12 Trees and Graphs

12.1 Rooted and Unrooted Trees

We’ve all seen trees. No, not that sprightly spruce in your garden, but your family tree.

A tree consists of a collection of vertices, some of which are joined by edges. A rooted tree is a tree with one vertex designated the root. Rooted trees are normally drawn with the root at the top. The above example has 8 vertices, with Rachael the root.

For a rooted tree, we can talk of parents and children in the natural way. There are many other places that a rooted tree arises. One is the folder/directory structure on your computer. A parent directory contains child subdirectories. That tree is often drawn with the root on the top left and the branches growing left to right.

In general, a tree is just like a rooted tree, except it does not have a special vertex. A tree can also be defined recursively:

- A single vertex is a tree;
- Adding one new vertex and joining it to one vertex of a tree yields a tree.

For example, alkanes are chemical molecules consisting of carbon and hydrogen atoms, where each carbon atom has four bonds and each hydrogen atom has one bond. Specifically, all links are single bonds and there are no cycles or loops. So, here is a representation of butane: four carbons and ten hydrogen.

©Wayne Goddard, Clemson University, 2013
For mathematical purposes, we can suppress the hydrogen atoms, since we can always infer where they go. Chemists care about how many different isomers occur for a particular alkane. This is equivalent to counting the trees that can be made up of the carbon atoms. For example, there is only one isomer of methane, ethane and propane (which have 1, 2, and 3 carbon atoms respectively), but there are two isomers of butane.

▶ For you to do! ◀

1. Draw the other isomer of butane.

12.2 Graphs

A (simple) graph is a collection of vertices and edges such that each edge joins two vertices. People sometimes allow multiple edges between vertices (for example, to represent double-bonds) or loops (edges both of whose ends are the same vertex), but we exclude those here—that is the meaning of “simple” in simple graph.

A typical place where a graph arises is with a map: the cities are the vertices; the roads are the edges. In this situation, the point is that the graph abstracts everything one needs to know. The actual direction or location of the road doesn’t matter; all we care about is how long does it take to traverse that road. Another graph is used in project planning: the vertices are the tasks, and there is a directed edge (we call this an arc) from one task to another if the first has to be completed before the second one starts. This allows for scheduling of resources, and also for critical path analysis, which tells one whether a particular task running late would cause the whole project to be delayed. Another (very large) graph is the Internet.

We need some terminology for graphs. A walk is a sequence of vertices such that consecutive vertices are joined by an edge. The length of a walk is the number of edges on it. A path is a walk without repeated vertices. A cycle is a walk of at least three edges without repeated vertices except that the first and last vertex are the same. The terms path and cycle also refer to the specific graphs that have that structure.

Two vertices are connected if there is a walk between them. Being-connected is an equivalence relation; the equivalence classes form the components of the graph. A graph is connected if there is only one component.
Here is a graph with three components: a cycle and two trees (one of which is a path).

12.3 Properties of Trees

We discuss next some properties of trees in general.

**Lemma 12.1** A tree is connected and contains no cycle.

Indeed, this is usually used as the definition of a tree.

**Lemma 12.2** (a) Between any two vertices in a tree there is a unique path.
(b) Removing any edge disconnects the tree.

**Proof.** (a) Because a tree is connected, there is at least one path between every pair of vertices. If there were multiple paths between two vertices, then there would be a cycle.

(b) This follows from (a).  

In fact the converse of (a) is true: if a graph has the property that between every two vertices there is a unique path, then the graph must be a tree.

How many carbon–carbon bonds are there in an alkane? One can readily see that the number of bonds goes up by 1 each time we add a carbon. This gives us the following result:

**Lemma 12.3** If a tree has \( n \) vertices, then it has \( n - 1 \) edges.

(Note that the above proof is really a lazy form of induction.)

In fact the converse is true. If a graph is connected and has one less edge than vertices, then it must be a tree.

There is also a natural way to **color** the vertices of a tree with two colors. Start by coloring the root with one color, say red. Color its children the other color, say blue. Color their children (the root’s grandchildren) with red. And so on, alternating. If we number the
generations with the root as 0, then the even generations are red and the odd generations are blue. This has the property that every edge has one end red and one end blue. This is called a bipartite coloring.

**Exercises**

12.1. (a) Show that there are exactly two trees on 4 vertices if the vertices are indistinguishable.

(b) How many different trees are there with 4 vertices if the 4 vertices are all distinguishable (say the vertices are labeled A, B, C, D)?

(c) How many different rooted trees are there with 4 vertices if the 4 vertices are indistinguishable (and the ordering of children does not matter)?

(d) How many different rooted trees are there with 4 vertices if the 4 vertices are all distinguishable (but the ordering of children does not matter)?

12.2. Determine the number of isomers of pentane and hexane (alkanes with 5 and 6 carbon atoms respectively).

12.3. Prove that a cycle has a bipartite coloring if and only if the number of vertices is even.

12.4. Draw a rooted tree with 5 vertices labeled A, B, C, D, and E such that all of the following conditions hold:
   (i) E has exactly two ancestors
   (ii) A and C are siblings
   (iii) No vertex has exactly one child
   (iv) B is neither an ancestor nor a descendant of C
   (v) B is not the grandparent of D

12.5. Consider a simple graph with 100 vertices.

   (a) Explain why such a graph has at most \( \binom{100}{2} \) edges.

   (b) Describe such a graph that has \( \binom{99}{2} \) edges but is not connected.

   (c) Prove that if such a graph has more than \( \binom{99}{2} \) edges then it is connected.
Solutions to Practice Exercises

1.