Graph Kernels

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

- Overview of Graph Kernels.
- Graph Kernels methods:
  - Graphlet kernel.
  - Shortest path kernel
  - Random walk kernel.
  - Weisfeiler-Lehman (WL) graph kernel: WL relabelling process.
- Subgraph Matching Kernel.
- Sample code of Graph Kernels.

Motivation

- From an algorithmic perspective, graphs are the most general data structures, as all common data types are simple instances of graphs.
  - E.g. 1, A time series of vectors can be represented as a graph that contains one node per time step, and consecutive steps are linked by an edge.
  - E.g. 2, A string is a graph in which each node represents one character, and consecutive characters are connected by an edge.

- Given their generality, the natural question to ask is:

  Why have graphs not been the common data structure in computer science for decades?

- The answer is simple:

  Their comparison is computationally expensive.

  Graphs are prisoners of their own their flexibility.

Why Graph Kernels?

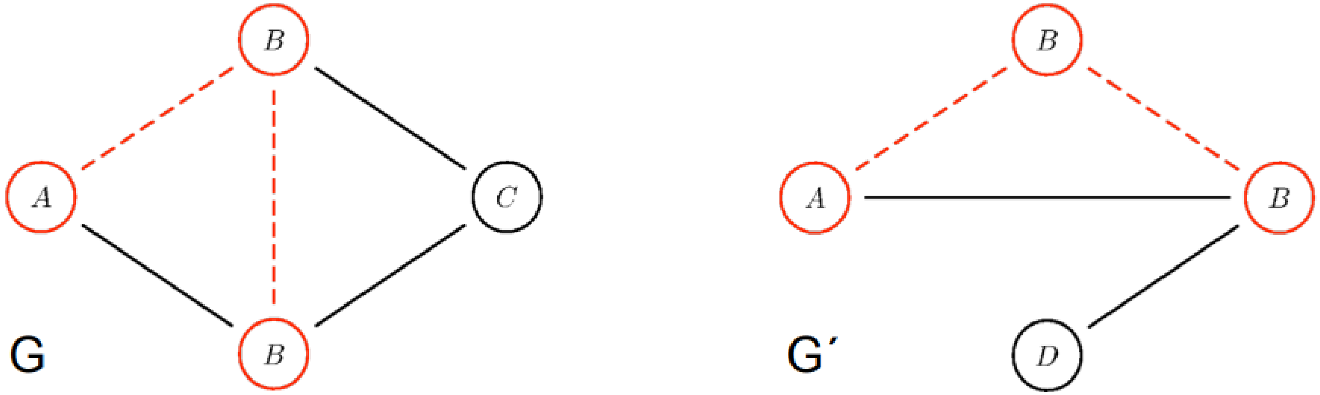
- Graph kernels are one of the most recent approaches to graph comparison.
- Interestingly, graph kernels employ concepts from all three traditional branches of graph comparison:
    - Measure similarity in terms of isomorphic substructures of graphs.
    - Allow for inexact matching of nodes, edges, and labels.
    - Treat graphs as vectors in a Hilbert space of graph features.

Graph Comparison

- Given two graphs G and G'. The problem of graph comparison is to find a mapping:

$$s : \mathcal{G} \times \mathcal{G} \rightarrow \mathbb{R}$$

- Such that $s(G, G')$ quantifies the similarity (dissimilarity) of G and G'

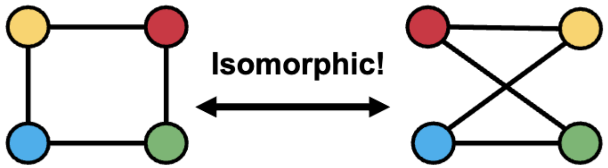


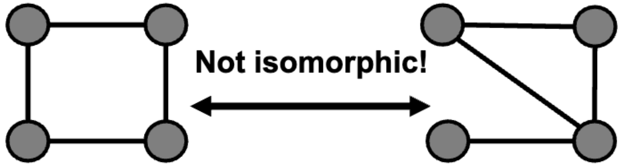
Applications of Graph Comparison

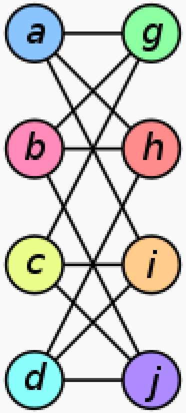
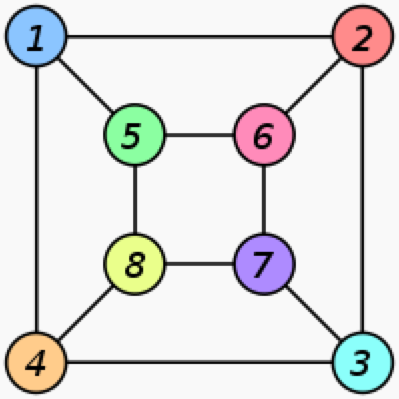
- Function prediction of chemical compounds.
- Structural comparison and function prediction of protein structures.
- Comparison of social networks.
- Analysis of semantic structures in Natural Language Processing.
- Comparison of UML diagrams.

Graph Isomorphism

- Graph isomorphism:
  - Find a mapping f of the vertices of G_1 to the vertices of G_2 such that G_1 and G_2 are identical.
  - i.e. (x, y) is an edge of G_1 if $(f(x), f(y))$ is an edge of G_2. Then f is an isomorphism, and G_1 and G_2 are called isomorphic.
  - No polynomial-time algorithm is known for graph isomorphism.
  - Neither is it known to be NP-hard.

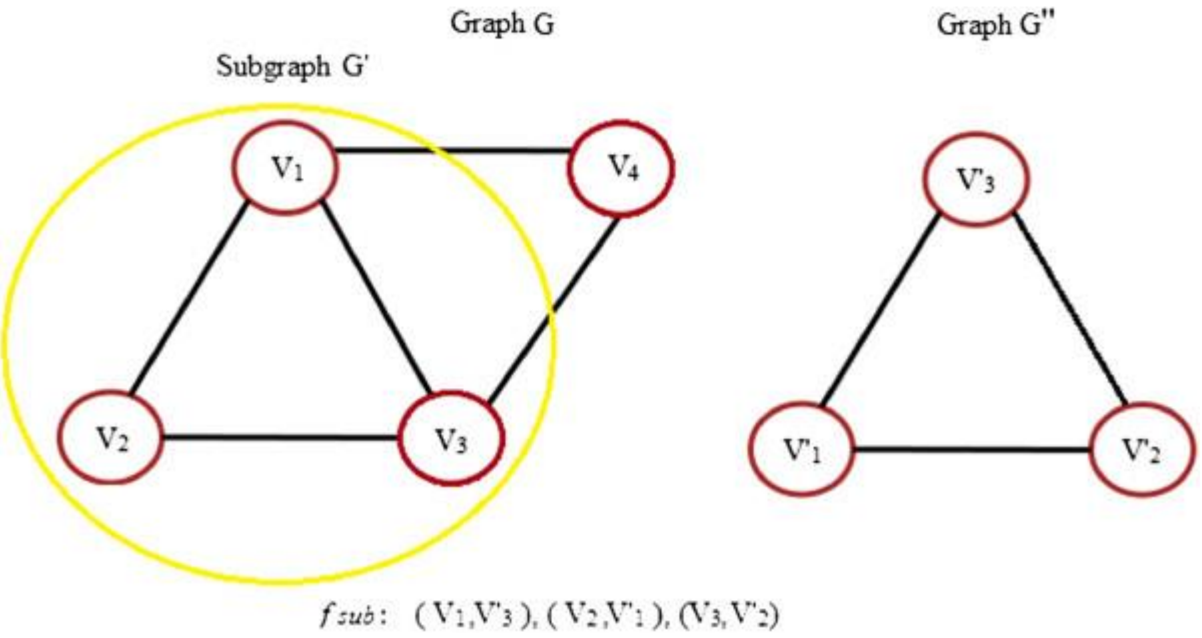




Graph G	Graph H	An isomorphism between G and H
		$f(a) = 1$ $f(b) = 6$ $f(c) = 8$ $f(d) = 3$ $f(g) = 5$ $f(h) = 2$ $f(i) = 4$ $f(j) = 7$

Graph Isomorphism

- Subgraph isomorphism:
  - Subgraph isomorphism asks if there is a subset of edges and vertices of G_1 that is isomorphic to a smaller graph G_2.
  - Subgraph isomorphism is **NP-complete**.


Graph G
Graph G''
Subgraph G'
V_1
V_4
V_2
V_3
V'_3
V'_1
V'_2
f_{sub}: (V_1, V'_3), (V_2, V'_1), (V_3, V'_2)

Subgraph Isomorphism Challenges

- **NP-completeness:**
  - A decision problem C is NP-complete if
    - C is in NP.
    - C is NP-hard, i.e. every other problem in NP is reducible to it.

- **Problems for the practitioner:**
  - Excessive runtime in worst case.
  - Runtime may grow exponentially with the number of nodes.
  - For larger graphs with many nodes and for large datasets of graphs, this is an enormous problem.

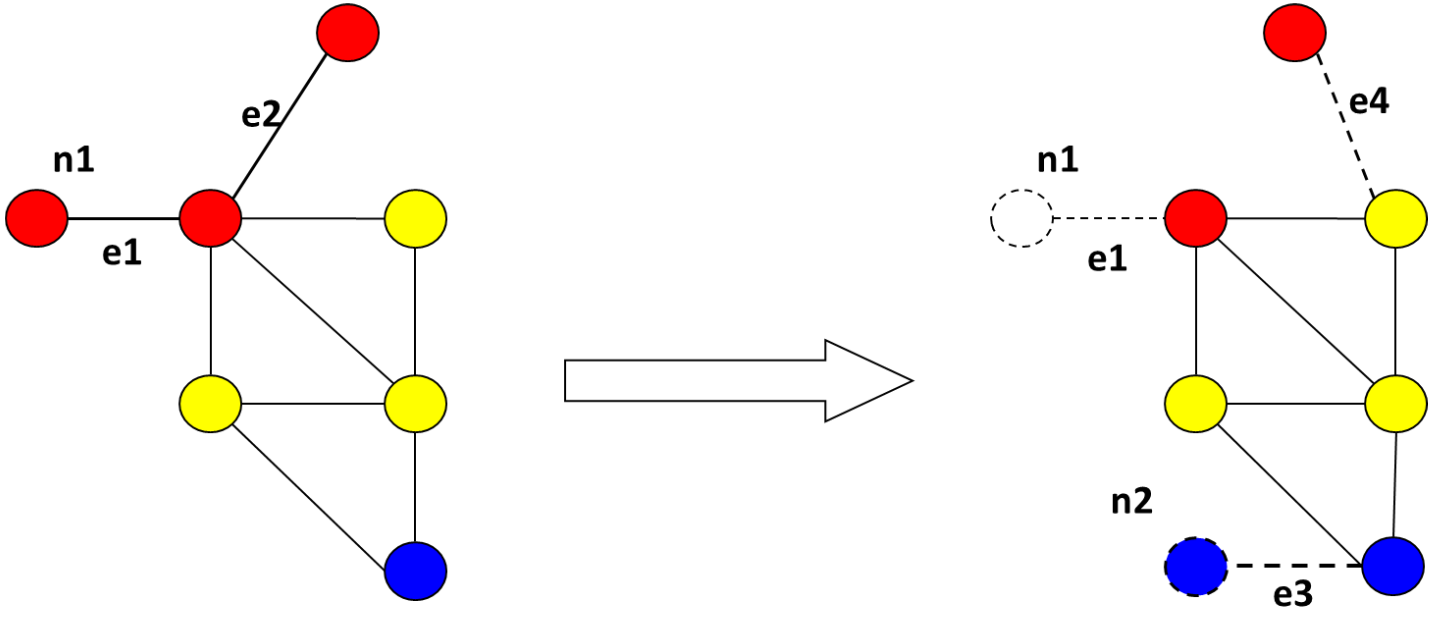
➡ Wanted: Polynomial-time similarity measure for graphs.

Graph Edit Distances

- Principle:
  - Count operations that are necessary to transform g_1 into g_2.
  - Assign costs to different types of operations (edge/node insertion/deletion, modification of labels).

$$GED(g_1, g_2) = \min_{(e_1,\ldots,e_k)\in\mathcal{P}(g_1,g_2)} \sum_{i=1}^{k} c(e_i)$$

Where $P(g_1, g_2)$ denotes the set of edit paths transforming g_1 into g_2 and $c(e) \geq 0$ is the cost of each graph edit operation e.



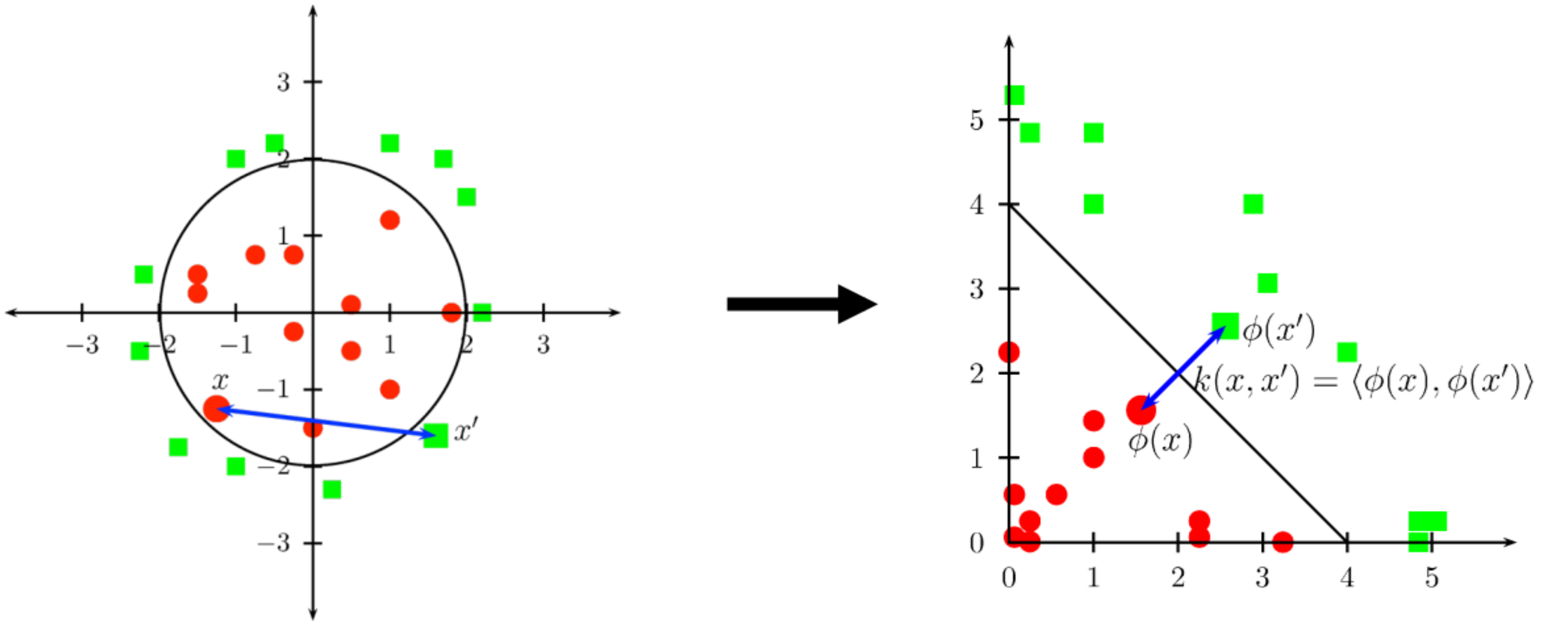
Graph Edit Distances Pros and Cons

- Advantages:
    - Captures partial similarities between graphs.
    - Allows for noise in the nodes, edges and their labels.
    - Flexible way of assigning costs to different operations.
- Disadvantages:
    - Contains subgraph isomorphism check as one intermediate step.
    - Choosing cost function for different operations is difficult.

What is a Kernel? (Schölkopf ,1997)

- Kernel is a type of measures of similarity.
- Mapping two objects x and x’ via mapping $\boxed{\phi}$ into feature space *H.*
- Measure their similarity in *H* as $\langle\phi(x),\phi(x')\rangle$.
- **Kernel Trick**: Compute inner product in *H* as kernel in input space

$$\boxed{k(x,x') = \langle\phi(x),\phi(x')\rangle.}$$

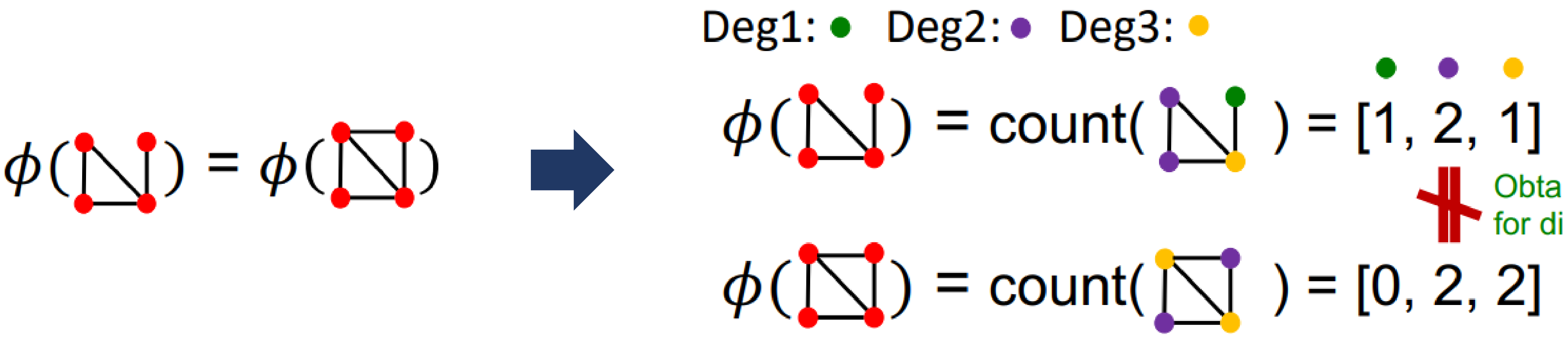

3
2
1
-3
-2
-1
1
2
3
-1
-2
-3
x
x'
5
4
3
2
1
0
0
1
2
3
4
5
$\phi(x')$
$k(x,x') = \langle\phi(x),\phi(x')\rangle$
$\phi(x)$

https://link.springer.com/chapter/10.1007/BFb0020217

What is a Kernel? (Schölkopf ,1997)

- Kernel is a type of measures of similarity.
- Mapping two objects x and x’ via mapping $\boxed{\phi}$ into feature space *H.*
- Measure their similarity in *H* as $\langle \phi(x), \phi(x') \rangle.$
- **Kernel Trick**: Compute inner product in *H* as kernel in input space

$$\boxed{k(x, x') = \langle \phi(x), \phi(x') \rangle.}$$



Deg1: ●
Deg2: ●
Deg3: ●
ϕ( ) = ϕ( )
ϕ( ) = count( ) = [1, 2, 1]
Obta
for di
ϕ( ) = count( ) = [0, 2, 2]

What is a Graph Kernel?

- Instance of R-convolution kernels by Haussler (1999):
  - R-convolution kernels compare decompositions of two structured objects.

$$k_{convolution}(x, x') = \sum_{(x_d, x) \in R} \sum_{(x'_d, x') \in R} k_{parts}(x_d, x'_d)$$

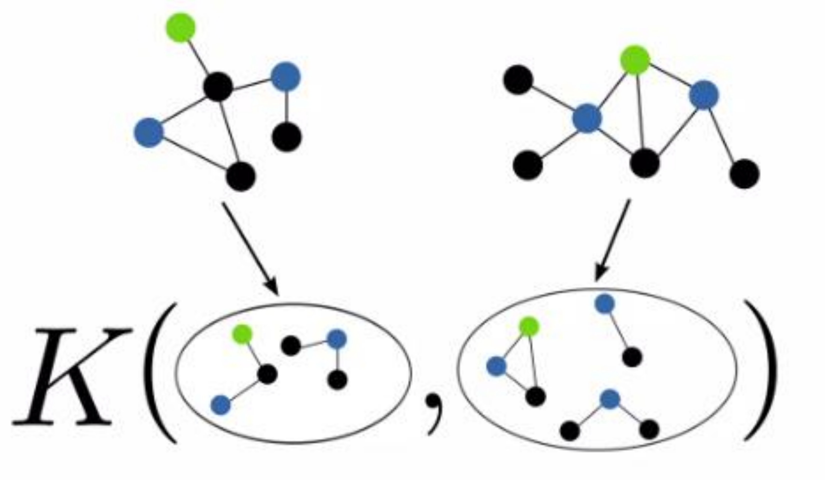
  - Decompose graphs into their substructures and add up the pairwise similarities between these substructures.

- Concept:
  - Kernel function to measure the similarity of pairs of graphs by computing an inner product on graphs.
  - Compare substructures of graphs that are computable in polynomial time.

https://citeseerx.ist.psu.edu/document?repid=rep1&type=pdf&doi=5ee0d8aeb2cb01ef4d8a858d234e72a7400c03ac

Kenels based on bags of patterns

- Graph kernels based on bags of patterns:
  - Extraction of a set of patterns from graphs.
  - Comparison between patterns.
  - Comparison between bags of patterns.



Hardness Results (Gaertner, Flach, Wrobel, COLT 2003)

- Link to graph isomorphism
  - Let $k(G, G') = < \phi(G), \phi(G') >$ be a graph kernel
  - If ϕ is injective (one-to-one), *k* is called a complete graph kernel

Proposition 1.

- Computing any complete graph kernel is at least as hard as deciding whether two graphs are isomorphic.

- Criteria for a good graph kernel:
  - Expressive
  - Efficient to compute
  - Positive definite
  - Applicable to wide range of graphs

https://link.springer.com/chapter/10.1007/978-3-540-45167-9_11

Example

- Let X represent the alphabet where each element of X is a set.
- Define the intersection kernel to be $K(X_1, X_2) = |X_1 \cap X_2|$.
- Given a graph G, obtain the set of all its subgraphs, denoted by $X(G)$.
- Then the following is a graph kernel

$$K(G_1, G_2) = K(X(G_1), X(G_2)) = |\, X(G_1) \cap X(G_2)|$$

- This kernel looks for all overlapping substructures between two graphs.
- High complexity.

Graph Kernel Applications: Chemoinformatics (Ralaivola et al., 2005)

- Graph kernels inspired by concepts from chemoinformatics:
  - Define three new kernels (Tanimoto, MinMax, Hybrid) for function prediction of chemical compounds,
  - Based on the idea of molecular fingerprints and
  - Counting labeled paths of depth up to d using depth-first search from each possible vertex.

- **Properties**:
  - Tailored for applications in chemical informatics,
  - Exploit the small size and low average degree of these molecular graphs.

Graph Kernel Applications: Chemoinformatics (Ralaivola et al., 2005)

- Graph kernels inspired by concepts from chemoinformatics:
  - Define three new kernels (Tanimoto, MinMax, Hybrid) for function prediction of chemical compounds,
  - Based on the idea of molecular fingerprints and
  - Counting labeled paths of depth up to d using depth-first search from each possible vertex.

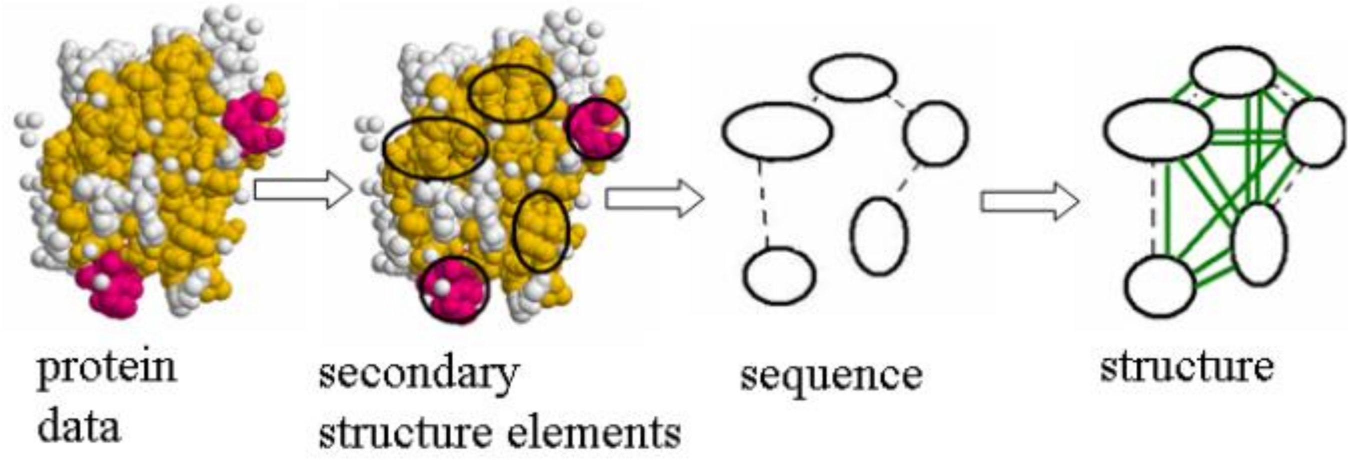
- **Properties**:
  - Tailored for applications in chemical informatics,
  - Exploit the small size and low average degree of these molecular graphs.

Chemical Compound Classification (Wale et al, ICDM 2006)

- New kernels and experimental comparison of existing techniques:
  - Define a kernel that considers *graph fragments*: Subgraphs with a maximum of l edges
  - Fragment-based kernels outperform kernels using frequent subgraphs and walk-based kernels.
- **Four choices in kernel design for chemical compound**:
  - Generation of patterns (learnt from dataset versus defined by expert).
  - 'Preciseness' of the patterns (whether subgraph features map to the same dimension in feature space).
  - Complete coverage (whether the patterns occur in all of the instances of the dataset).
  - Complexity of patterns (walks and cycles versus frequent subgraphs).

Applications: Protein Function Prediction (B. et al, ISMB 2005)

- Predict the function of a protein from its structure.
- Model protein structure as graph.
- Use graph kernels to measure structural similarity and SVM to predict functional class.
- Reaches competitive results on benchmark datasets.

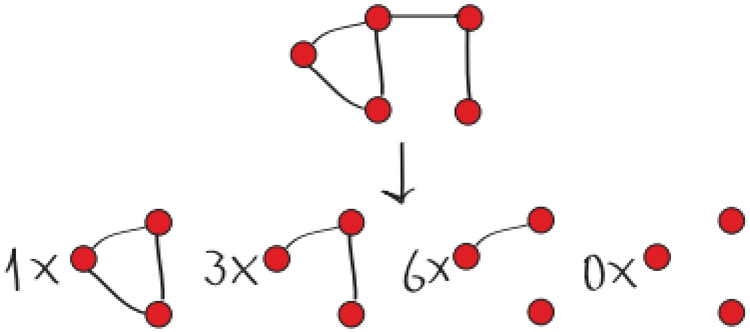

protein data
secondary structure elements
sequence
structure

Base Kernels

- **Graphlet kernel** [Shervashidze et al., 2009]:
  - Counts identical pairs of graphlets.
    (i.e., subgraphs with k nodes where k = 3, 4, 5) in two graphs.
- **Shortest path kernel** [Borgwardt and Kriegel, 2005]:
  - Counts pairs of shortest paths in two graphs having the same source and sink labels and identical length.
- **Random walk kernel** [Kashima et al.,2003; Gärtner et al., 2003]:
  - Counts pairs of random walks and compare walks in two input graphs.
- **Weisfeiler-Lehman** [Weisfeiler-Lehman isomorphic testing, 1968]:
  - WL relabelling process.
- **Pyramid match graph kernel** [Nikolentzos et al.,2017b]:
  - Embeds the vertices of the input graphs in a vector space.
  - It then partitions the feature space into regions of increasingly larger size and takes a weighted sum of the matches that occur at each level.

Graphlet Kernel (B., Petri, et al., MLG 2007)

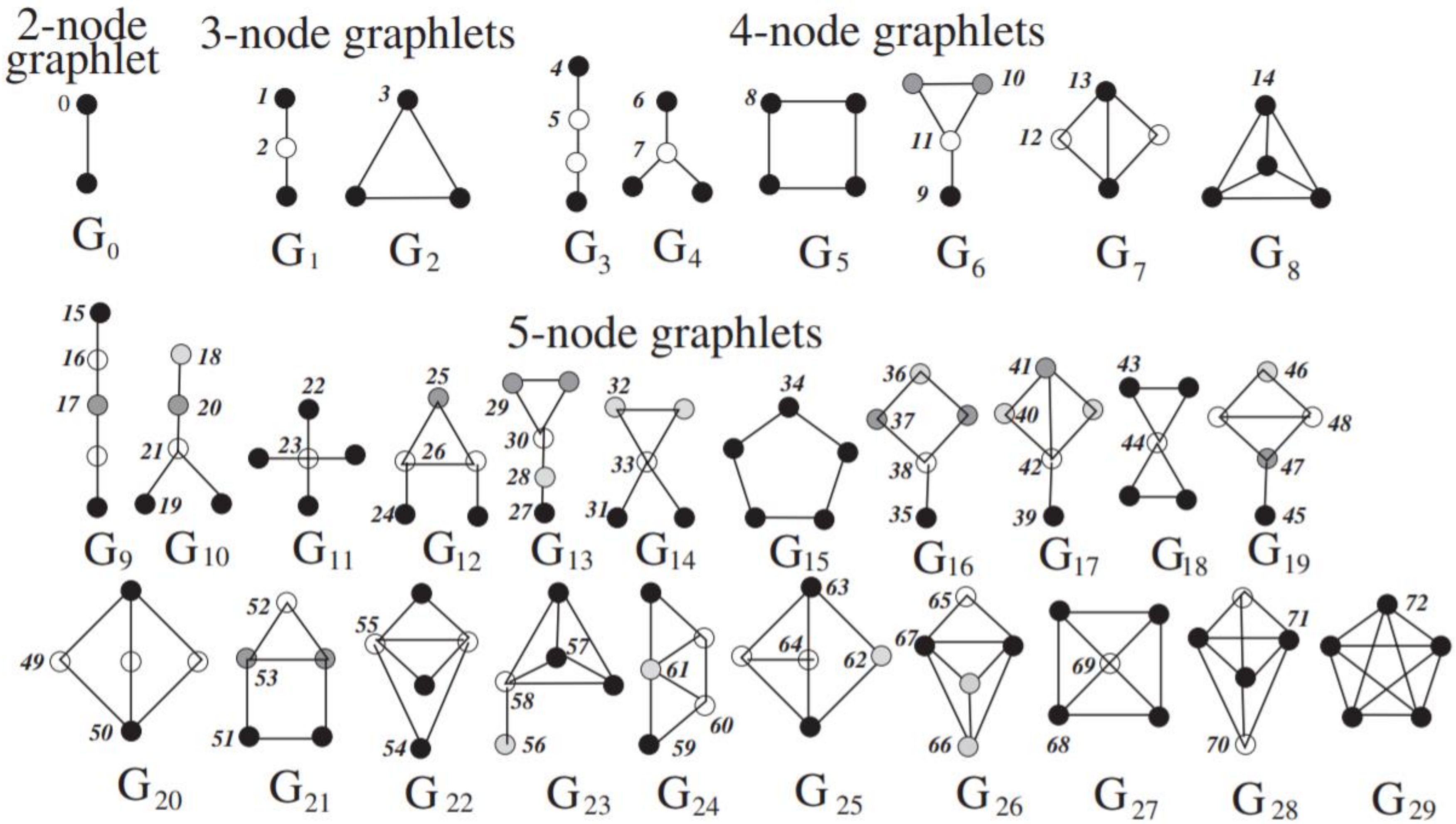
- Principle:
  - Count subgraphs of limited size k in G and G'.
  - These subgraphs are referred to as graphlets (Przulj, Bioinformatics 2007).
  - Define graph kernel that counts isomorphic graphlets in two graphs.
- Runtime problems:
  - Pairwise test of isomorphism is expensive.
  - Number of graphlets scales as $O(n^k)$.
- Two solutions on unlabelled graphs:
  - Precompute isomorphisms.
  - Sample graphlets.
- Disadvantage:
  - Same solutions not feasible on labelled graphs.



Size k-graphlet = 3, number of node n = 5

Graphlet Kernel (B., Petri, et al., MLG 2007)

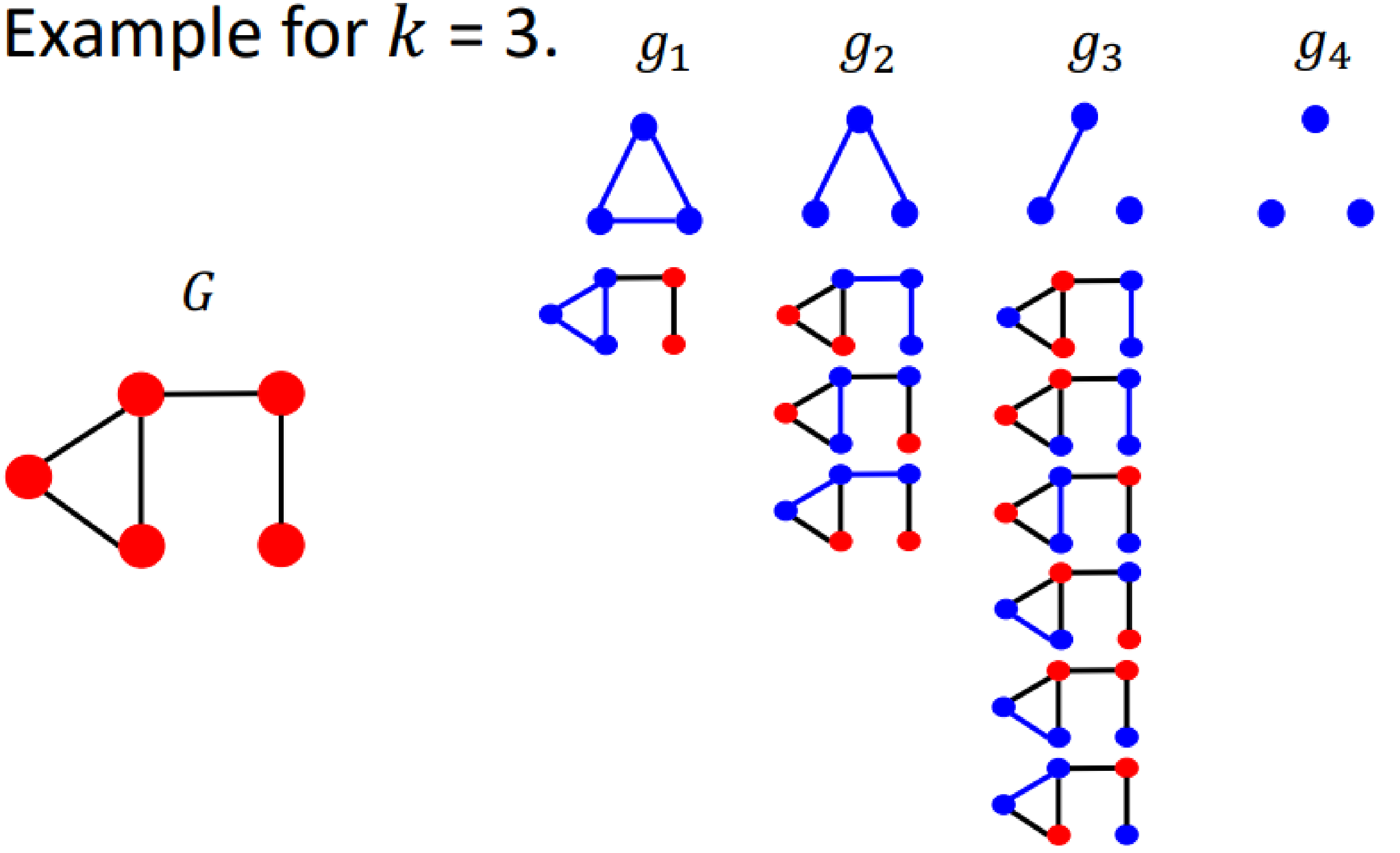
- Variety of subgraphs according to size *k*:


2-node graphlet
3-node graphlets
4-node graphlets
5-node graphlets
G0 G1 G2 G3 G4 G5 G6 G7 G8
G9 G10 G11 G12 G13 G14 G15 G16 G17 G18 G19
G20 G21 G22 G23 G24 G25 G26 G27 G28 G29
0 1 2 3 4 5 6 7 8 9 10 11 12 13 14
15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48
49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72

Graphlet Kernel (B., Petri, et al., MLG 2007)

- Count subgraphs of limited size 3:

  - Example for k = 3.



$$f_G = (1, \quad 3, \quad 6, \quad 0)^T$$

Shortest Path Kernel: More General Form

Floyd-transformation:

- Given an input graph G, outputs a shortest-path graph S.
  - S contains the same set of nodes as the input graph G.
  - There exists an edge between all nodes in S which are connected by a path in G.
  - Every edge in S between two nodes is labelled by the shortest distance between these two nodes.
  - This transformation can be done in $O(n^3)$ time.

Shortest Path Kernel: More General Form

Definition (Shortest-path graph kernel):

- Let G_1 and G_2 be two graphs that are Floyd-transformed into S_1 and S_2.
- We can then define shortest-path graph kernel on S_1 = (G_1, E_1) and S_2 = (G_2, E_2) as:

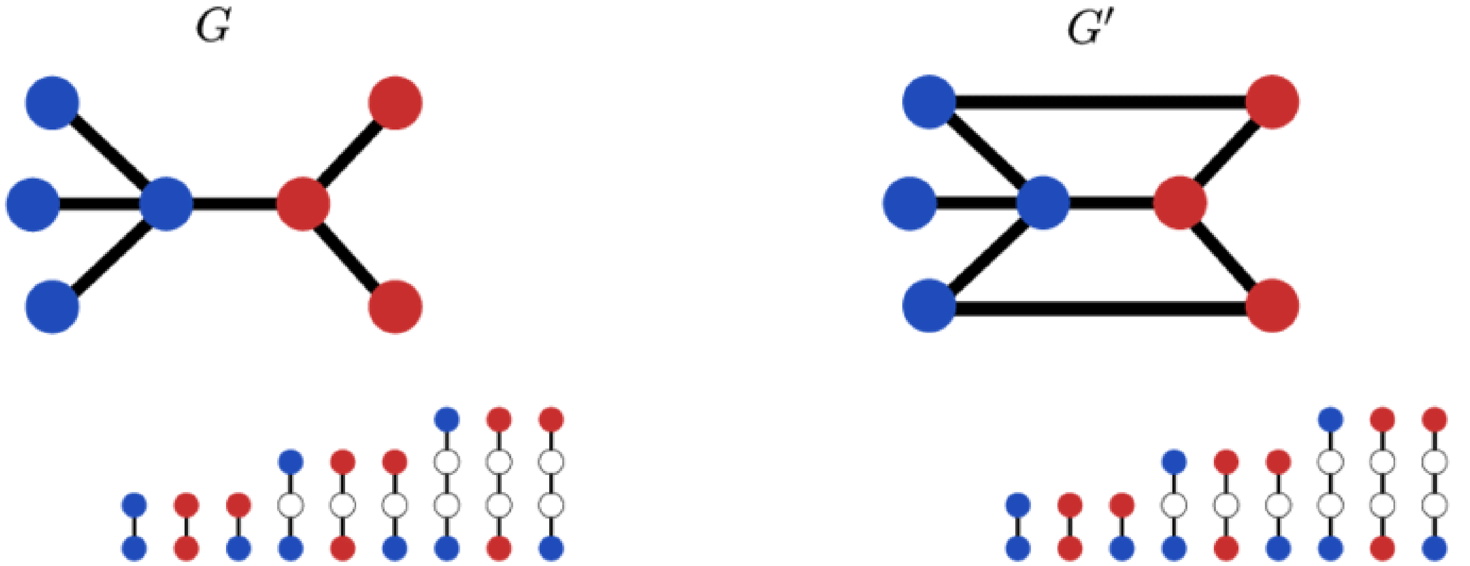
$$k_{shortest\ paths}(S_1, S_2) = \sum_{e_1 \in E_1} \sum_{e_2 \in E_2} k_{walk}^{(1)}(e_1, e_2),$$

where K_{walk} is a positive definite kernel on edge walks of length 1.

Shortest Path Kernel: More General Form

Shortest-path graph kernel:

$$k_{shortest\ paths}(S_1, S_2) = \sum_{e_1 \in E_1} \sum_{e_2 \in E_2} k_{walk}^{(1)}(e_1, e_2),$$



$$\phi_{\text{path}}(G) = [\, 3 \;\; 2 \;\; 1 \;\; 3 \;\; 1 \;\; 5 \;\; 0 \;\; 0 \;\; 6 \,] \qquad \phi_{\text{path}}(G') = [\, 3 \;\; 2 \;\; 3 \;\; 3 \;\; 1 \;\; 5 \;\; 0 \;\; 0 \;\; 4 \,]$$

Random Walk Kernel

- Random walk-kernels are based on the idea to count the number of matching walks in two input graphs. All pairs of matching walks in two input graphs G_1 and G_2 via a direct product graph G_X:

$$k_\times(G_1, G_2) = \sum_{i,j=1}^{|V_\times|} \left[\sum_{n=0}^{\infty} \lambda_n A_\times^n\right]_{ij},$$

where A_X is the adjacency matrix of G_X, defined from

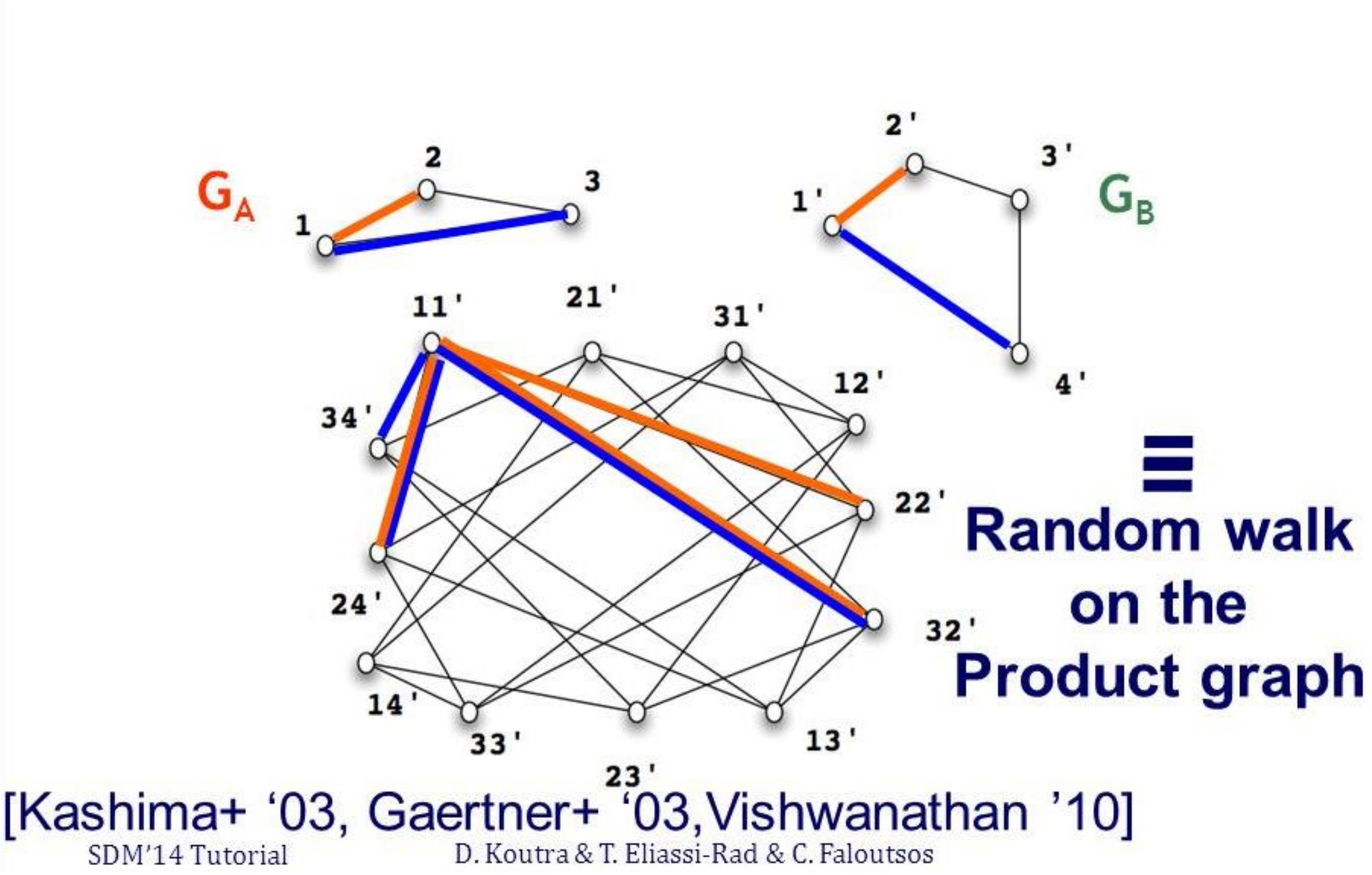
$$\begin{aligned} V_\times(G_1 \times G_2) = \quad & \{(v_1, w_1) \in V_1 \times V_2 : \\ & label(v_1) = label(w_1)\} \end{aligned}$$

$$\begin{aligned} E_\times(G_1 \times G_2) = \quad & \{((v_1, w_1), (v_2, w_2)) \in V^2(G_1 \times G_2) : \\ & (v_1, v_2) \in E_1 \wedge (w_1, w_2) \in E_2 \\ & \wedge(label(v_1, v_2) = label(w_1, w_2))\} \end{aligned}$$

λ_n must be chosen appropriately for k_X to converge

Random Walk Kernel

- Random walk-kernels are based on the idea to count the number of matching walks in two input graphs.


G_A
1
2
3
G_B
1'
2'
3'
4'
11'
21'
31'
12'
34'
22'
24'
32'
14'
33'
23'
13'

≡ Random walk on the Product graph

[Kashima+ '03, Gaertner+ '03, Vishwanathan '10]

SDM'14 Tutorial D. Koutra & T. Eliassi-Rad & C. Faloutsos

Isomorphism of Graphs

Definition:

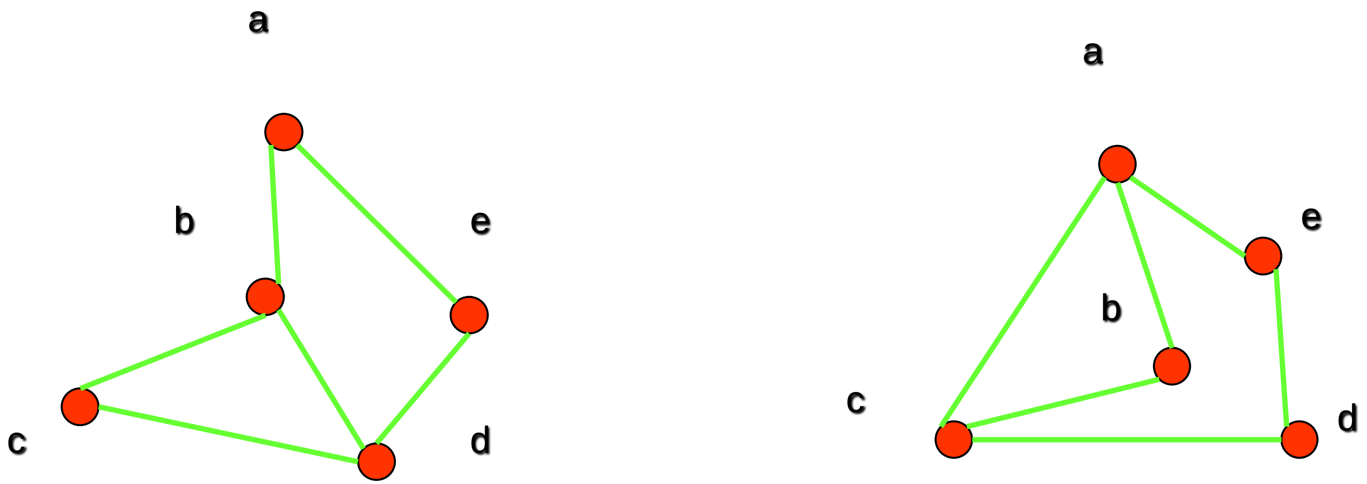
- The simple graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ are isomorphic if there is a bijection (a one-to-one and onto function) f from V_1 to V_2 with the property that a and b are adjacent in G_1 if and only if $f(a)$ and $f(b)$ are adjacent in G_2, for all a and b in V_1.
- Such a function f is called an isomorphism.
- In other words, G_1 and G_2 are isomorphic if their vertices can be ordered in such a way that the adjacency matrices $M(G_1)\ and\ M(G_2)$ are identical.

Isomorphism of Graphs

- For this purpose, we can check invariants, that is, properties that two isomorphic simple graphs must both have.
- For example, they must have
  - The same number of nodes,
  - the same number of edges,
  - And the same degrees of nodes.
- Note that two graphs that differ in any of these invariants are not isomorphic, but two graphs that match in all of them are not necessarily isomorphic.

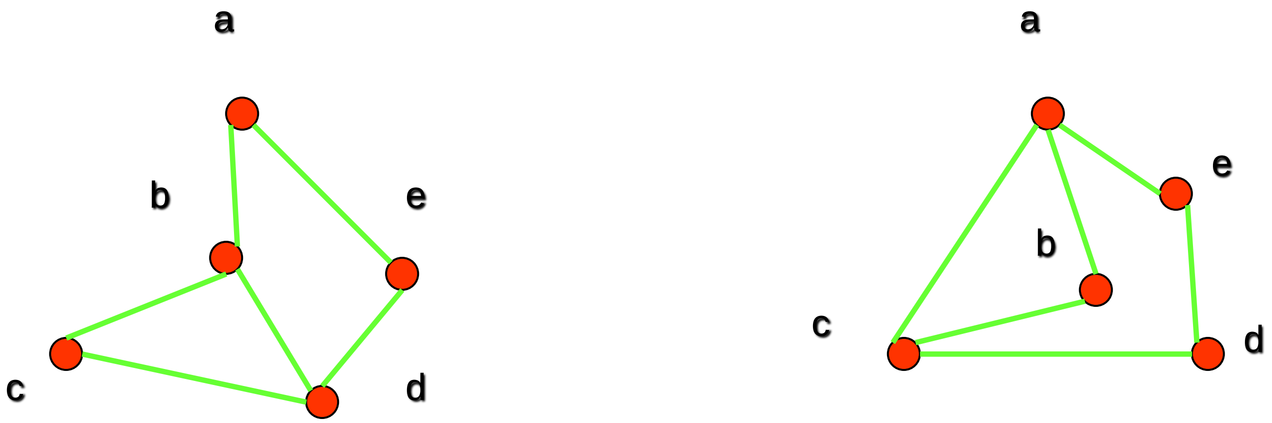
Isomorphism of Graphs: Example 1

- Are the following two graphs isomorphic?



Isomorphism of Graphs: Example 1

- Are the following two graphs isomorphic?

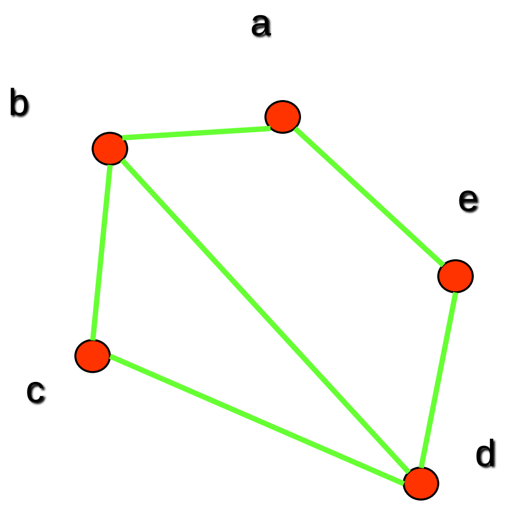


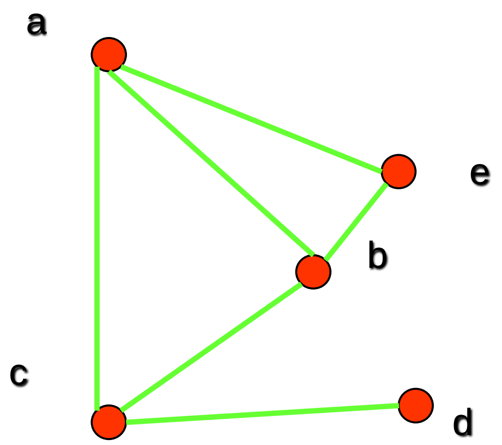
- **Solution**: Yes, they are isomorphic, because they can be arranged to look identical.
- You can see this if in the right graph you move vertex b to the left of the edge {a, c}. Then the isomorphism f from the left to the right graph is

$$f(a) = e, f(b) = a, f(c) = b, f(d) = c, f(e) = d.$$

Isomorphism of Graphs: Example 2

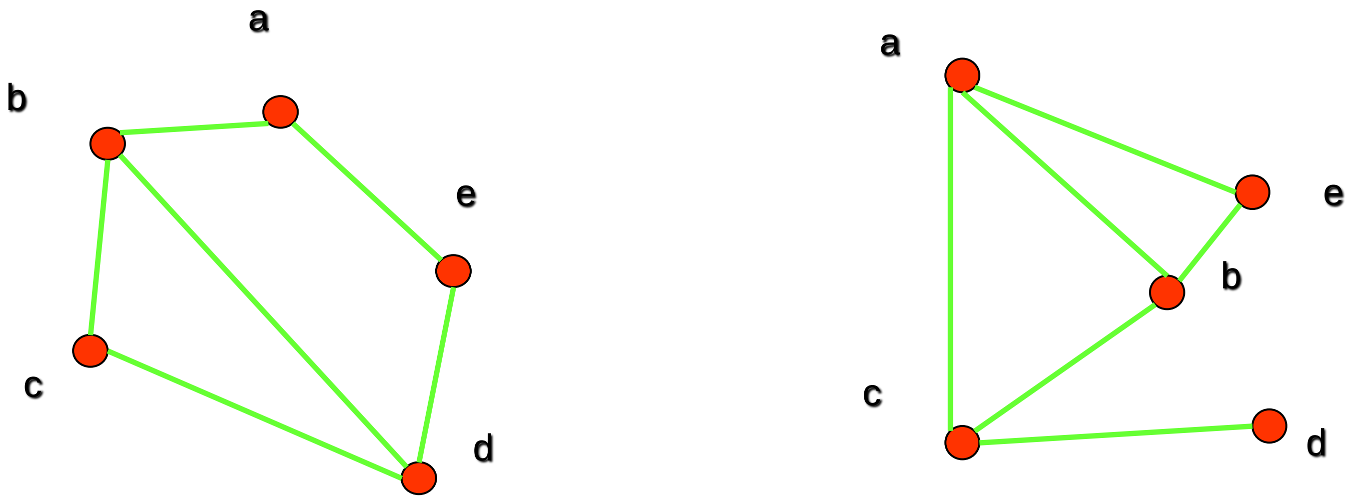
- Are the following two graphs isomorphic?





Isomorphism of Graphs: Example 2

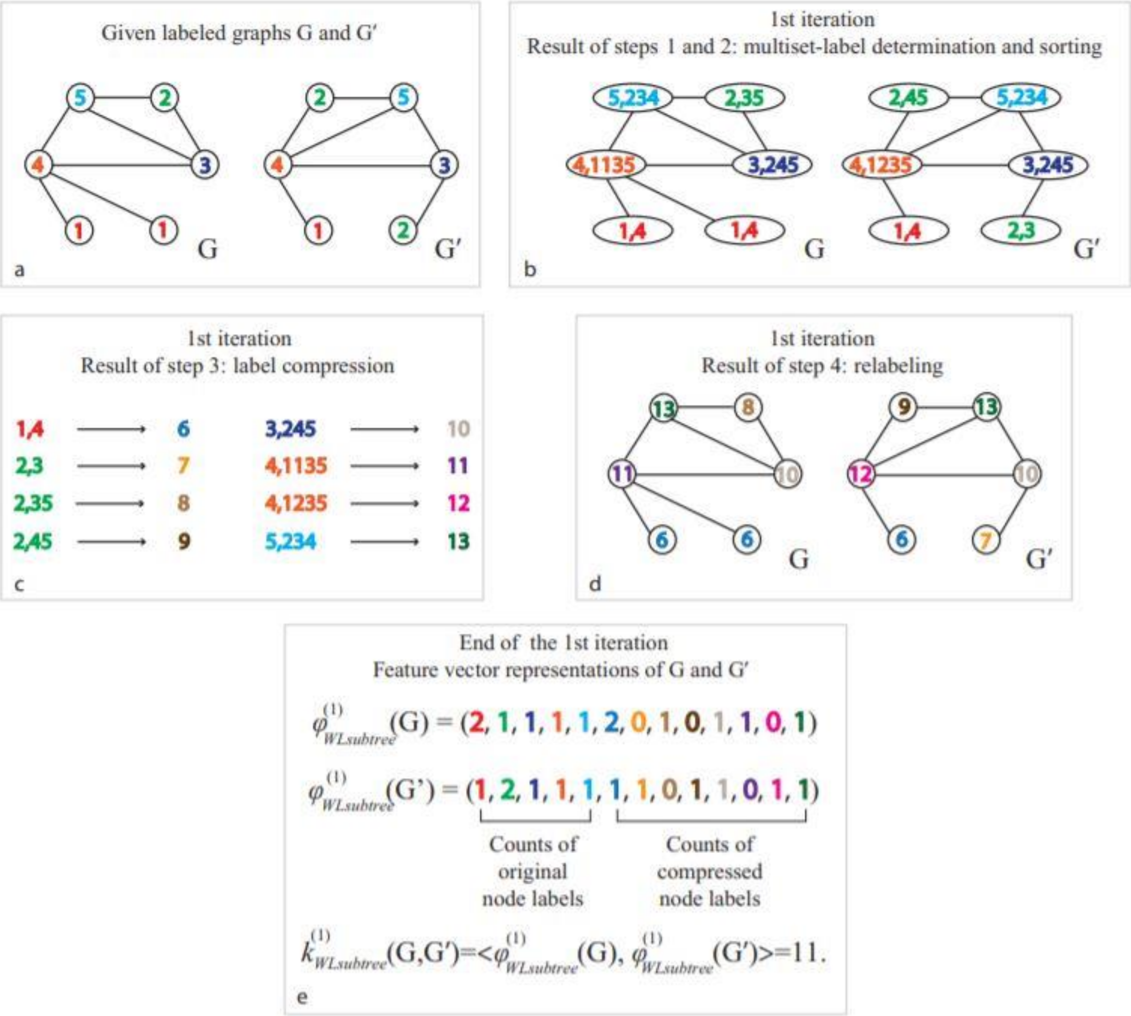
- Are the following two graphs isomorphic?

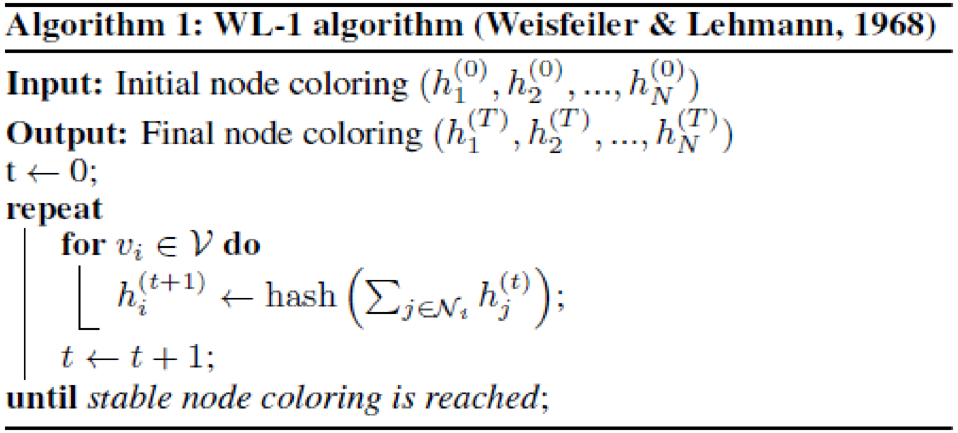


- **Solution**: No, they are not isomorphic, because they differ in the degrees of their vertices.
- Vertex d in right graph is of degree one, but there is no such vertex in the left graph.

The Weisfeiler-Lehman Isomorphism Test

- Weisfeiler-Lehman Isomorphism Testing:

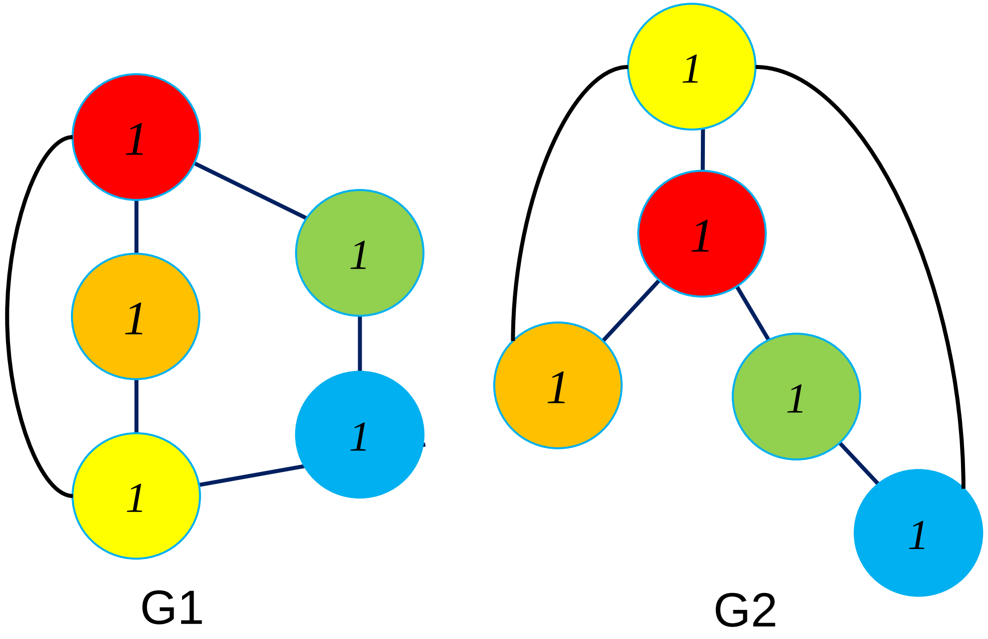

Given labeled graphs G and G′
G
G′
a
1st iteration
Result of steps 1 and 2: multiset-label determination and sorting
5,234
2,35
4,1135
3,245
1,4
2,45
4,1235
2,3
b
1st iteration
Result of step 3: label compression
1,4 ⟶ 6
2,3 ⟶ 7
2,35 ⟶ 8
2,45 ⟶ 9
3,245 ⟶ 10
4,1135 ⟶ 11
4,1235 ⟶ 12
5,234 ⟶ 13
c
1st iteration
Result of step 4: relabeling
d
End of the 1st iteration
Feature vector representations of G and G′
$\varphi^{(1)}_{WLsubtree}(G) = (2, 1, 1, 1, 1, 2, 0, 1, 0, 1, 1, 0, 1)$
$\varphi^{(1)}_{WLsubtree}(G') = (1, 2, 1, 1, 1, 1, 1, 0, 1, 1, 0, 1, 1)$
Counts of original node labels
Counts of compressed node labels
$k^{(1)}_{WLsubtree}(G,G') = \langle \varphi^{(1)}_{WLsubtree}(G), \varphi^{(1)}_{WLsubtree}(G') \rangle = 11.$
e



```
Algorithm 1: WL-1 algorithm (Weisfeiler & Lehmann, 1968)
Input: Initial node coloring $(h_1^{(0)}, h_2^{(0)}, ..., h_N^{(0)})$
Output: Final node coloring $(h_1^{(T)}, h_2^{(T)}, ..., h_N^{(T)})$
$t \leftarrow 0$;
repeat
    for $v_i \in \mathcal{V}$ do
        $h_i^{(t+1)} \leftarrow \text{hash}\left(\sum_{j \in \mathcal{N}_i} h_j^{(t)}\right)$;
    $t \leftarrow t + 1$;
until stable node coloring is reached;
```

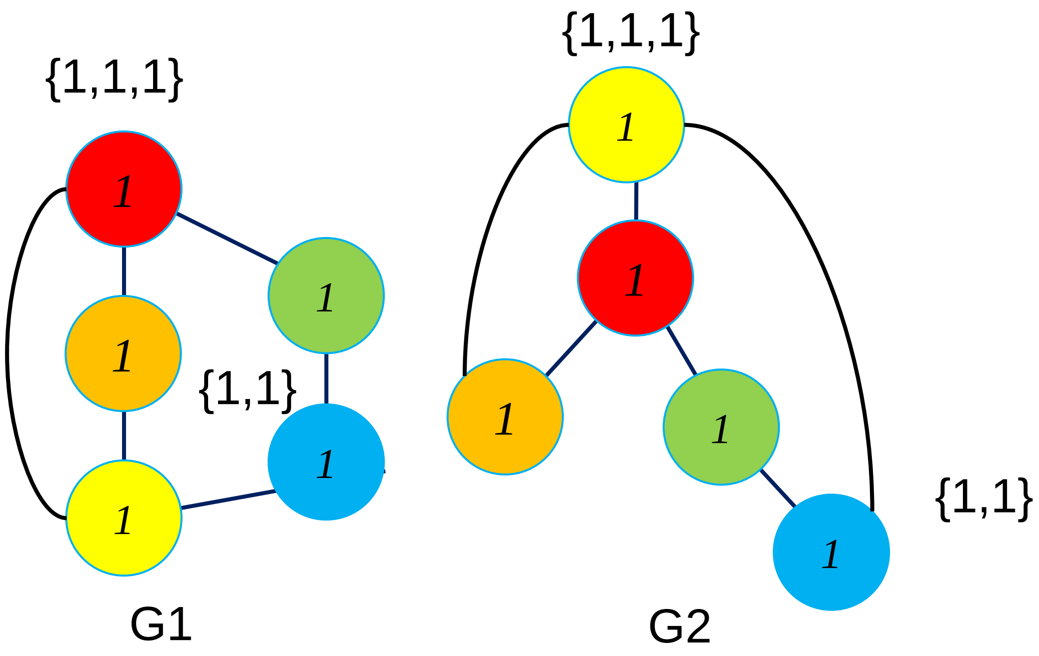
The Weisfeiler-Lehman Isomorphism Test

- We will apply the Weisfeiler-Lehman isomorphism test to these graphs as a means of illustrating the test.
- Step 1: Set node label =1 for all nodes



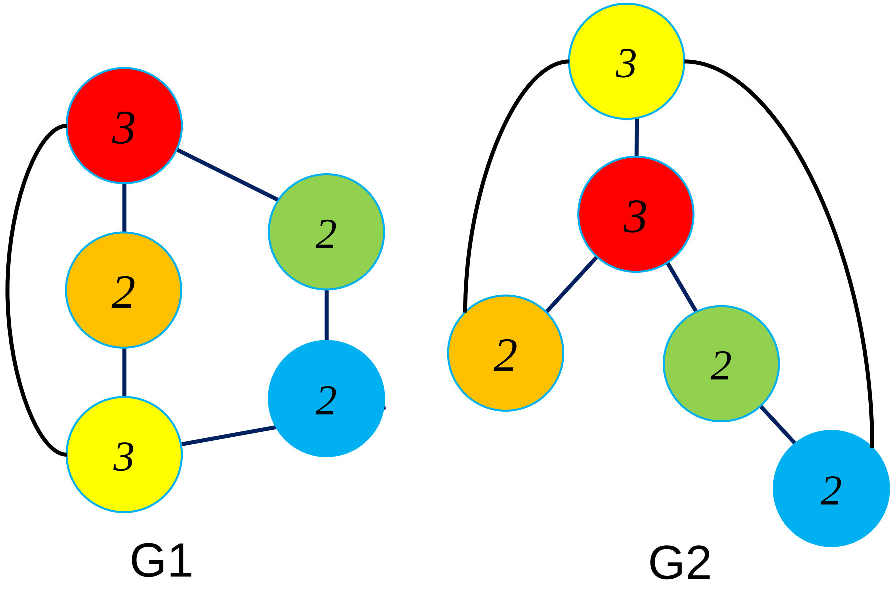
The Weisfeiler-Lehman Isomorphism Test

- We will apply the Weisfeiler-Lehman isomorphism test to these graphs as a means of illustrating the test.
- Step 1: Set node label =1 for all nodes
- Step 2: Compute multiset of the neighboring nodes' compressed labels.


{1,1,1}
1
1
1
{1,1}
1
1
G1
{1,1,1}
1
1
1
1
{1,1}
1
G2

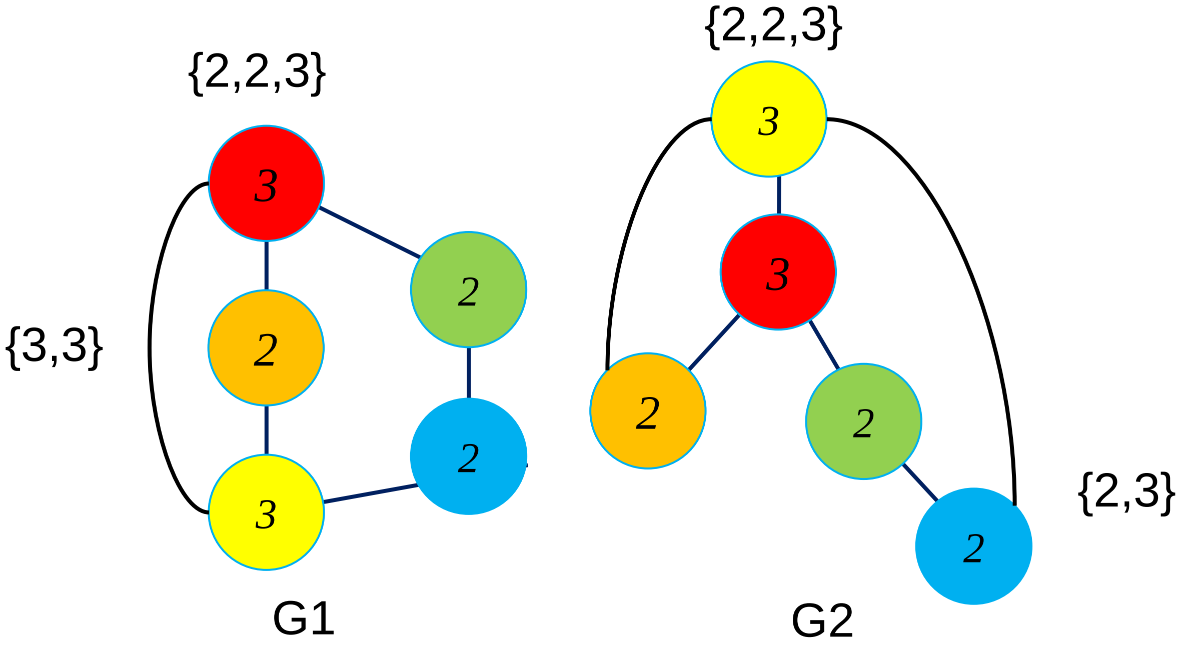
The Weisfeiler-Lehman Isomorphism Test

- We will apply the Weisfeiler-Lehman isomorphism test to these graphs as a means of illustrating the test.
- Step 1: Set node label =1 for all nodes
- Step 2: Compute multiset of the neighboring nodes' compressed labels.



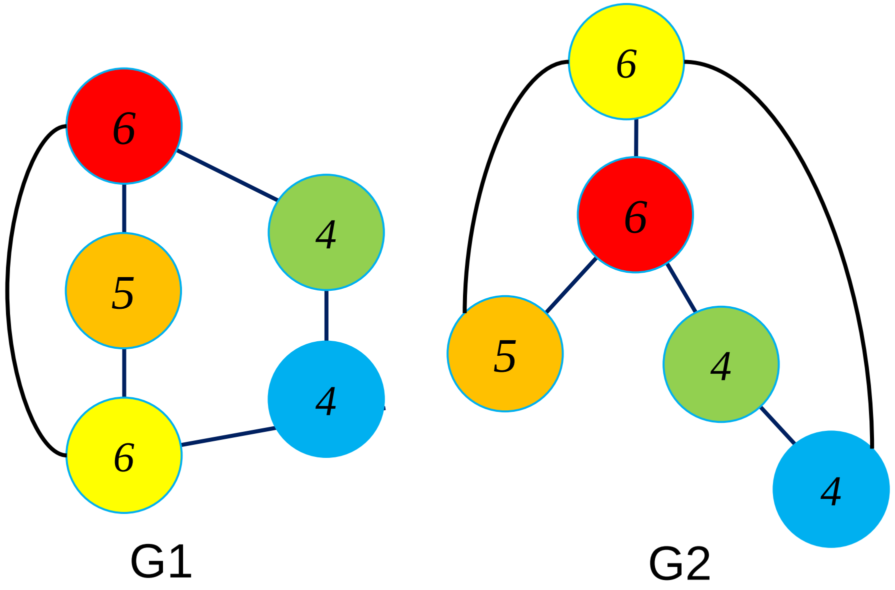
The Weisfeiler-Lehman Isomorphism Test

- We will apply the Weisfeiler-Lehman isomorphism test to these graphs as a means of illustrating the test.
- Step 1: Set node label =1 for all nodes
- Step 2: Compute multiset of the neighboring nodes' compressed labels.
- Step 3: Continuous.



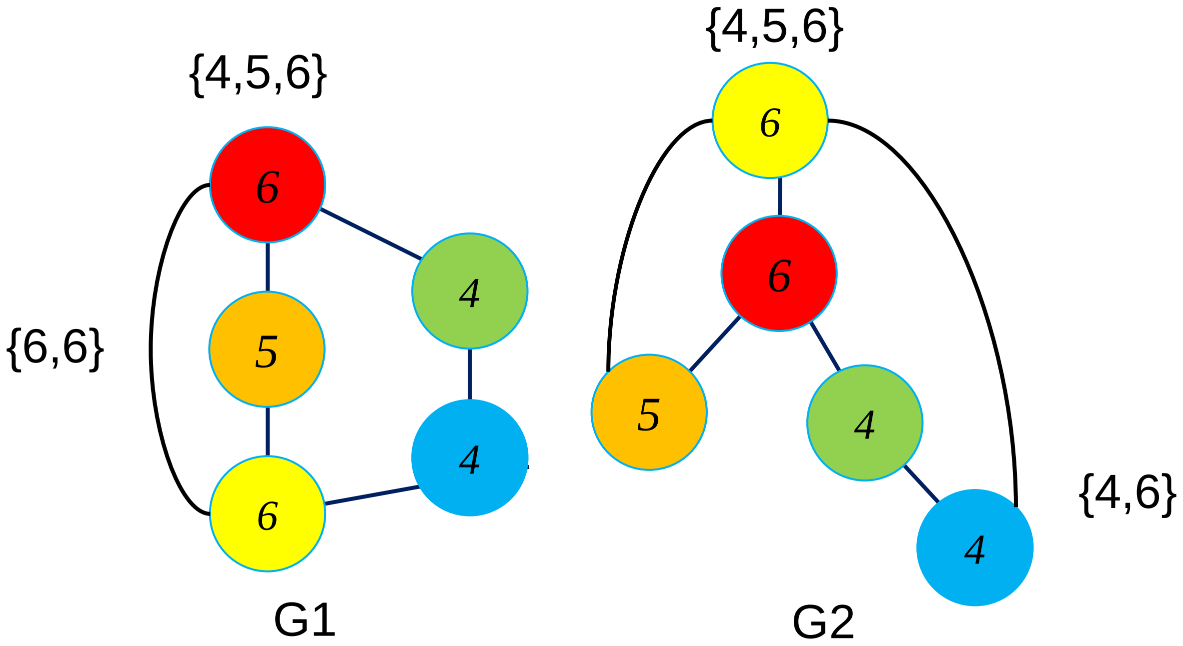
The Weisfeiler-Lehman Isomorphism Test

- We will apply the Weisfeiler-Lehman isomorphism test to these graphs as a means of illustrating the test.
- Step 1: Set node label =1 for all nodes
- Step 2: Compute multiset of the neighboring nodes' compressed labels.
- Step 3: Continuous….



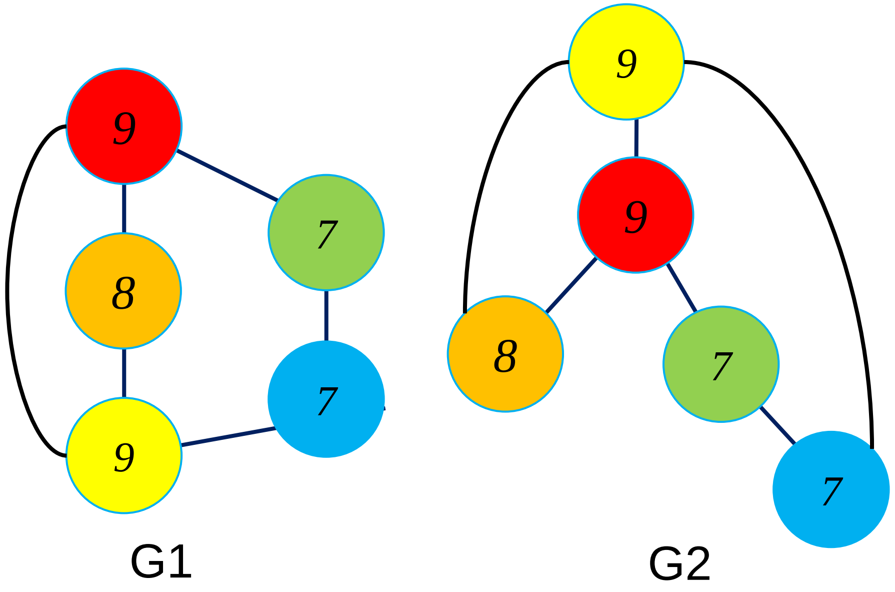
The Weisfeiler-Lehman Isomorphism Test

- We will apply the Weisfeiler-Lehman isomorphism test to these graphs as a means of illustrating the test.
- Step 1: Set node label =1 for all nodes
- Step 2: Compute multiset of the neighboring nodes' compressed labels.
- Step 3: Continuous…



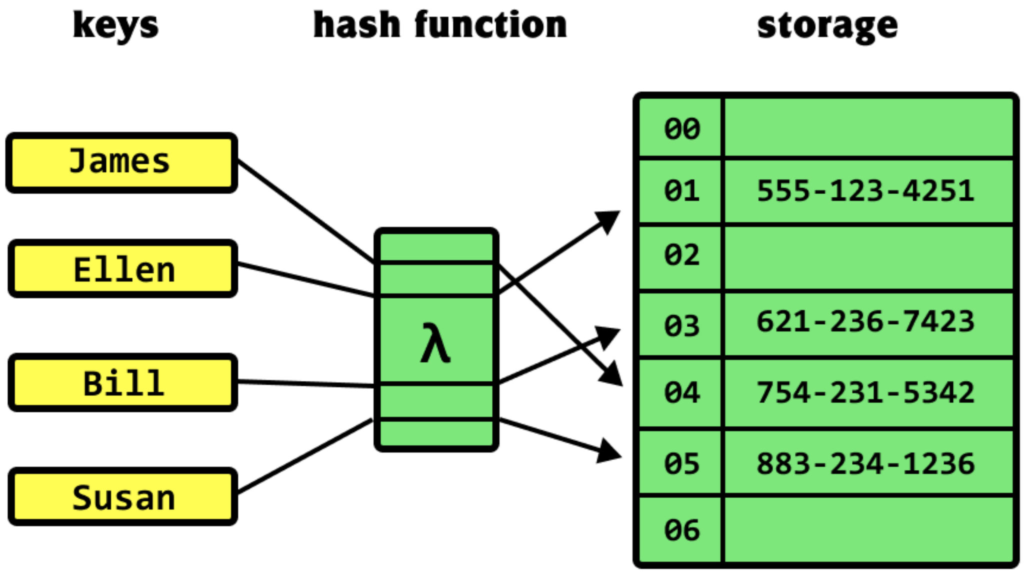
The Weisfeiler-Lehman Isomorphism Test

- We will apply the Weisfeiler-Lehman isomorphism test to these graphs as a means of illustrating the test.
- Step 1: Set node label =1 for all nodes
- Step 2: Compute multiset of the neighboring nodes' compressed labels.
- Step 3: Continuous….
- Step 4: Since the partition of nodes by compressed label has not changed, we may terminate the algorithm here



Hash Function

- Converts a given numeric or alphanumeric key to a small practical integer value.
- Hash function $h: (\{0,1\}^k \rightarrow \{0,1\}^{t(k)})$
  - Compresses.
- Main goal: a little bit of difference in inputs will cause a big difference in outputs.


keys
hash function
storage
James
Ellen
Bill
Susan
λ
00
01
555-123-4251
02
03
621-236-7423
04
754-231-5342
05
883-234-1236
06

Subgraph Matching Kernel

- Counts the number of matchings between subgraphs of bounded size in two graphs.
    - Can apply to graphs that contain node labels, edge labels, node attributes or edge attributes.

- Given two graphs $G = (V, E)$ and $G' = (V', E')$.
- Let $B(G, G')$ denote the set of all bijections between sets $S \subseteq V$ and $S' \subseteq V'$. $\lambda: B(G, G') \to \mathbb{R}^{+}$ be a weight function.
- The subgraph matching kernel is

$$k(G, G') = \sum_{\phi \in B(G, G')} \lambda(\phi) \prod_{v \in S} \kappa_V(v, \phi(v)) \prod_{e \in S \times S} \kappa_E(e, \psi(e))$$

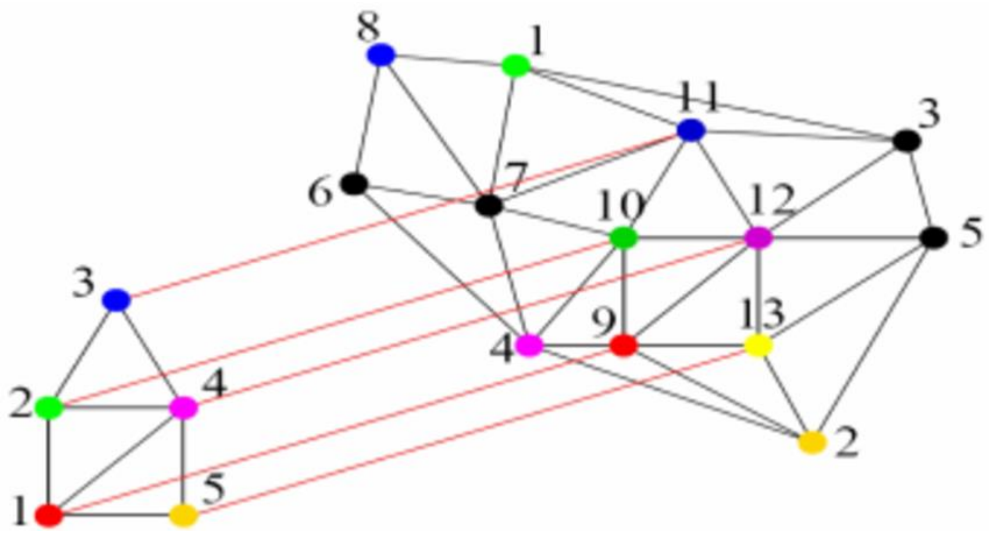
Where $S = dom(\phi)$ and K_V, K_E are kernel functions defined on vertices and edges.

Subgraph Matching Kernel

- The common subgraph isomorphism kernel:

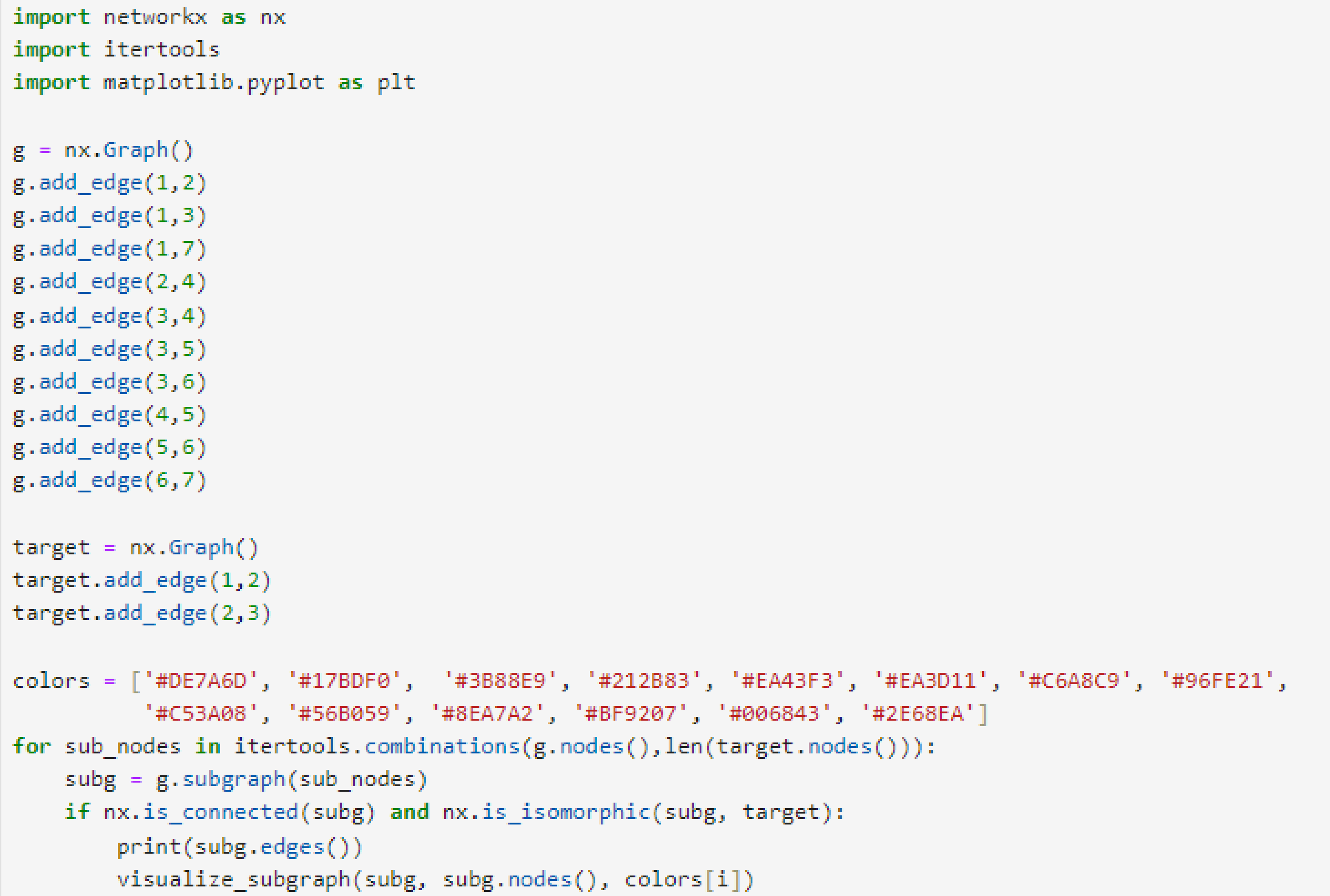
$$\kappa_V(v, v') = \begin{cases} 1, & \text{if } \ell(v) \equiv \ell(v'), \\ 0, & \text{otherwise and} \end{cases}$$
$$\kappa_E(e, e') = \begin{cases} 1, & \text{if } e \in E \wedge e' \in E' \wedge \ell(e) \equiv \ell(e') \text{ or } e \notin E \wedge e' \notin E', \\ 0, & \text{otherwise.} \end{cases}$$

➡ counts the number of isomorphic subgraphs contained in two graphs.

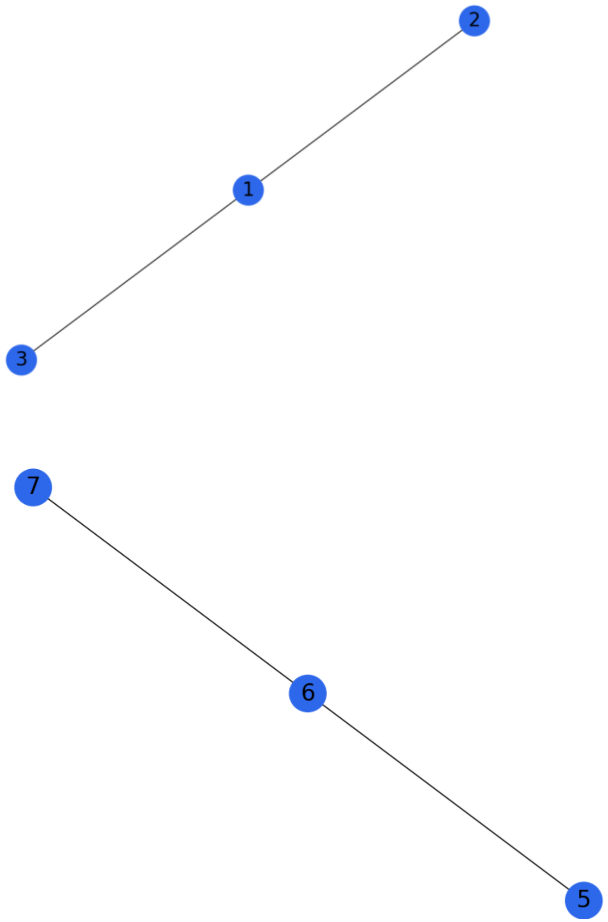


Sample code: Graphlet kernels

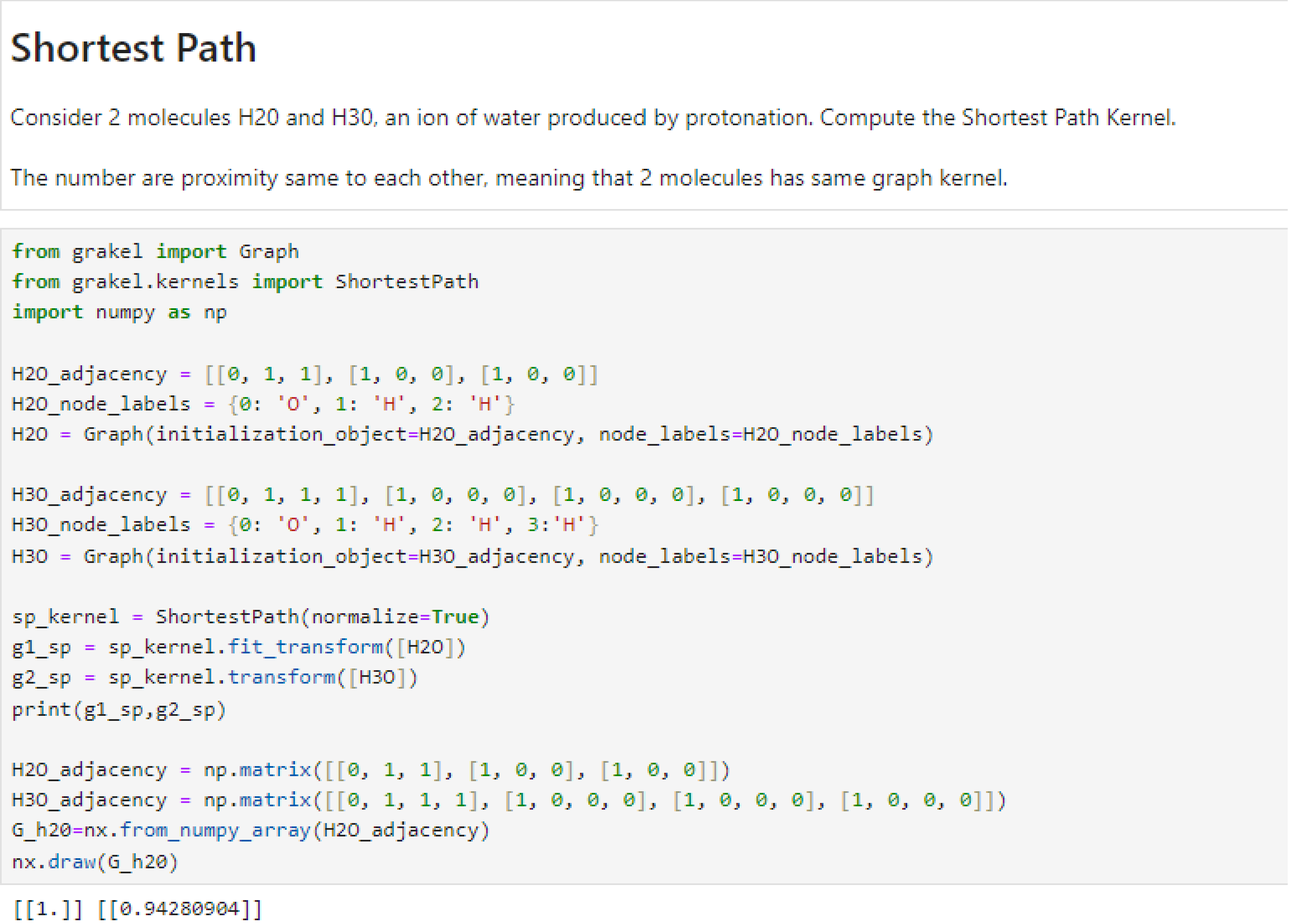
- Find Graphlet kernels size 3:



```
import networkx as nx
import itertools
import matplotlib.pyplot as plt

g = nx.Graph()
g.add_edge(1,2)
g.add_edge(1,3)
g.add_edge(1,7)
g.add_edge(2,4)
g.add_edge(3,4)
g.add_edge(3,5)
g.add_edge(3,6)
g.add_edge(4,5)
g.add_edge(5,6)
g.add_edge(6,7)

target = nx.Graph()
target.add_edge(1,2)
target.add_edge(2,3)

colors = ['#DE7A6D', '#17BDF0',  '#3B88E9', '#212B83', '#EA43F3', '#EA3D11', '#C6A8C9', '#96FE21',
          '#C53A08', '#56B059', '#8EA7A2', '#BF9207', '#006843', '#2E68EA']
for sub_nodes in itertools.combinations(g.nodes(),len(target.nodes())):
    subg = g.subgraph(sub_nodes)
    if nx.is_connected(subg) and nx.is_isomorphic(subg, target):
        print(subg.edges())
        visualize_subgraph(subg, subg.nodes(), colors[i])
```



Shortest Path kernels



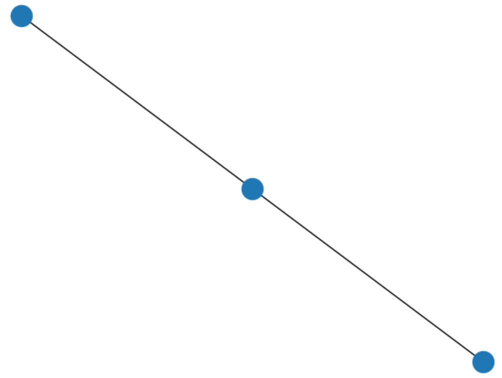
Shortest Path

Consider 2 molecules H20 and H30, an ion of water produced by protonation. Compute the Shortest Path Kernel.

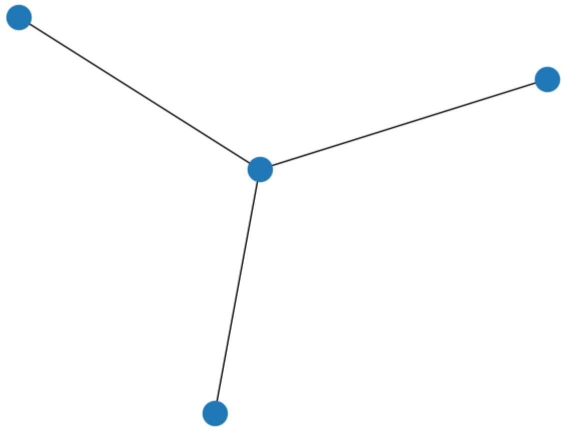
The number are proximity same to each other, meaning that 2 molecules has same graph kernel.

```python
from grakel import Graph
from grakel.kernels import ShortestPath
import numpy as np

H2O_adjacency = [[0, 1, 1], [1, 0, 0], [1, 0, 0]]
H2O_node_labels = {0: 'O', 1: 'H', 2: 'H'}
H2O = Graph(initialization_object=H2O_adjacency, node_labels=H2O_node_labels)

H3O_adjacency = [[0, 1, 1, 1], [1, 0, 0, 0], [1, 0, 0, 0], [1, 0, 0, 0]]
H3O_node_labels = {0: 'O', 1: 'H', 2: 'H', 3:'H'}
H3O = Graph(initialization_object=H3O_adjacency, node_labels=H3O_node_labels)

sp_kernel = ShortestPath(normalize=True)
g1_sp = sp_kernel.fit_transform([H2O])
g2_sp = sp_kernel.transform([H3O])
print(g1_sp,g2_sp)

H2O_adjacency = np.matrix([[0, 1, 1], [1, 0, 0], [1, 0, 0]])
H3O_adjacency = np.matrix([[0, 1, 1, 1], [1, 0, 0, 0], [1, 0, 0, 0], [1, 0, 0, 0]])
G_h20=nx.from_numpy_array(H2O_adjacency)
nx.draw(G_h20)
```

```
[[1.]] [[0.94280904]]
```

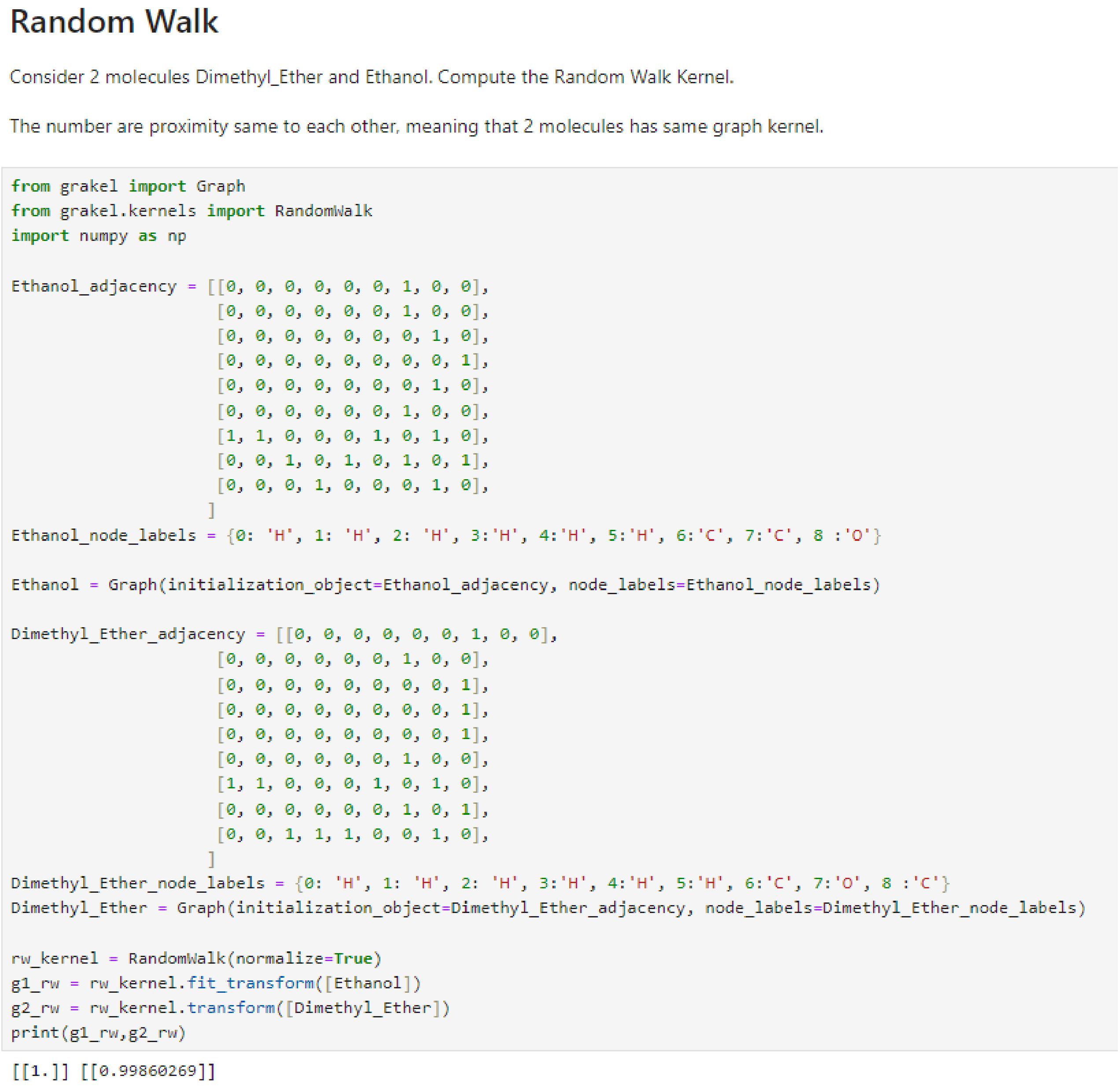


H_2O



H_3O

Random Walk kernels



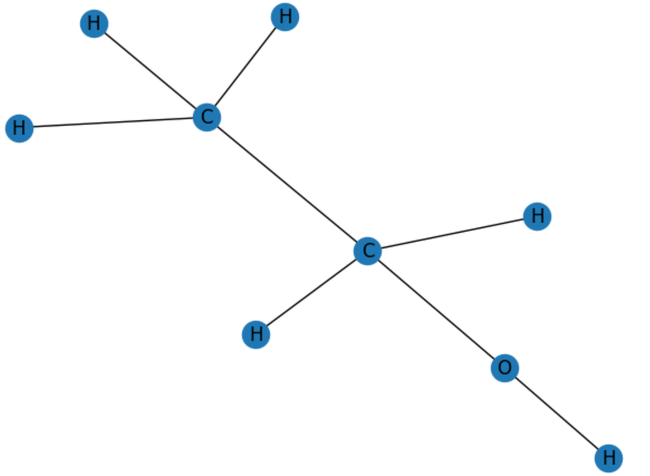
Random Walk

Consider 2 molecules Dimethyl_Ether and Ethanol. Compute the Random Walk Kernel.

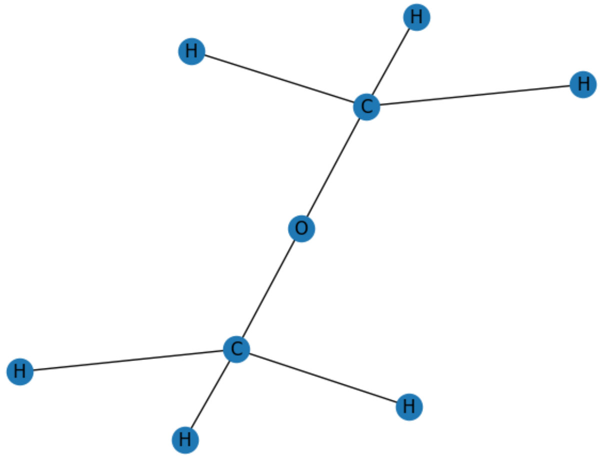
The number are proximity same to each other, meaning that 2 molecules has same graph kernel.

```
from grakel import Graph
from grakel.kernels import RandomWalk
import numpy as np

Ethanol_adjacency = [[0, 0, 0, 0, 0, 0, 1, 0, 0],
                     [0, 0, 0, 0, 0, 0, 1, 0, 0],
                     [0, 0, 0, 0, 0, 0, 0, 1, 0],
                     [0, 0, 0, 0, 0, 0, 0, 0, 1],
                     [0, 0, 0, 0, 0, 0, 0, 1, 0],
                     [0, 0, 0, 0, 0, 0, 1, 0, 0],
                     [1, 1, 0, 0, 0, 1, 0, 1, 0],
                     [0, 0, 1, 0, 1, 0, 1, 0, 1],
                     [0, 0, 0, 1, 0, 0, 0, 1, 0],
                    ]
Ethanol_node_labels = {0: 'H', 1: 'H', 2: 'H', 3:'H', 4:'H', 5:'H', 6:'C', 7:'C', 8 :'O'}

Ethanol = Graph(initialization_object=Ethanol_adjacency, node_labels=Ethanol_node_labels)

Dimethyl_Ether_adjacency = [[0, 0, 0, 0, 0, 0, 1, 0, 0],
                     [0, 0, 0, 0, 0, 0, 1, 0, 0],
                     [0, 0, 0, 0, 0, 0, 0, 0, 1],
                     [0, 0, 0, 0, 0, 0, 0, 0, 1],
                     [0, 0, 0, 0, 0, 0, 0, 0, 1],
                     [0, 0, 0, 0, 0, 0, 1, 0, 0],
                     [1, 1, 0, 0, 0, 1, 0, 1, 0],
                     [0, 0, 0, 0, 0, 0, 1, 0, 1],
                     [0, 0, 1, 1, 1, 0, 0, 1, 0],
                    ]
Dimethyl_Ether_node_labels = {0: 'H', 1: 'H', 2: 'H', 3:'H', 4:'H', 5:'H', 6:'C', 7:'O', 8 :'C'}
Dimethyl_Ether = Graph(initialization_object=Dimethyl_Ether_adjacency, node_labels=Dimethyl_Ether_node_labels)

rw_kernel = RandomWalk(normalize=True)
g1_rw = rw_kernel.fit_transform([Ethanol])
g2_rw = rw_kernel.transform([Dimethyl_Ether])
print(g1_rw,g2_rw)
```

```
[[1.]] [[0.99860269]]
```



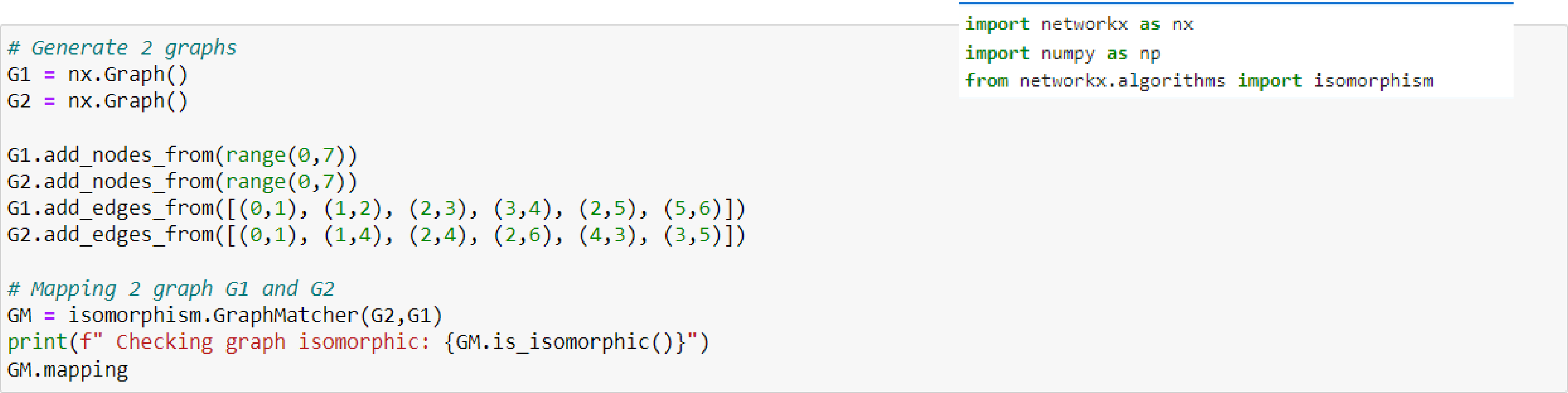
Ethanol (C_2H_5OH)



Dimethyl Ether (CH_3OCH_3)

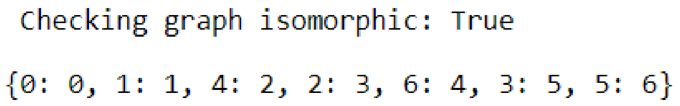
Graph isomorphism testing in NetworkX

- Check isomorphism mapping from undirected graph G1 to undirected graph G2

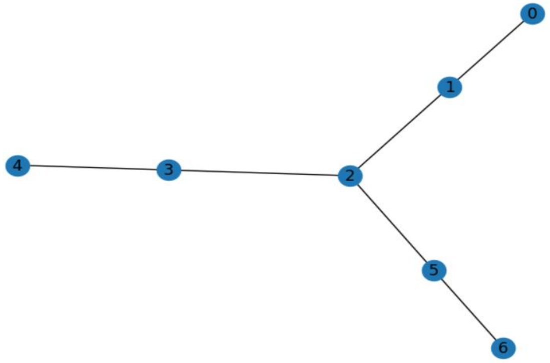


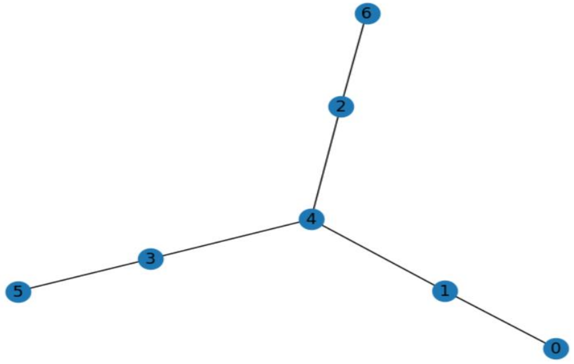
```
import networkx as nx
import numpy as np
from networkx.algorithms import isomorphism
```

```
# Generate 2 graphs
G1 = nx.Graph()
G2 = nx.Graph()

G1.add_nodes_from(range(0,7))
G2.add_nodes_from(range(0,7))
G1.add_edges_from([(0,1), (1,2), (2,3), (3,4), (2,5), (5,6)])
G2.add_edges_from([(0,1), (1,4), (2,4), (2,6), (4,3), (3,5)])

# Mapping 2 graph G1 and G2
GM = isomorphism.GraphMatcher(G2,G1)
print(f" Checking graph isomorphic: {GM.is_isomorphic()}")
GM.mapping
```



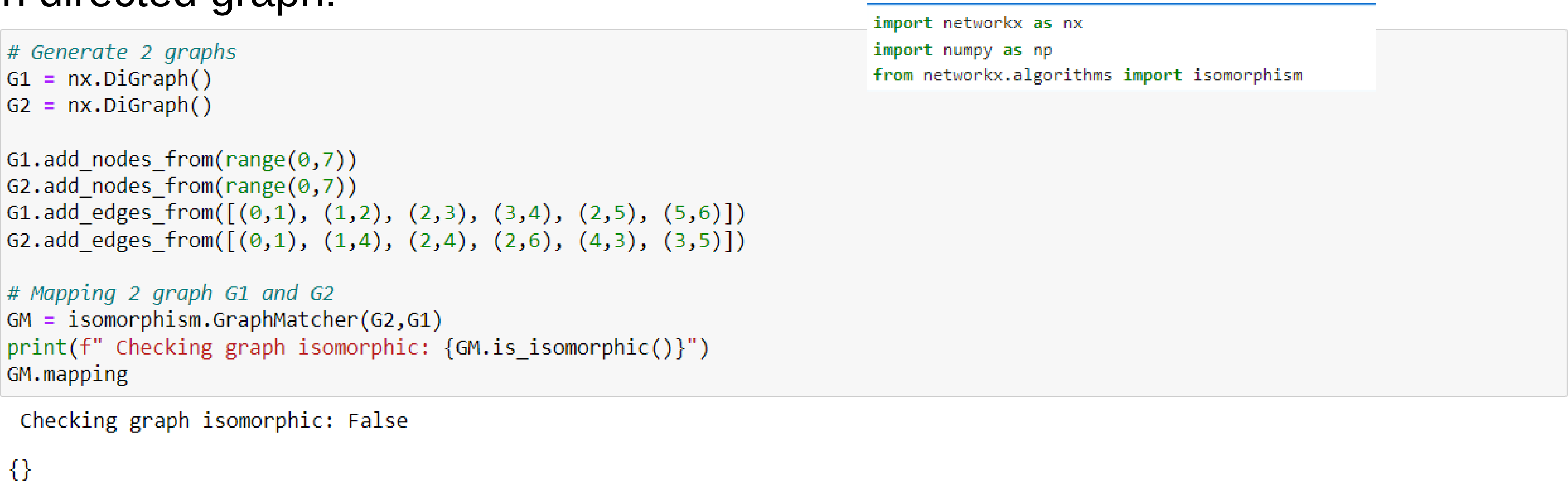
```
 Checking graph isomorphic: True

{0: 0, 1: 1, 4: 2, 2: 3, 6: 4, 3: 5, 5: 6}
```





Graph isomorphism testing in NetworkX

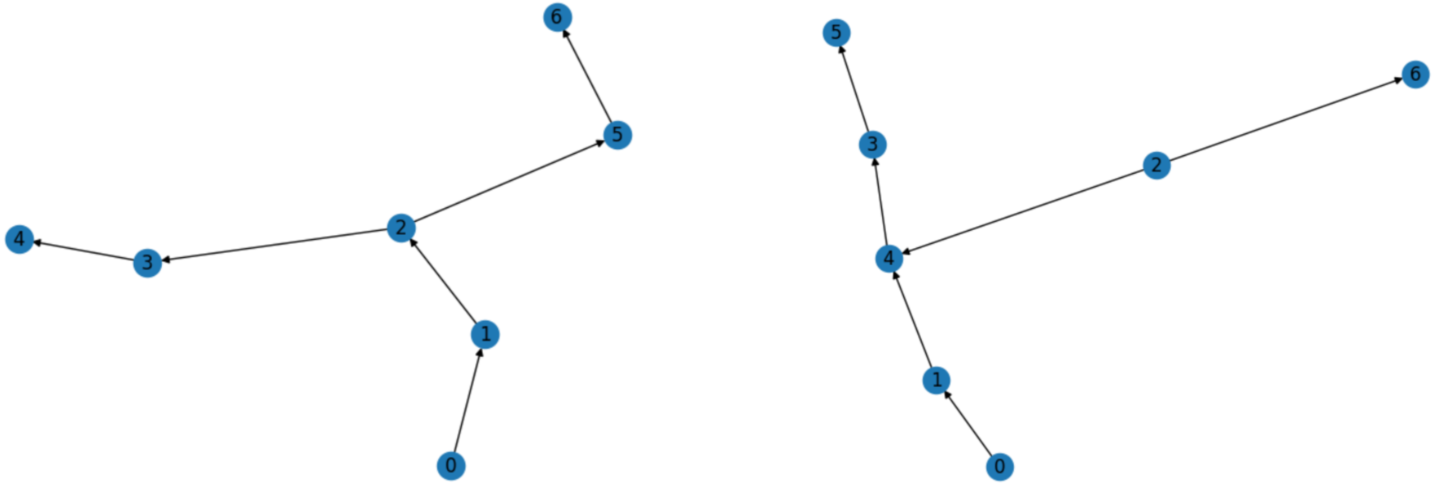
- In directed graph:



```
import networkx as nx
import numpy as np
from networkx.algorithms import isomorphism
```

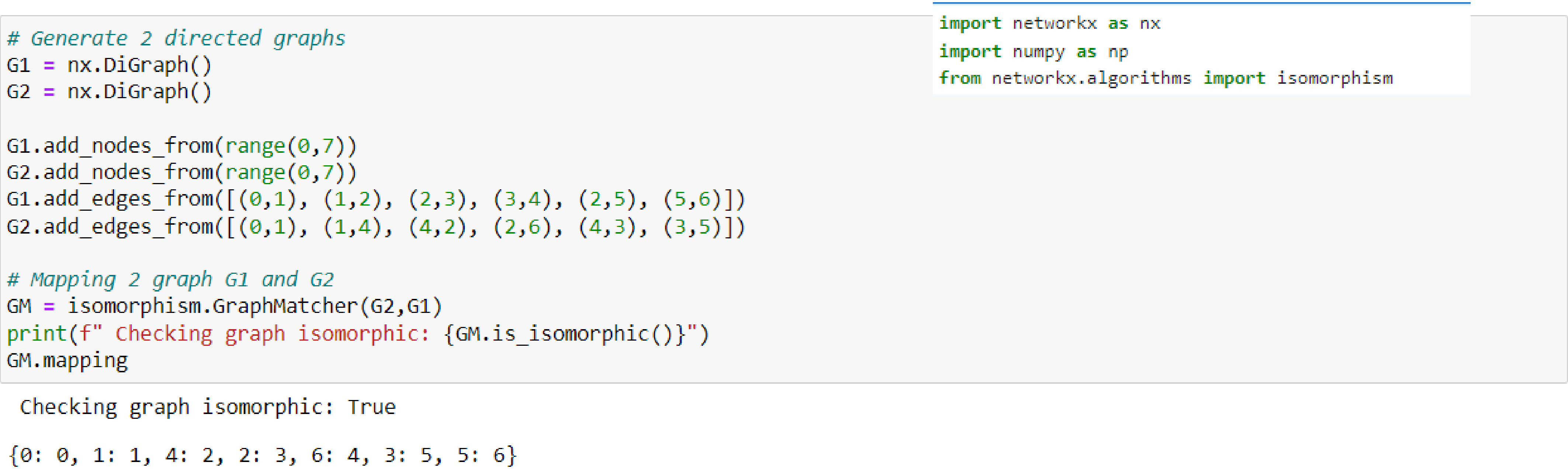
```
# Generate 2 graphs
G1 = nx.DiGraph()
G2 = nx.DiGraph()

G1.add_nodes_from(range(0,7))
G2.add_nodes_from(range(0,7))
G1.add_edges_from([(0,1), (1,2), (2,3), (3,4), (2,5), (5,6)])
G2.add_edges_from([(0,1), (1,4), (2,4), (2,6), (4,3), (3,5)])

# Mapping 2 graph G1 and G2
GM = isomorphism.GraphMatcher(G2,G1)
print(f" Checking graph isomorphic: {GM.is_isomorphic()}")
GM.mapping
```

```
 Checking graph isomorphic: False

{}
```



Graph isomorphism testing in NetworkX

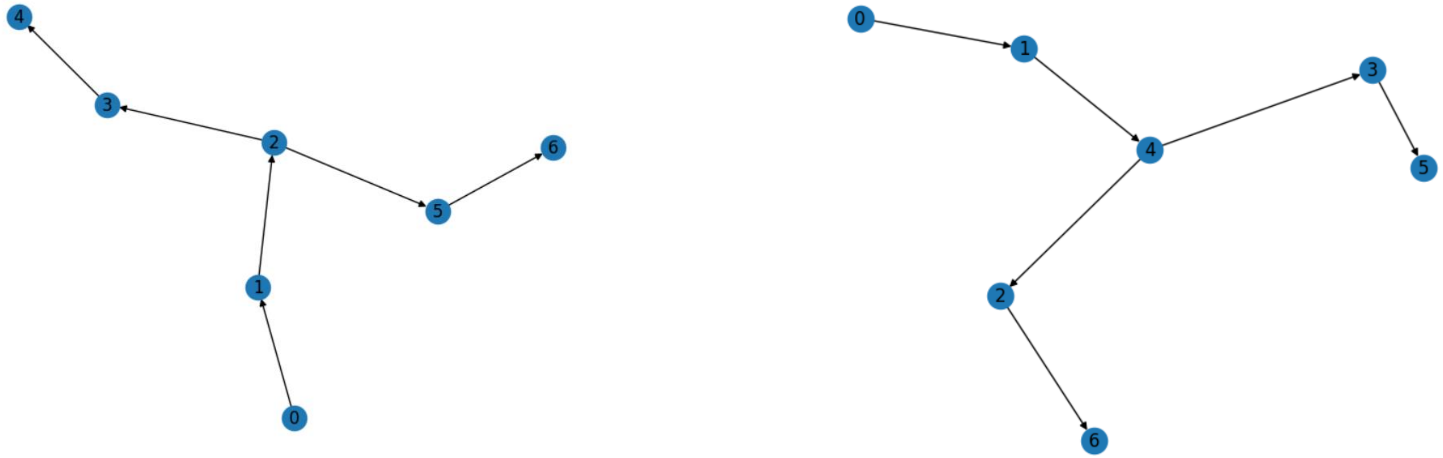
- Another example for directed graph



```
import networkx as nx
import numpy as np
from networkx.algorithms import isomorphism
```

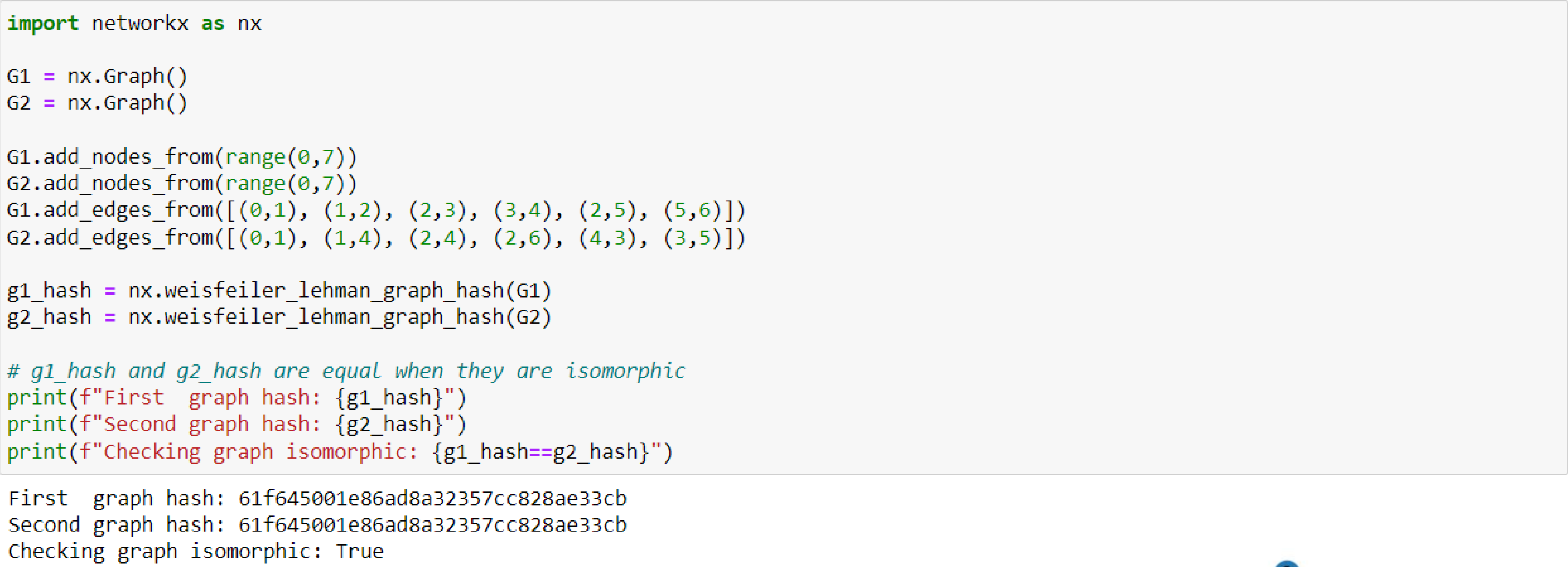
```
# Generate 2 directed graphs
G1 = nx.DiGraph()
G2 = nx.DiGraph()

G1.add_nodes_from(range(0,7))
G2.add_nodes_from(range(0,7))
G1.add_edges_from([(0,1), (1,2), (2,3), (3,4), (2,5), (5,6)])
G2.add_edges_from([(0,1), (1,4), (4,2), (2,6), (4,3), (3,5)])

# Mapping 2 graph G1 and G2
GM = isomorphism.GraphMatcher(G2,G1)
print(f" Checking graph isomorphic: {GM.is_isomorphic()}")
GM.mapping
```

```
 Checking graph isomorphic: True

{0: 0, 1: 1, 4: 2, 2: 3, 6: 4, 3: 5, 5: 6}
```



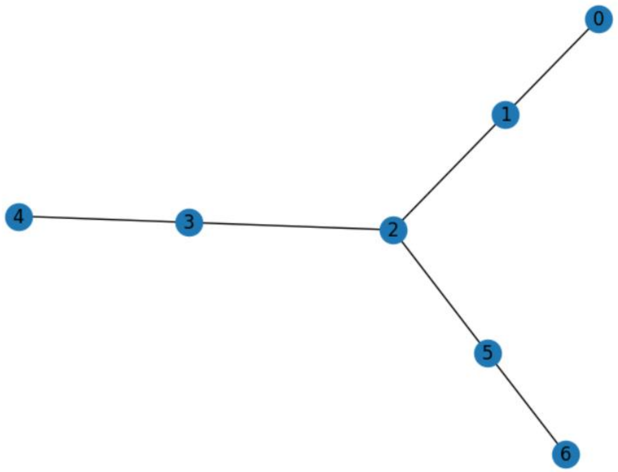
Graph kernels using WL relabelling process in NetworkX

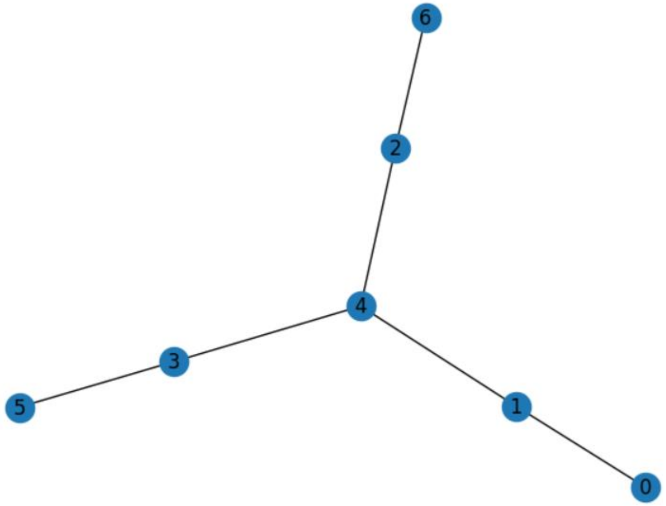
- Weisfeiler Lehman (WL) – hash function: Undirected graph



```python
import networkx as nx

G1 = nx.Graph()
G2 = nx.Graph()

G1.add_nodes_from(range(0,7))
G2.add_nodes_from(range(0,7))
G1.add_edges_from([(0,1), (1,2), (2,3), (3,4), (2,5), (5,6)])
G2.add_edges_from([(0,1), (1,4), (2,4), (2,6), (4,3), (3,5)])

g1_hash = nx.weisfeiler_lehman_graph_hash(G1)
g2_hash = nx.weisfeiler_lehman_graph_hash(G2)

# g1_hash and g2_hash are equal when they are isomorphic
print(f"First  graph hash: {g1_hash}")
print(f"Second graph hash: {g2_hash}")
print(f"Checking graph isomorphic: {g1_hash==g2_hash}")
```

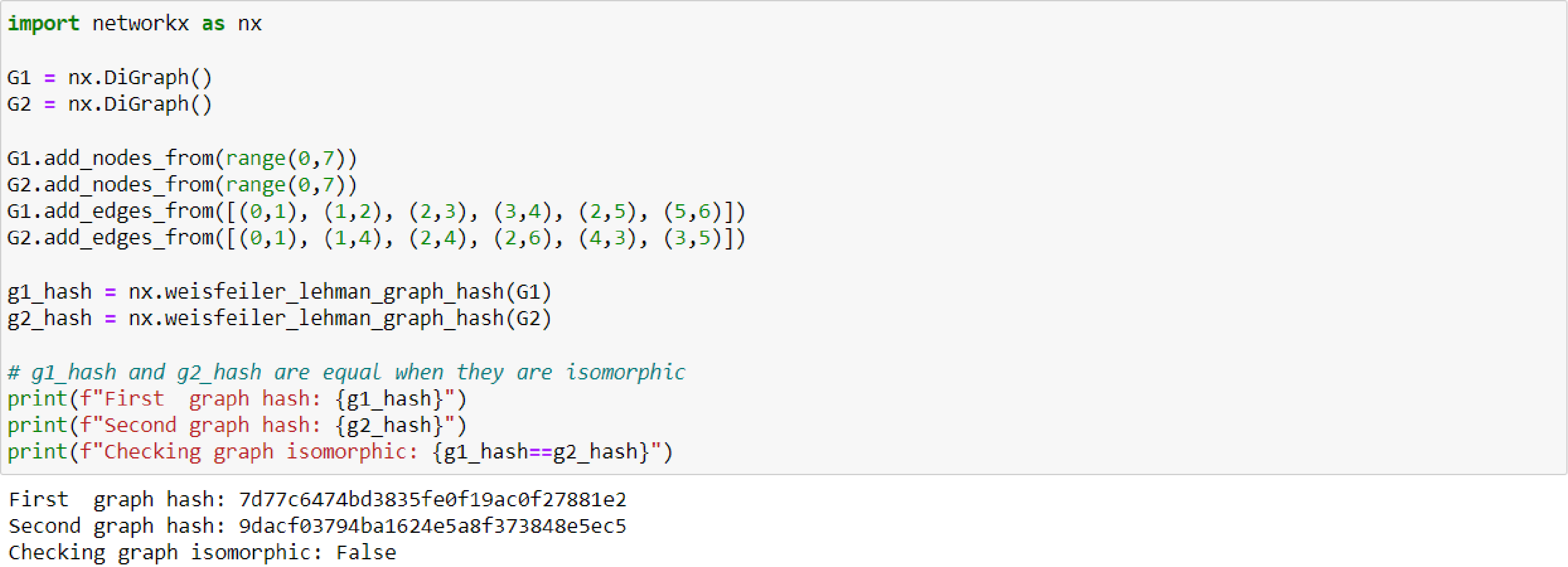
```
First  graph hash: 61f645001e86ad8a32357cc828ae33cb
Second graph hash: 61f645001e86ad8a32357cc828ae33cb
Checking graph isomorphic: True
```





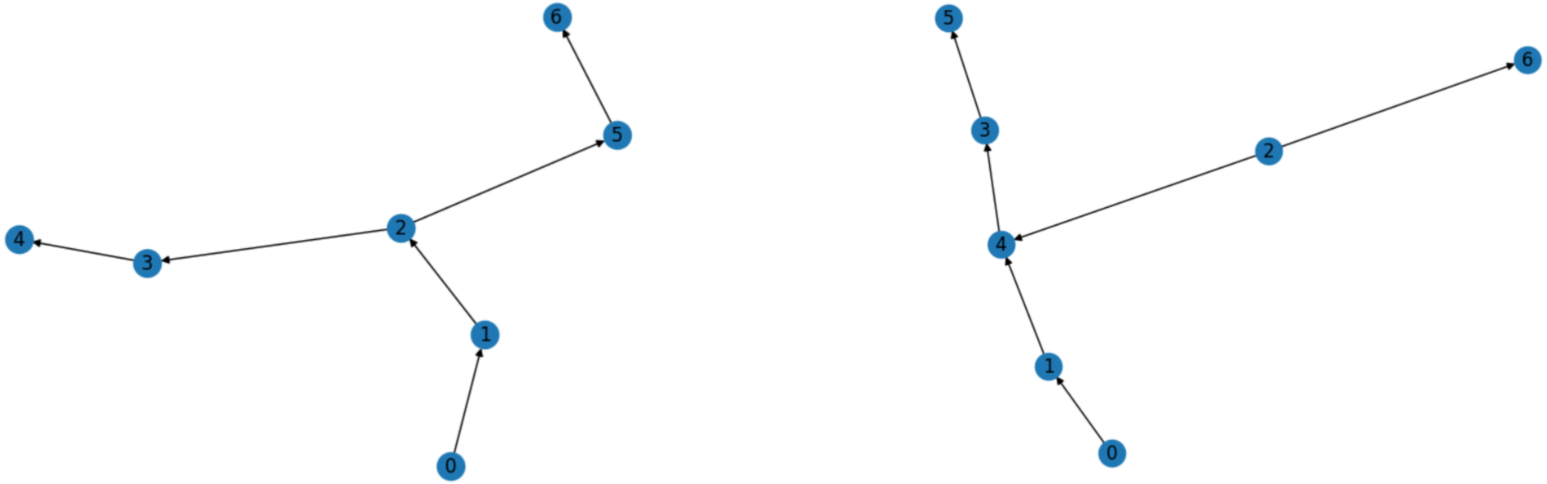
Graph kernels using WL relabelling process in NetworkX

- Weisfeiler Lehman (WL) – hash function : Directed graph



```python
import networkx as nx

G1 = nx.DiGraph()
G2 = nx.DiGraph()

G1.add_nodes_from(range(0,7))
G2.add_nodes_from(range(0,7))
G1.add_edges_from([(0,1), (1,2), (2,3), (3,4), (2,5), (5,6)])
G2.add_edges_from([(0,1), (1,4), (2,4), (2,6), (4,3), (3,5)])

g1_hash = nx.weisfeiler_lehman_graph_hash(G1)
g2_hash = nx.weisfeiler_lehman_graph_hash(G2)

# g1_hash and g2_hash are equal when they are isomorphic
print(f"First  graph hash: {g1_hash}")
print(f"Second graph hash: {g2_hash}")
print(f"Checking graph isomorphic: {g1_hash==g2_hash}")
```

```
First  graph hash: 7d77c6474bd3835fe0f19ac0f27881e2
Second graph hash: 9dacf03794ba1624e5a8f373848e5ec5
Checking graph isomorphic: False
```



Q
A