IV: Section (ii) Trees, Directed Graphs & Isomorphisms

Def: A Tree is a connected, acyclic (i.e., contains no cycles) graph.

Ex.

- Tree w/ 7 vertices
- Tree w/ 5 vertices

7) Essential Facts about Trees

Trees are often characterized according to the following (4) equivalences:

1) G is connected & contains no cycles, n vertices
2) G is connected & contains n-1 edges
3) G has n-1 edges & no cycles
4) For each u, v ε V(G), there exists a unique path from u to v contained in G.

Note that by equivalences we mean that, say, if property (1) holds for a graph with n vertices, then so does (2), (3), (4), etc.

Observe that in the previous example, the tree on the left has 7 vertices & 6 edges; the tree on the right consists of 5 vertices & 4 edges - each tree is acyclic & connected, confirming the above-noted equivalences.
Additional pertinent facts about trees:
(a) Every edge of a tree is a so-called cut-edge, meaning that its deletion increases the number of components in the graph.

Ex.  
\[ e_1 \quad e_2 \quad e_3 \quad e_4 \]

A tree with 5 vertices, 4 edges; note graph is connected & acyclic.

Observe that the deletion/removal of any edge of this tree increases the number of components of the graph.

Deletion of \( e_1 \):

\[ e_1 \quad e_2 \quad e_3 \quad e_4 \]

2 components

(b) Adding one edge to a tree forms exactly one cycle.

Ex.  
\[ e_1 \quad e_2 \quad e_3 \quad e_4 \quad e^* \]

Note that adding any of the edges \( e^* \) forms exactly one cycle in the graph.

def. A spanning tree of a graph \( G \) is a subgraph of \( G \) with vertex set \( V(G) \) satisfying the tree criteria (i.e., it is connected & acyclic).
Example: Considering \( G = K_4 \):

A spanning tree of \( G \) is given by:

Note that this choice is not unique, and that a graph in general possesses many spanning trees.

(c) Every connected graph contains a spanning tree. (See the example above).

Definition: A **directed graph** (or "digraph" for short) is a graph whose edges are directed/oriented from one incident vertex to the other. Conventionally, for a directed edge: \( u \to v \), we say that \( u \) is the **tail** of \( v \) is the **head**, so that an edge is from its tail to its head. Frequently, graphs are presented as **weighted** if each edge is attributed a real-valued weight. Such weights often represent "flow" (e.g., traffic/current modeling), "cost", "distance", or some such real-world measure.

Example: A digraph.

Here the arrows indicated the orientation of each edge in the graph.
Ex. 1. Digraphs & weighted digraphs.

A finite simulation for two light switches: D - Down, U - Up.

A "Markov chain" digraph.

Def. The incidence matrix, \( M(G) \), of an (undirected) graph \( G \) is an \( n \times m \) matrix where \( |V(G)| = n \) & \( |E(G)| = m \), respectively, such that \( m_{ij} = 1 \) if vertex \( v_i \) & edge \( e_j \) are incident, & \( m_{ij} = 0 \) otherwise.

Ex. 2. For a directed graph \( G \), the incidence matrix is defined analogously; we define \( m_{ij} = +1 \) if \( v_i \) is the tail of \( e_j \); similarly, we define \( m_{ij} = -1 \) if \( v_i \) is the head of \( e_j \).
Ex.

Def. The adjacency matrix, \( A(G) \), of an undirected/directed graph \( G \) is an \( n \times n \) matrix where the entry \( a_{ij} \) equals the number of edges from \( v_i \) to \( v_j \) in \( G \).

Ex.

Def. A **walk** in a graph is a sequence \( v_0, e_1, v_1, e_2, v_2, \ldots, v_k \) of graph vertices and edges such that edge \( e_i \) has endpoints \( v_{i-1} \) and \( v_i \).

Next we show how the adjacency matrix of a graph can be used to count all the walks in a graph of a specified length.
Theorem

Let \( A(6) \) be the adjacency matrix of a graph having vertices \( v_1, \ldots, v_6 \). The number of distinct \( v_0 - v_i \) walks of length \( k \) (\( k \geq 1 \)) is equal to the \((0,i)\) element of \( A^k \).

Example

Consider the graph:

\[
\begin{align*}
    v_0 & \rightarrow v_1, v_2, v_3, v_4, v_5, v_6 \\
    v_1 & \rightarrow 0, 1, 0, 1 \\
    v_2 & \rightarrow 1, 0, 2, 1 \\
    v_3 & \rightarrow 0, 2, 0, 0 \\
    v_4 & \rightarrow 1, 1, 0, 0 \\
    v_5 & \rightarrow 0, 1, 0, 1 \\
    v_6 & \rightarrow 0, 0, 1, 1 \\
\end{align*}
\]

\( A(6) \)

Note that for walks of length 2 (i.e. \( k = 2 \)), say,

the number of walks from \( v_2 \rightarrow v_3 \) is \((a_{23}) \times 2 \); similarly no walks of length 2 exist for \( v_3 \rightarrow v_4 \) and we see that \((a_{34}) = 0\), etc.

Now consider walks of length 2 (\( k = 2 \)).

\[
A^2 = \begin{bmatrix}
2 & 1 & 2 & 1 \\
1 & 6 & 0 & 1 \\
2 & 0 & 4 & 3 \\
1 & 1 & 2 & 2 \\
\end{bmatrix}
\]

So, for instance, this shows that there are two unique walks of length 2 from \( v_0 \rightarrow v_4 \):

walk 1: \( v_0 \rightarrow v_1 \rightarrow v_4 \)
walk 2: \( v_0 \rightarrow v_2 \rightarrow v_4 \)

In addition, we see from \( A^2 \) that there are no walks of length 2 from \( v_2 \rightarrow v_3 \), etc.
$A^2$ also reveals, for instance, the presence of six unique walks from $v_2$ to $v_2$; we enumerate this list to verify:

- Walk 1: $v_2 \rightarrow v_3 \rightarrow v_2$
- Walk 2: $v_2 \rightarrow v_3 \rightarrow v_2$
- Walk 3: $v_2 \rightarrow v_3 \rightarrow v_2$
- Walk 4: $v_2 \rightarrow v_3 \rightarrow v_2$
- Walk 5: $v_2 \rightarrow v_4 \rightarrow v_2$
- Walk 6: $v_2 \rightarrow v_1 \rightarrow v_2$

These examples are relatively trivial due to the small length size. However, suppose we wanted to count the number of unique walks between two vertices in $G$ for length 10 ($k=10$).

Exponentiating $A$ yields:

$$A^{10} = \begin{bmatrix}
3218 & 4329 & 4382 & 3217 \\
4329 & 10,870 & 4276 & 4329 \\
4382 & 4276 & 6486 & 4382 \\
3217 & 4329 & 4382 & 3218
\end{bmatrix}$$

Incredibly, this shows, for instance, that there are 4,276 unique walks in $G$ between $v_2$ and $v_3$! Clearly it would be tremendously onerous (if not impossible) to count all of these walks by hand or even with the aid of a computer, for that matter.

N.B.: In statistics and applied mathematics, the notion of a "random walk" in a graph has become something of a sine qua non for estimating complex probabilities. In this vein, if we wanted
To determine how many random walks of length 10 emanating from $v_1$ exist in $G$, we would simply add the components from row 1 of $A^{10}$.

This gives: $3218 + 4329 + 4382 + 3217 = 15,146$.

In summary, there are a total of 15,146 random walks of length 10 (beginning at $v_1$) in $G$ — we note again that such a computation would, naturally, be extremely difficult to achieve by hand.

**Graph Isomorphism**

Informally, two graphs are said to be isomorphic if they are "structurally identical" — in other words, if a re-labeling of the vertices of graph $G$ yields graph $H$. Thus, the graphs are isomorphic if we write: $G \cong H$.

**Ex.**

$G: \begin{array}{c} \text{w} \\ \text{x} \end{array}$   $H: \begin{array}{c} \text{a} \\ \text{b} \end{array}$

Note that if we impose the following vertex re-labeling on $G$: $\begin{array}{c} \text{w} & \rightarrow & \text{a} \\ \text{x} & \rightarrow & \text{b} \\ \text{y} & \rightarrow & \text{d} \\ \text{z} & \rightarrow & \text{c} \end{array}$, we get the graph $H$. Thus, $G \cong H$. 
Def. More formally, we say G is \textbf{isomorphic} to H (i.e. \( G \cong H \)) if there exists a bijection \( f \) (one-to-one, onto) from \( V(G) \) to \( V(H) \) such that \( u \in E(G) \) if \( f(u)f(v) \in E(H) \). Put another way, \( f \) "preserves" edge incidence in \( H \).

From the previous example, then, let \( f: V(G) \rightarrow V(H) \) with:
\( f(w) = a, \ f(x) = d, \ f(y) = b \ \& \ f(z) = c \). This defines an isomorphism between \( G \) & \( H \).

Def. If a graph is isomorphic to itself, we say that there exists an \textbf{automorphism} on \( G \).

Note that the (trivial) identity map is an automorphism on \( G \) always. Such an automorphism is consequently said to be \textit{trivial}.

Ex. Consider \( G = K_3 \).

\[ \begin{array}{c}
\text{Note that any permutation of the vertices of } K_3 \text{ yields an automorphism.}
\end{array} \]

For instance:
\[ \begin{align*}
f(a) &= b \\
f(w) &= c \\
f(z) &= a
\end{align*} \]

is an automorphism of \( K_3 \).

In total, there are 3 such automorphisms.

In general, \( G = K_n \) has \( n! \) total automorphisms. We say the "automorphism class" of \( K_n \) is of size \( n! \).
Lastly, let's explore a deep connection between isomorphic graphs and their adjacency matrices.

**Theorem:** Two simple graphs $G$ and $H$ are isomorphic iff there exists a permutation matrix $P$ such that $A(G) = P \cdot A(H) \cdot P^T$, where $A(G)$ is the adjacency matrix of $G$, and $A(H)$ is the adjacency matrix of $H$.

**Q:** Why does this work?

If $G \cong H$, then some re-labeling of the vertices of $G$ yields $H$. Equivalently, re-labeling the rows/cols. of $A(G)$ appropriately gives $A(H)$ (or vice versa).

Note that $P \cdot A(H) \cdot P^T$ effectively performs row swaps of $A(H)$, while $A^T(G) \cdot P^T$ performs transpose column swaps on $A(H)$.

Consequently, $A(G) = P \cdot A(H) \cdot P^T$ means that we can effectively relabelify of row vertices (to equivalent column vertices) on $A(G)$ to yield $A(H)$ (or vice versa).

We demonstrate with an earlier example.
Recall the example:

\[ G: \]
\[
\begin{array}{cccc}
\text{x} & \text{w} & \text{y} & \text{z} \\
\hline
\text{x} & 1 & 0 & 1 \\
\text{y} & 0 & 1 & 0 \\
\text{z} & 0 & 1 & 0 \\
\text{w} & 0 & 0 & 0 \\
\end{array}
\]

\[ H: \]
\[
\begin{array}{cccc}
\text{a} & \text{c} & \text{b} & \text{d} \\
\hline
\text{a} & 1 & 0 & 0 & 0 \\
\text{b} & 0 & 1 & 0 & 0 \\
\text{c} & 0 & 0 & 1 & 0 \\
\text{d} & 0 & 0 & 0 & 1 \\
\end{array}
\]

Where \( G \cong H \) with the explicit isomorphism:

\[
\begin{aligned}
w & \rightarrow a \\
x & \rightarrow b \\
y & \rightarrow c \\
z & \rightarrow d
\end{aligned}
\]

Consider the respective adjacency matrices:

\[
A(G) = \begin{bmatrix}
0 & 1 & 0 & 0 \\
1 & 0 & 1 & 0 \\
0 & 1 & 0 & 1 \\
0 & 0 & 1 & 0 \\
\end{bmatrix}
\]

\[
A(H) = \begin{bmatrix}
0 & 0 & 0 & 1 \\
0 & 0 & 0 & 1 \\
0 & 0 & 0 & 1 \\
0 & 0 & 0 & 1 \\
\end{bmatrix}
\]

As indicated, the isomorphism is achieved. Thusly:

\[
\begin{aligned}
P &= \begin{bmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 \\
\end{bmatrix}, & P^T &= \begin{bmatrix}
1 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 \\
\end{bmatrix}
\end{aligned}
\]

\[
\begin{bmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 \\
\end{bmatrix}
\]

\[
\begin{bmatrix}
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 \\
\end{bmatrix}
\]

\[
\begin{bmatrix}
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 1 \\
0 & 1 & 0 & 0 \\
1 & 0 & 0 & 0 \\
\end{bmatrix}
\]

\[
P \cdot A(G) \cdot P^T = A(H)
\]