NetworkX: Network Analysis Subgraph Isomorphism

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Discrete Math Bridging Course, HSE University

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- Vertices in social network graphs represent *actors:* people, social entities etc.
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- The standard example is the friendship relation in social networks.

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- We are going to get acquainted with specialized software for calculating them.

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- We shall see that the so called *clustering coefficients* tend to be quite high.
- This reflects the fact that friends of one person are much more likely to be friends also.

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- On the other hand, being highly clusterized, the social network happens to be tightly connected.
- The well-known theory of *six degrees of separation* ("six handshakes") claims that any two people in the world are no more than six social connections from each other.
- In graph-theoretic terms, this means that the **diameter** of the social connections graph should be ≤ 6.

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- This makes the dataset relatively small.
- All data is of course anonymized.

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- Capable of handling big graphs (real-world datasets): 10M nodes / 100M edges and more.
- Highly portable and scalable.

Getting NetworkX

- NetworkX, along with libraries necessary for visualization, can be installed with `pip`:

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- We've renamed `networkx` to `nx` for convenience.

Defining a Graph: Manual

- In NetworkX, one can define a graph manually, by adding edges one by one.

```
mygraph = nx.Graph()

mygraph.add_edge('A','B')
mygraph.add_edge('B','C')
mygraph.add_edge('C','A')
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- Vertices can be of arbitrary type (strings, numbers, ...).

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- Graphs in NetworkX can also be *weighted*.
- In a weighted graph, each edge receives a number called its weight.
- E.g., time (or cost) of driving along a road.
- Weight is added just as an optional parameter to `add_edge`:

```
mygraph.add_edge('A','B', weight=6)
```

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- In the file `facebook_combined.txt` one finds the list of edges as pairs of numbers (vertices are numbered).
- The data gets imported by the `nx.read_edgelist` method.

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- NetworkX is capable of visualizing graphs, both in 2D and 3D.

Visualization: Small Example

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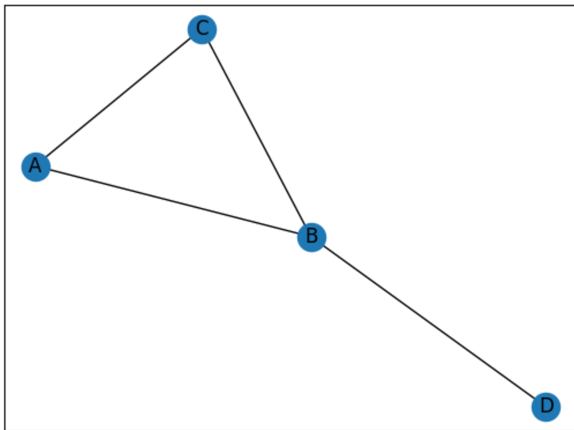
- The method is called `nx.draw_networkx`:

```
nx.draw_networkx(mygraph)
matplotlib.pyplot.savefig("mygraph.png")
```

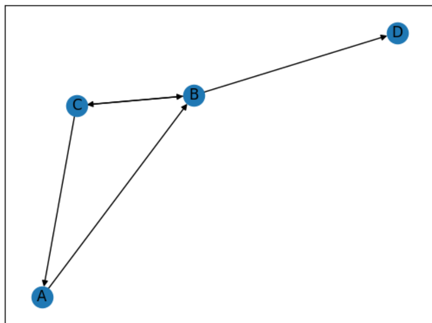
Visualization: Small Example



NetworkX output

Visualization: Small Example

This is how a directed graph is visualized. Two opposite edges between B and C are drawn as one edge with two arrows.



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Visualization of Real Data

- We remove labels, because there are too many vertices:

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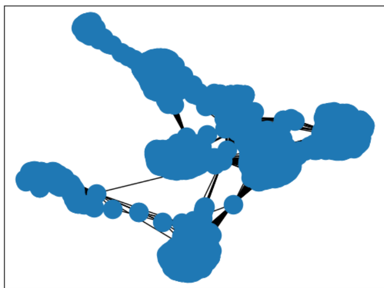
- Visualization makes clustering visible:



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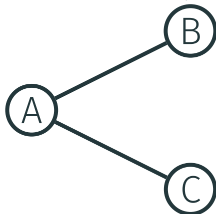

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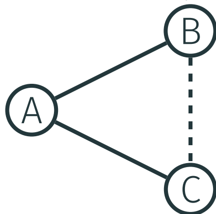

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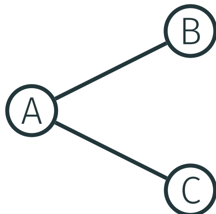
- A *triplet* is a pair of edges going from one vertex A:



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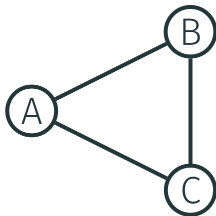

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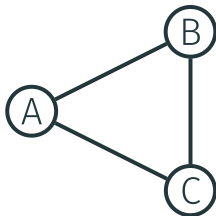

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- Thus, the GCC is the *probability* for a random triplet A, B, C in $\mathcal{G}$ to be closed (that is, B and C connected).

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- If A is an isolated vertex (degree = 0), then $LCC(A)$ is undefined (zero-by-zero division).

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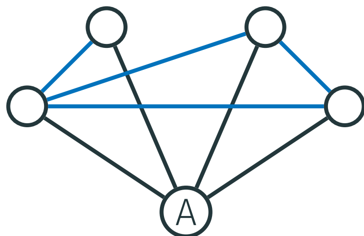

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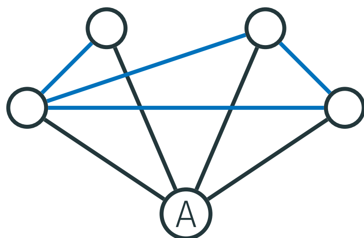

In this example, $LCC(A) = \frac{2 \cdot 4}{4 \cdot 3} = \frac{2}{3}$.

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- Global parameters of the graph are just functions of it.
- For example, if we wish to calculate the *average clustering coefficient* (the average value of local clustering coefficients), we just run

```
av_clust = nx.average_clustering(fb_gr)
```

Clustering: Real vs Random

```
import networkx as nx
from random import random

G_fb = nx.read_edgelist("facebook_combined.txt")

av_clust_coeff =  nx.average_clustering(G_fb)
print ("acc = "+str(av_clust_coeff))

edges = G_fb.number_of_edges()
nodes = G_fb.number_of_nodes()
max_edges = nodes*(nodes-1)/2
edge_probab = edges / max_edges
G_rand = nx.Graph();
k = nodes-1
for i in range(0,k) :
    for j in range(0,i) :
        if (random() <= edge_probab) :
            G_rand.add_edge(i,j)

av_clust_coeff = nx.average_clustering(G_rand)
print("rgraph_acc = " + str(av_clust_coeff));
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- This experiment yields the following results:

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- This shows that (unsurprisingly) the social network tends to cluster more than the random graph (with the same probability of edge).
- Thus, one has to be cautious with stochastic modelling of social graphs.

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- This is quite a good result, recalling that we have just a fusion of 10 ego nets, not the full Facebook graph.

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- **Caveat!** If there is no path, NetworkX throws an exception.
- To be on the safe side, use `nx.has_path` before.

Preparing for HW 3

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- Good luck!

Graph and Subgraph Isomorphism

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- First, let us recall the notion of isomorphic graphs.

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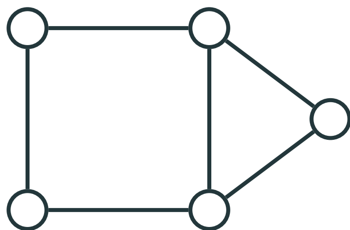

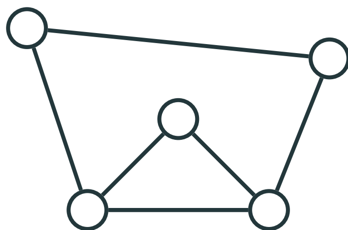

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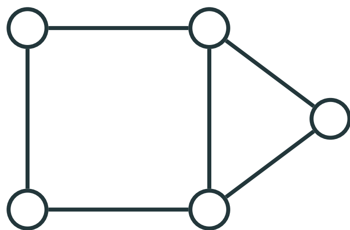

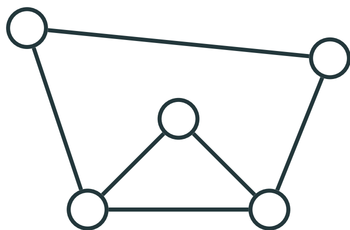

Here both graphs can be described as “a triangle and a quadrangle sharing a common edge.”

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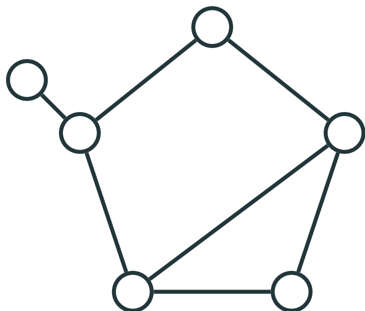

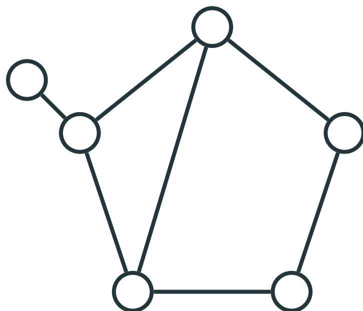

Graph Isomorphism

Isomorphic Graphs

Two graphs, $\mathcal{G}$ and $\mathcal{H}$, are *isomorphic*, if they have the same number n of vertices and vertices of each graph can be enumerated by numbers from 1 to n, so that vertices with numbers i and j are connected in $\mathcal{G}$ if and only if vertices with these numbers are connected in $\mathcal{H}$.

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Isomorphic graphs can be seen as *different representations of the same graph.*

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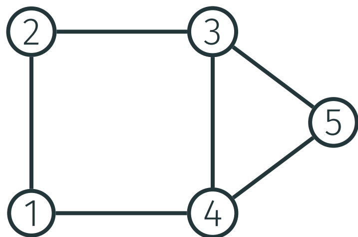
$\mathcal{G}$



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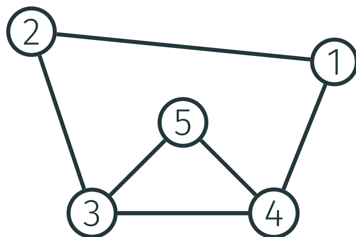

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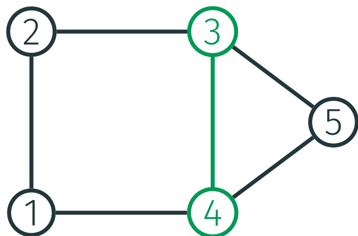

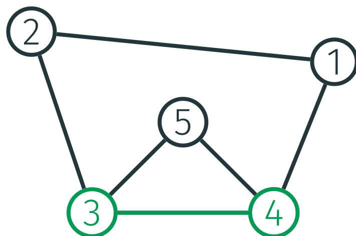

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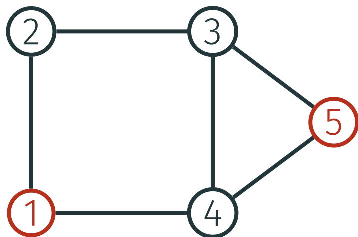

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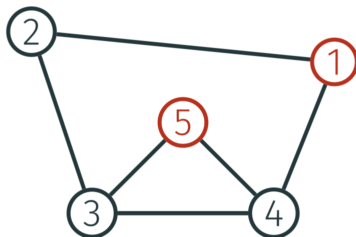

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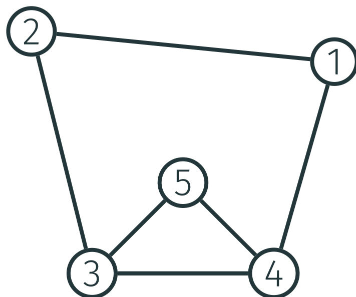

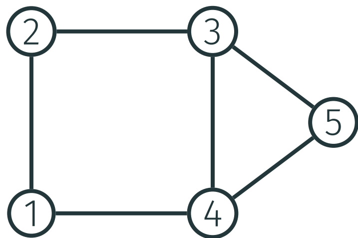

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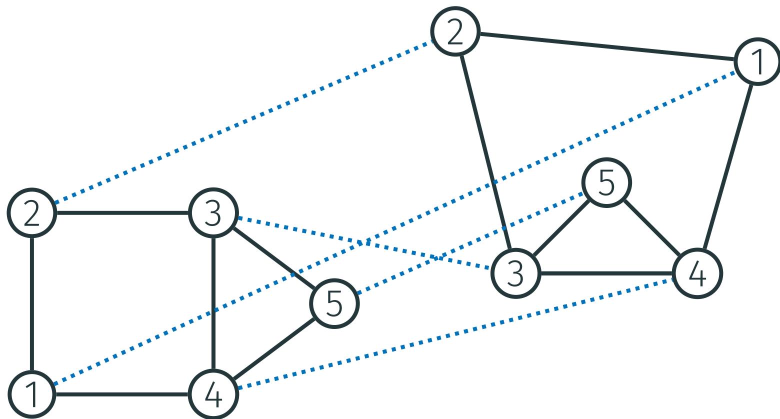

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- However, graph isomorphism is a quite rare species of NP problem: we know neither that it is NP-complete, nor that it belongs to P.

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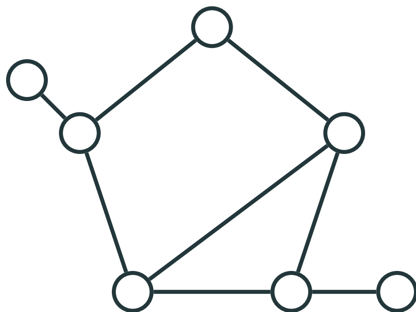

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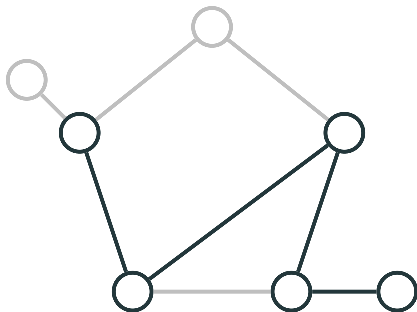

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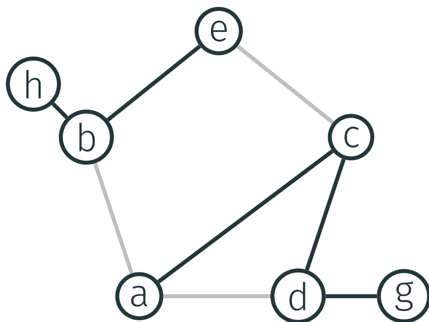

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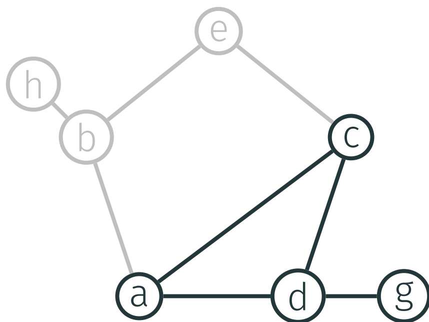

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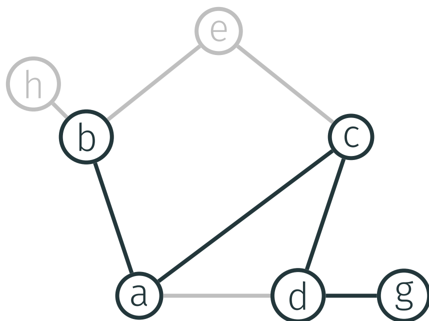

neither

Subgraph Isomorphism Problem

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- There is also a variant of this problem without requiring the subgraph to be an induced one.

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- The subgraph isomorphism problem is NP-complete (in both variants).

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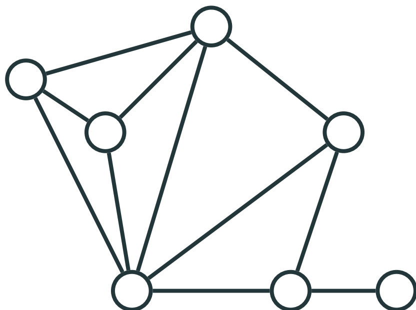

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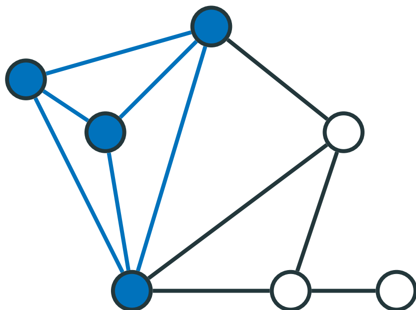

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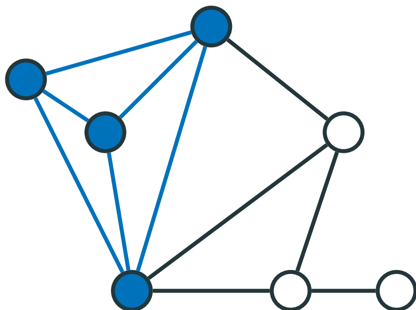

- Clique in social network graph = group of users who are friends with each other.

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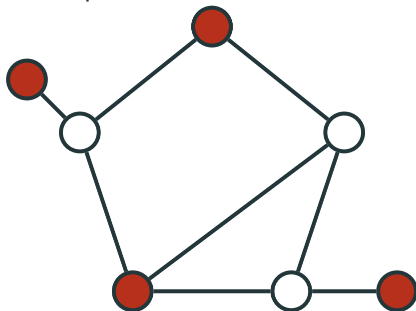

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- Therefore, CLIQUE is also NP-complete.

Hamiltonian Paths

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- This is also a subcase of subgraph isomorphism: whether $\mathcal{H}$ includes a subgraph (not an induced one), which is a chain of $|V|$ vertices.
- We shall prove NP-completeness for Hamiltonian path if we have time, but first we'll sketch its applications to genomics.

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- The two notions look similar, but there is a complexity gap: finding an Euler path is polynomial, while existence of a Hamiltonian one is NP-complete.

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- Finding a Euler cycle is easy (can be done in polynomial time).
- What if, for a specific class of graphs, the problem of finding a Hamiltonian cycle could be *reduced* to the problem of finding a Euler cycle?

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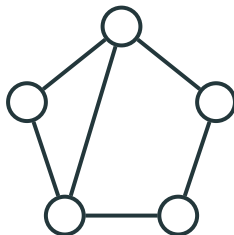

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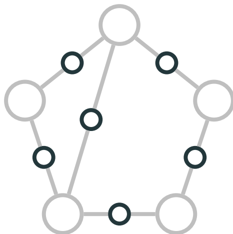

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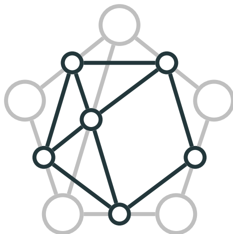

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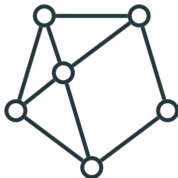

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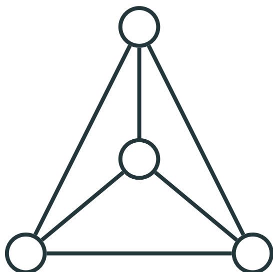

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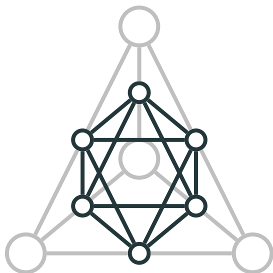

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- Nevertheless, in some practically important cases representation of a given graph as $L(G)$ allows efficient construction of Hamiltonian cycles.

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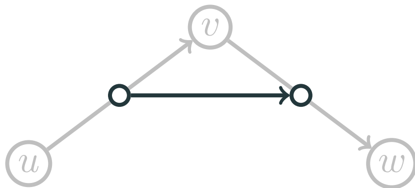

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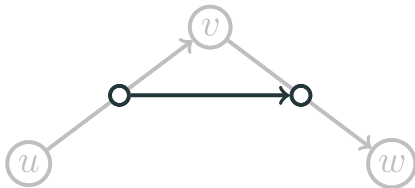

- Again, a directed Euler path in G induces a directed Hamiltonian path in $L(G)$.

Application: Genome and Its Fragments

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- Our goal is to reassemble the genome.

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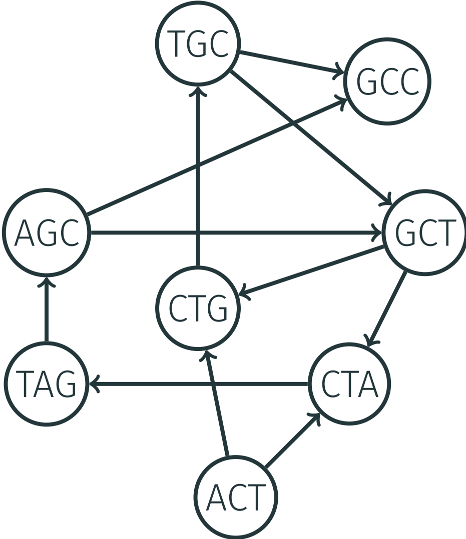
- In this graph, triplet u is connected to triplet v, if the last two letters of u are the first two letters of v:

$$\text{CTA} \rightarrow \text{TAG}.$$

Reassembly as Hamiltonian Path



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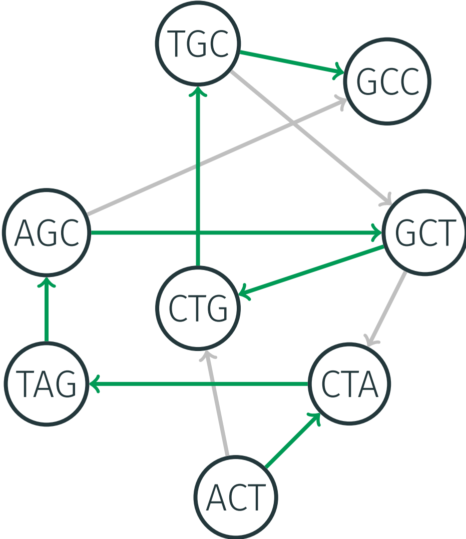

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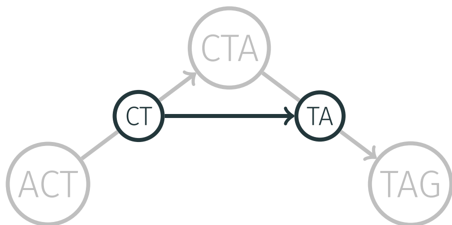
- It would be much better if we could use Euler path instead.

De Bruijn Graph

- Fortunately, the overlap graph is $L(G)$ for some other graph G:



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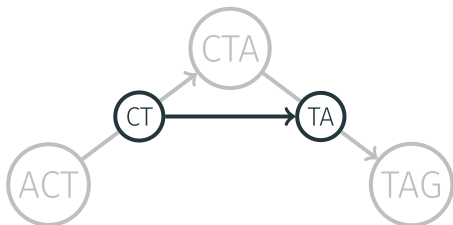
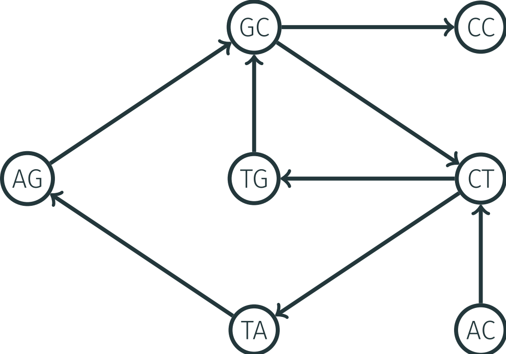


- After identifying vertices with the same annotation in G and adding AC and CC (start and end), we get **de Bruijn graph.**

De Bruijn Graph

A Euler path in de Bruijn graph induces a Hamiltonian path in overlap graph.

Reassembly as Euler Path



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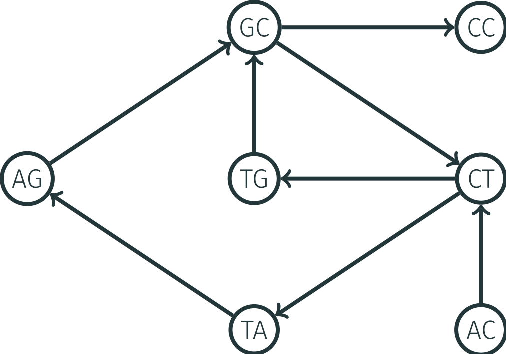

Two possible ways to reassemble: ACTAGCTGCC and ACTGCTAGCC.

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- De Bruijn graph is used in real-world genome assemblers.