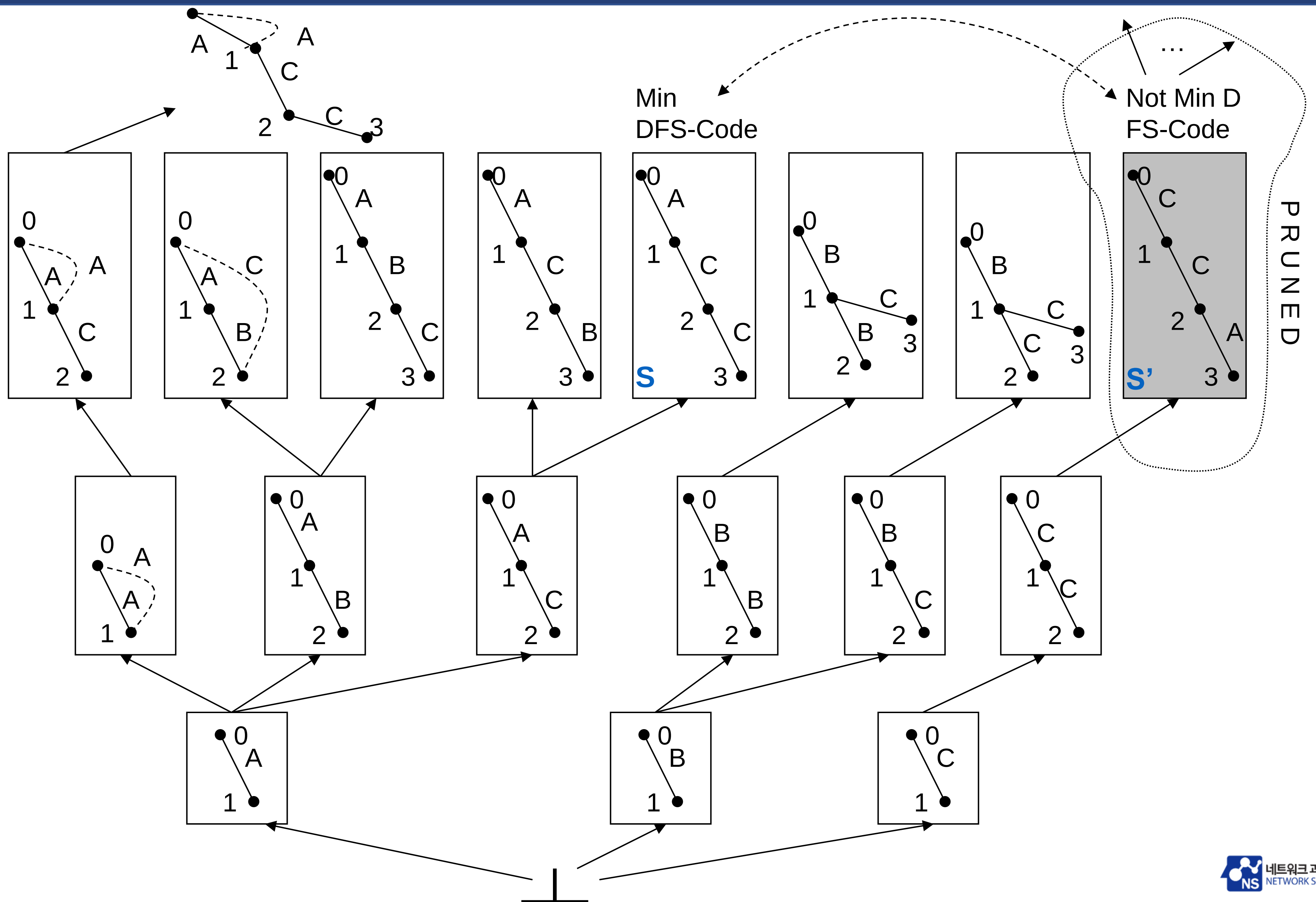
# Search Space: DFS Code Tree



- Organize DFS Code nodes as parent-child
- Sibling nodes organized in ascending DFS lexicographic order
- *In-Order* traversal follows DFS lexicographic order

# Search space: DFS code Tree





# Tree Pruning

- All the descendants of infrequent node are infrequent also

- All the descendants of a not minimal DFS code are also not minimal DFS codes

**Function gSpan(*D*, *F*, *g*):**

1: If $g \neq \min(g)$

return;

2: $F \leftarrow F \cup \{ g \}$

3: children($g$) $\leftarrow$ [generate all *g*’ potential children with one edge growth]

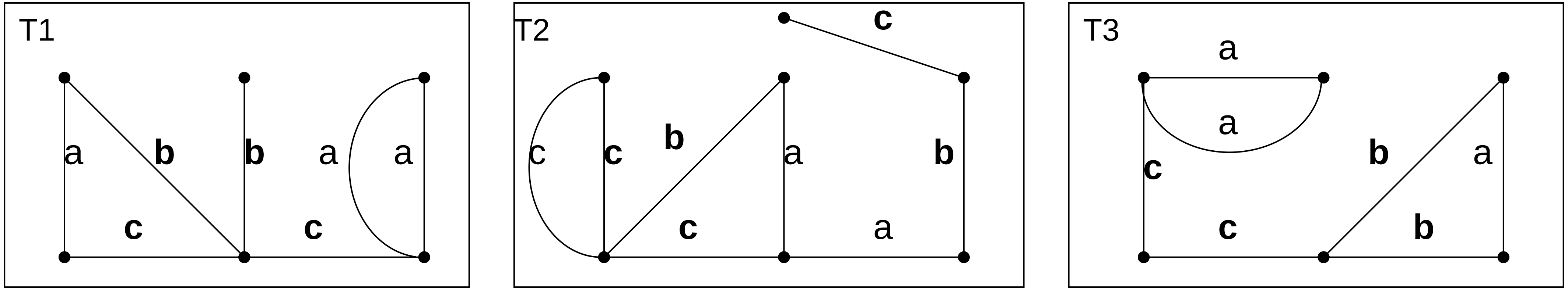
4: Enumerate(D, *g*, children(*g*))

5: for each $c \in$ children($g$)

If support($c$) $\geq$ #minSup

SubgraphMining (*D*, *F*, *c*)

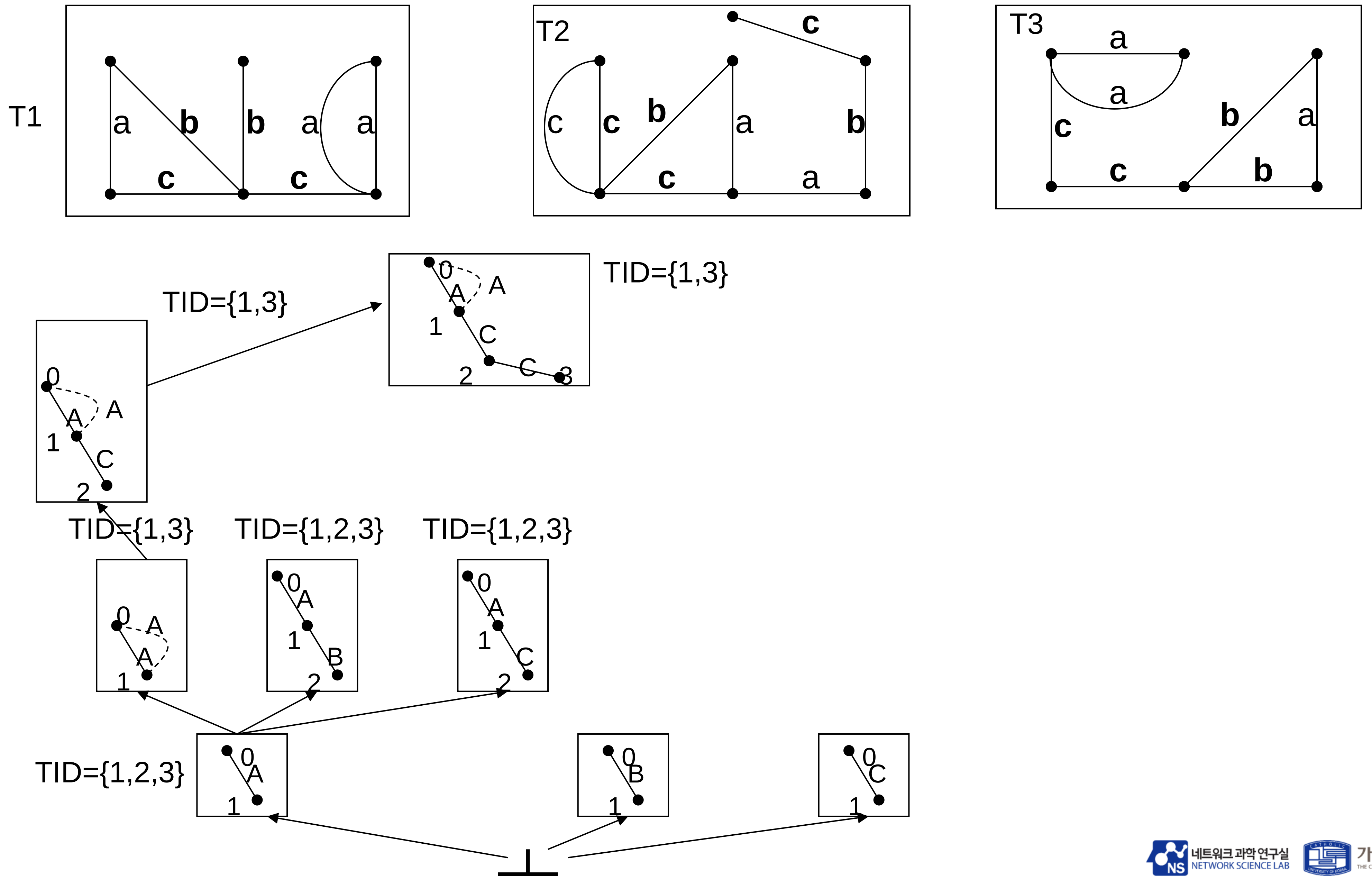
Given: database *D*




Task: Mine all frequent subgraphs with support ≥ 2 (#minSup)

# Example





T1
a
b
b
a
a
c
c
T2
c
c
c
b
a
b
c
a
T3
a
a
c
b
a
c
b
TID={1,3}
TID={1,3}
TID={1,3}
TID={1,2,3}
TID={1,2,3}
TID={1,2,3}

# gSpan Algorithm: Sample code

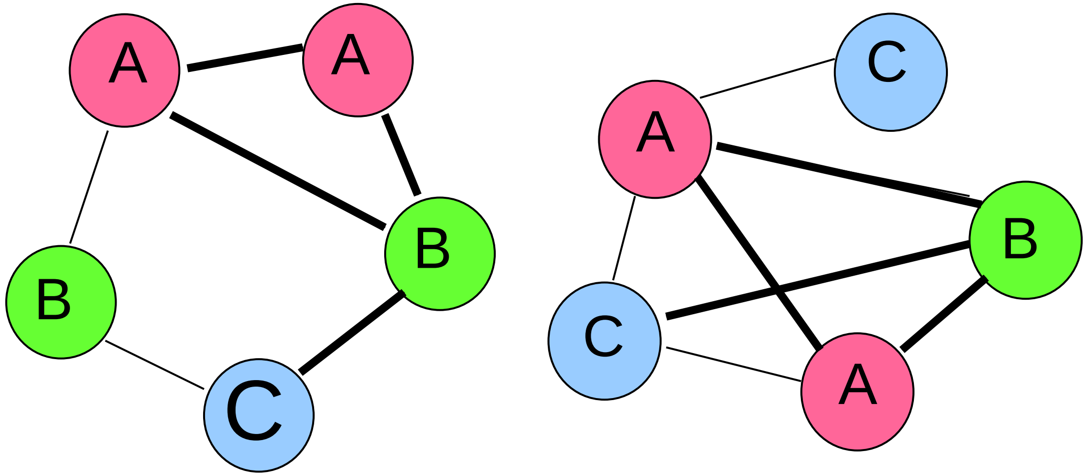
- Support: 2

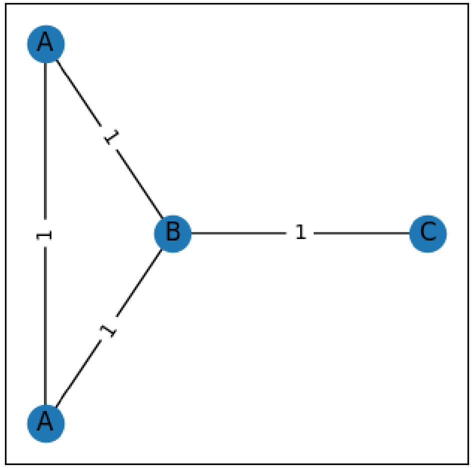
```python
from gspan_mining.config import parser
from gspan_mining.main import main
```

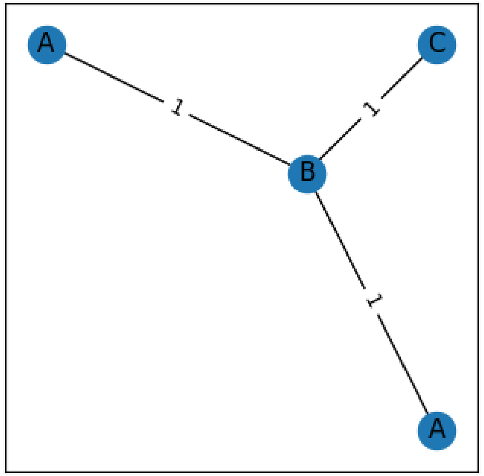
```python
%matplotlib inline
```

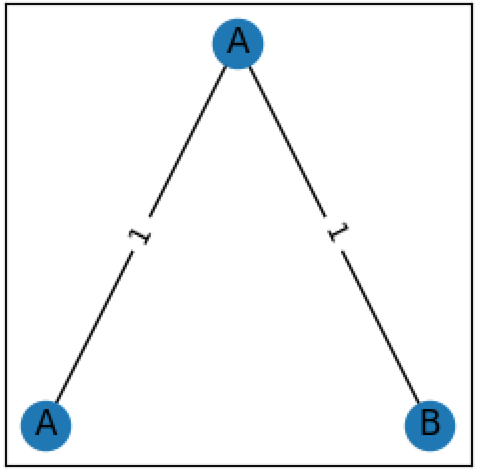
```python
args_str = '-s 2 -l 3 -p True graphdata/sample_data3'
FLAGS, _ = parser.parse_known_args(args=args_str.split())
```

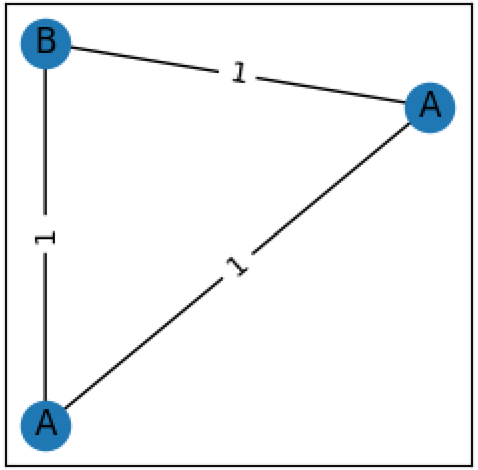
```python
gs = main(FLAGS)
print(gs)
```

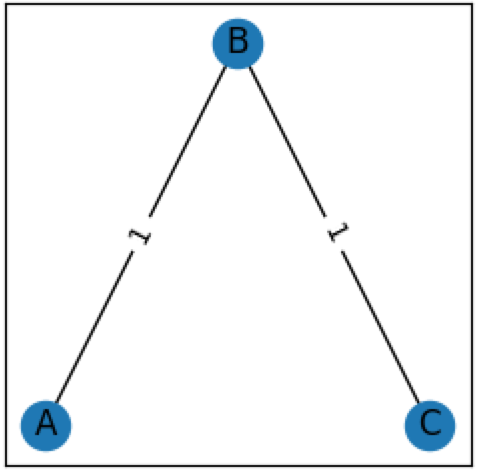


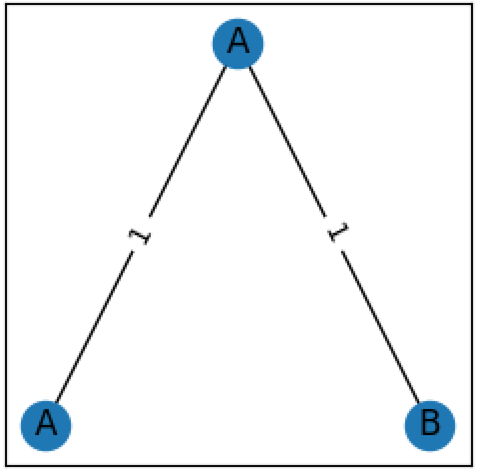



# Subdue Algorithm

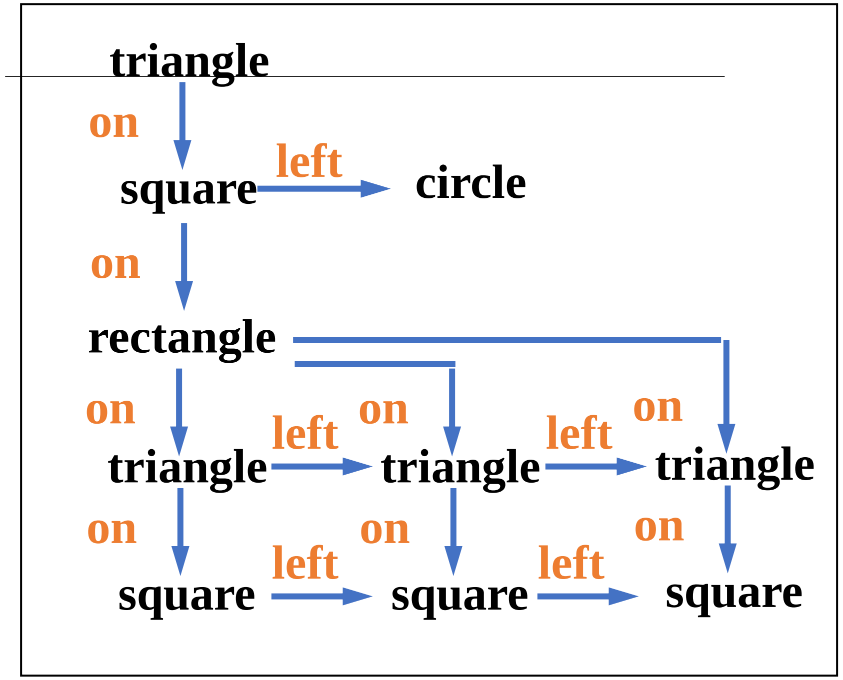


- A greedy algorithm for finding some of the most prevalent subgraphs
- This method is not complete
  - i.e. it may not obtain all frequent subgraphs, although it pays in fast execution
- It discovers substructures that compress the original data and represent structural concepts in the data
- Based on *Beam Search* - like BFS it progresses level by level. Unlike BFS, however, beam search moves downward only through the best *W* nodes at each level. The other nodes are ignored

# Subdue Algorithm: Step 1

- Step 1: Create substructure for each unique node label

DB:



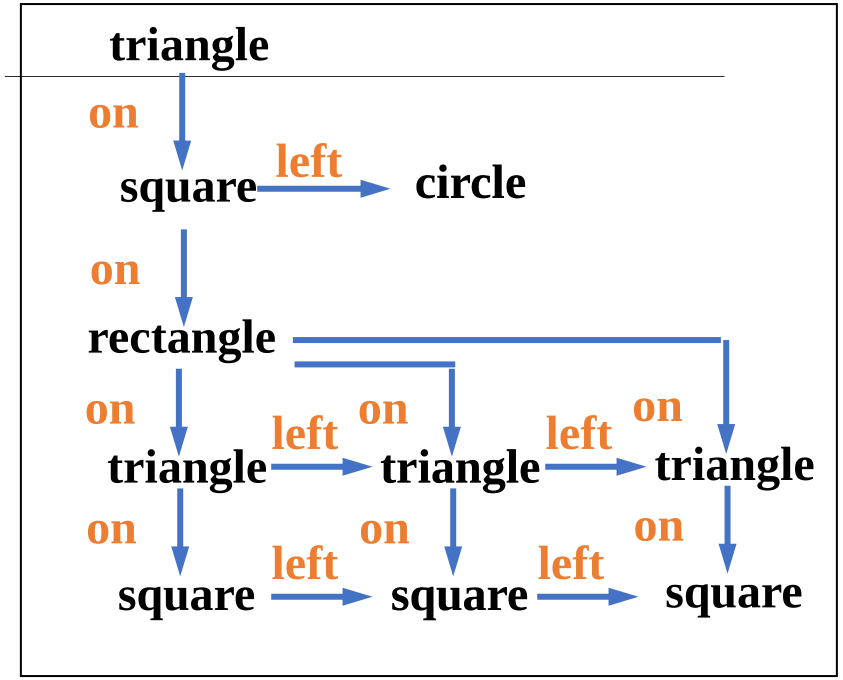

Substructures:

**triangle (4)**
**square (4)**
**circle (1)**
**rectangle (1)**

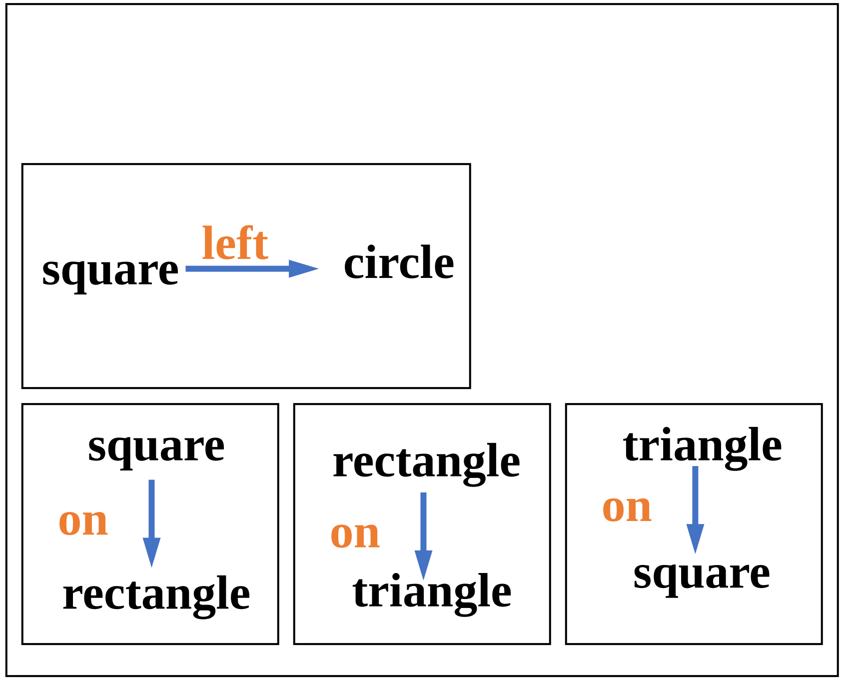
# Subdue Algorithm: Step 2

➢ Step 2: Expand best substructure by an edge or edge and neighboring node

DB:




Substructures:



# Subdue Algorithm: Steps 3-5



- Step 3:  Keep only best substructures on queue (specified by beam width)

- Step 4: Terminate when queue is empty or when the number of discovered substructures is greater than or equal to the limit specified

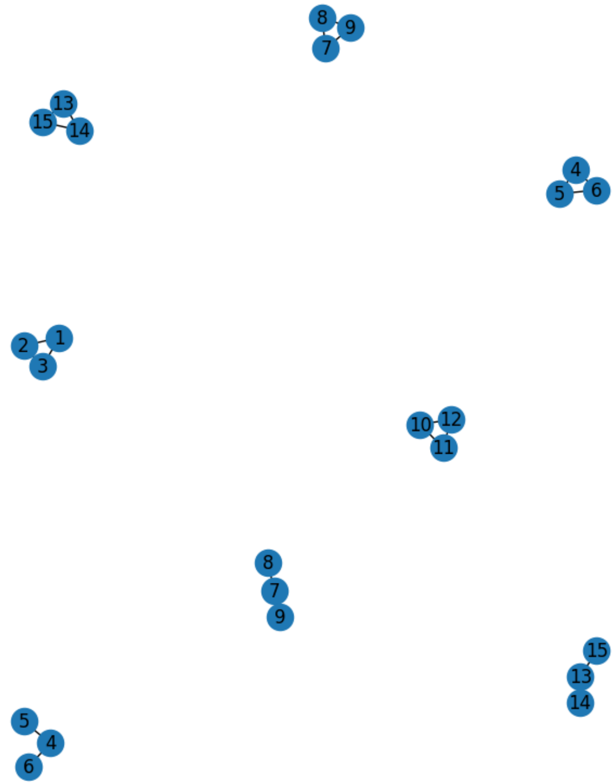
- Step 5: Compress graph and repeat to generate hierarchical description

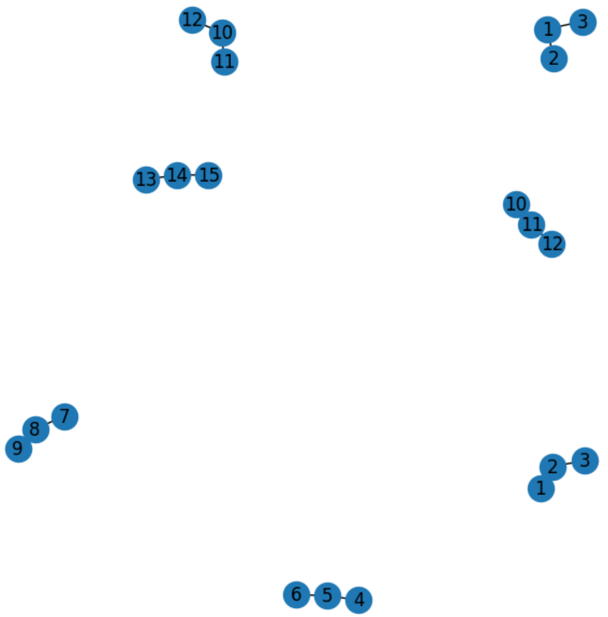
# Subdue Algorithm: Steps 3-5



```python
import os
import subprocess
import json
import re
import contextlib
import io
import sys
import networkx as nx

from Subdue_mining import Parameters
from Subdue_mining.Subdue import ReadGraph, Subdue, nx_subdue

subdue_example_path = './graphdata/inputgraph.json'
tolerance_pct = 0.1  # mainly due to non-deterministic nature of the algorithm

def subdue_json_to_undirected_nx_graph(subdue_json_path):
    with open(subdue_json_path, 'r') as subdue_json_file:
        subdue_format = json.load(subdue_json_file)

    graph = nx.Graph()
    for vertex_or_edge in subdue_format:
        if list(vertex_or_edge.keys()) == ['vertex']:
            node_attributes_loop = vertex_or_edge['vertex']['attributes']
            graph.add_node(
                vertex_or_edge['vertex']['id'],
                **node_attributes_loop,
            )
        elif list(vertex_or_edge.keys()) == ['edge']:
            edge_attributes_loop = vertex_or_edge['edge']['attributes']
            graph.add_edge(
                u_of_edge=vertex_or_edge['edge']['source'],
                v_of_edge=vertex_or_edge['edge']['target'],
                **edge_attributes_loop,
            )
        else:
            raise ValueError('Invalid entry type')

    return graph

# use networkx graph as an input
subdue_example_graph = subdue_json_to_undirected_nx_graph(subdue_example_path)
capture_prints = io.StringIO()
with contextlib.redirect_stdout(capture_prints):
    result = nx_subdue(graph=subdue_example_graph, verbose=True)
prints_nx_subdue = capture_prints.getvalue()
```

```python
import matplotlib.pyplot as plt

# Create a new graph for each list and add nodes and edges
graphs = []
for graph_data in result:
    G = nx.Graph()
    for subgraph_data in graph_data:
        G.add_nodes_from(subgraph_data['nodes'])
        G.add_edges_from(subgraph_data['edges'])
    graphs.append(G)

# Draw the graphs
for i, G in enumerate(graphs):
    plt.figure(i)
    nx.draw(G, with_labels=True)
plt.show()
```






네트워크 과학 연구실
NETWORK SCIENCE LAB

가톨릭대학교
THE CATHOLIC UNIVERSITY OF KOREA