

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 $V(S) \in V(G)$. 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 $V(S) \in V(G)$. 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 exist; e.g., triangles can be enumerated in $O(m^{\frac{2\omega}{\omega+1}})$ time, cycles can be found in $O(n^\omega \log n)$ time, and trees can be found in polynomial time (ω is the exponent of fast matrix multiplication – most recently, $\omega \approx 2.373$ by Alman and Williams, 2021).