2.1 Isomorphism

Two graphs: $G = (V, E)$ and $G' = (V', E')$ are called isomorphic if there is a one-to-one mapping $f$ from $V$ onto $V'$ such that any two vertices $v_i, v_j \in V$ are adjacent iff $f(v_i)$ and $f(v_j)$ are adjacent. We would say that $G$ is isomorphic to $G'$, or $G \cong G'$. Isomorphism can also be extended to non-simple graphs, through adding the language that there also must exist a one-to-one mapping from $E$ to $E'$, where every edge $v_i, v_j \in E$ must map to an edge $(f(v_i), f(v_j)) \in E'$.

By permuting the rows of the adjacency matrix of $G$ ($A$), we should be able to create the adjacency matrix of $G'$ ($A'$); i.e., there exists a permutation matrix $P$ such that $PAP^T = A'$.

If $G(V, E)$ and $G'(V', E')$ are isomorphic, then we can make general statements such as:

1. $|V| = |V'|$ and $|E| = |E'|$
2. the degree sequences of $G$ and $G'$ sorted in non-increasing order are identical
3. the lengths of the longest shortest paths (a graph’s diameter) in $G$ and $G'$ are equal
4. the lengths of the shortest cycles (a graph’s girth) in $G$ and in $G'$ are equal

Note that properties (1) - (4) are necessary but not sufficient conditions for isomorphism. We’ll discuss more about what this means soon.

The isomorphism relation on the set of ordered pairs from $G$ to $G'$ is:

- reflexive: $G \cong G$
- symmetric: if $G \cong H$, then $H \cong G$
- transitive: if $G \cong H$ and $H \cong J$, then $G \cong J$

An isomorphism class is an equivalence class of graphs that are all under an isomorphic relation.

An automorphism is an isomorphism from $G$ to itself. The set of automorphisms of $G$ is known as $G$’s automorphism group. This can be loosely thought of the ways in which a graph is symmetric. While the notion of isomorphism and automorphism appear quite similar on the surface, an automorphic permutation of $G$ will be equal to the original graph (i.e., the edge list is preserved).
2.1.1 Subgraph Isomorphism

Sometimes we may talk about the **subgraph isomorphism** problem, which is: Given a graph $G$ and a graph $H$ of equal or smaller size of $G$, does there exist a subgraph of $G$ that is isomorphic to $H$? Subgraph isomorphism and related problems (subgraph counting: how many different subgraphs of $G$ are isomorphic to $H$? subgraph enumeration: what are those subgraphs of $G$ that are isomorphic to $H$?) are common techniques of graph mining. We also might want to differentiate between **vertex-induced** subgraphs and **non-induced** subgraphs. For both, we consider a subgraph $S$ of $G$ that contains a set of vertices $V(S) \subseteq V(G)$. We would say that the subgraph is induced if $\forall e(u, v) \in E(G)$ s.t. $u, v \in V(S)$ $\implies e(u, v) \in E(S)$. The subgraph is non-induced if it only contains a subset of the edges $e(u, v) \in E(G)$ s.t. $u, v \in V(S)$.

Aside: we didn’t yet explicitly cover the difference between **induced** and **noninduced** subgraphs. For both, we consider a subgraph $S$ of $G$ that contains a set of vertices $V(S) \subseteq V(G)$. We would say that the subgraph is induced if $\forall e(u, v) \in E(G)$ s.t. $u, v \in V(S)$ $\implies e(u, v) \in E(S)$. The subgraph is noninduced if it only contains a subset of the edges $e(u, v) \in E(G)$ s.t. $u, v \in V(S)$.

In terms of computational complexity, graph isomorphism is thought to be solvable in quasi-polynomial time $[\exp((\log n)^{O(1)})$, Babai 2015], though it remains an open problem. Subgraph isomorphism is NP-complete. A naive algorithm for subgraph isomorphism would involve exhaustively checking the local neighborhood of all $v \in V(G)$ for an isomorphic relation to $H$, and requires $O(n^k)$ time, where $n = |V(G)|$ and $k = |V(H)|$. Although, several specialized algorithms exists; e.g., triangles can be enumerated in $O(m^{\frac{2}{\omega} + 1})$ time, cycles can be found in $O(n^\omega \log n)$ time, and trees can be found in polynomial time ($\omega$ is the exponent of fast matrix multiplication – most recently, $\omega \approx 2.373$ by Alman and Williams, 2021).