Lecture 3

Current plan: include algorithms

- Next week: Eulerian and Hamiltonian Graphs
- 4 Lectures each of the last 3 units

Today: three quick hits

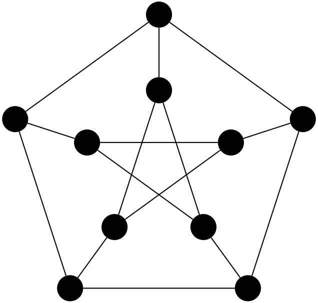
- Basic definitions
- Trees
- Applications to Chemistry

Basic Definitions

Basic graphs and concepts

- The *empty graph* E_n has n vertices and no edges
- The *complete graph* K_n has n vertices, and each vertex is connected to every other.
- The *path graph* P_n has n vertices $\{1, \ldots, n\}$ with an edge between i and $i + 1$
- The *cycle graph* C_n has n vertices $\{1, \ldots, n\}$ with an edge between i and $i + 1$ and between n and 1.

The Petersen Graph



Connected means we can "get from any vertex to another"

Definition (Walk)

Let G be a simple graph. A *walk* in G is a sequence of vertices $v_1, v_2, \ldots, v_n$ so that v_i is adjacent to v_{i+1}. We we say the walk goes from v_1 to v_n.

Definition (Connected)

A graph G is *connected* if there is a walk between any two vertices v and w in G.

Definitions I won't use without explaining:

- A *trail* is a walk that doesn't repeat any edges
- A *path* is a walk that doesn't repeat any vertices

Bipartite graphs

Definition (Bipartite graphs)

A graph G is *bipartite* if we can colour every vertex either blue or red so that every edge goes between a blue vertex and a red vertex.

Definition (Complete bipartite graphs)

The *complete bipartite graph* $K_{m,n}$ consists of $m + n$ vertices, m coloured red, n coloured blue, and an edge between any red vertex and and any blue vertex.

Examples

Another way to characterise bipartite graphs

Lemma

A graph G is bipartite if and only if it doesn't have any cycles of odd length (i.e., subgraphs of the form C_{2k+1}).

Bipartite $\implies$ no odd cycles:

Subgraphs of bipartite graphs are bipartite

No odd cycles $\implies$ Bipartite:

Try to colour G by distance from v

Definition (Distance)

Let G be connected, and let v, w be two vertices. The *distance from v to w* is the least number of edges in any walk from v to w.

Trees

A forest is a bunch of trees

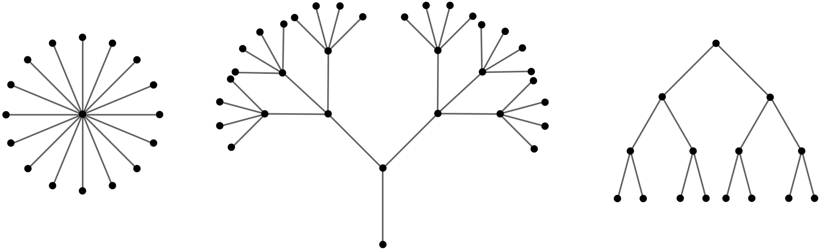


Figure: A forest of three trees

Definition

- A *forest* is a graph without cycles
- A *tree* is a connected graph without cycles

The Treachery of Definitions (After Magritte)

Figure: Ceci n'est pas un arbre (This is not a tree)

$\lfloor 13/2 \rfloor$ ways of looking a tree (After Wallace Stevens)

Proposition:

Let G be a graph with n vertices. The following are equivalent.

1. G is a tree (i.e., G connected but has no cycles)
2. There is a unique path in G between any two vertices
3. G is connected and has $n - 1$ edges
4. G has no cycles and has $n - 1$ edges
5. G is connected, but removing any edge disconnects G
6. G has no cycles, but adding any edge creates a cycle

Informally: Trees are Goldilocks graphs

- Trees have enough edges: they're connected
- Trees don't have too many edges: they have no cycles

Make like a tree and get out of here (After Biff Tannen)

Definition (Tree)

Let T be a tree. A vertex $v \in T$ is a *leaf* if it has degree 1.

Lemma

Let T be a tree with $2 \leq n < \infty$ vertices. Then T has at least two leaves.

Proof 1: See title of slide.

Pick an edge, and try to "leave" – that is, walk as far as you can.

- No loops, so you'll never return to where you are
- Finitely many vertices, so it can't go on forever

Eventually you'll get stuck – that's a leaf.

Pruning Trees

Part of Proposition:

If T is a tree with n vertices, then T has $n-1$ edges.

Proof: Induct on n

- Base case: $n = 1$
- Now assume that all trees with $n-1$ vertices have $n-2$ edges
- If T is a tree with n vertices, it has a leaf v (by Lemma)
- Delete v and the edge next to it to get a new tree T'
- T' has $n-1$ vertices, so $n-2$ edges, so T has $n-1$ edges.

Another use of the handshaking lemma

Part of Proposition:

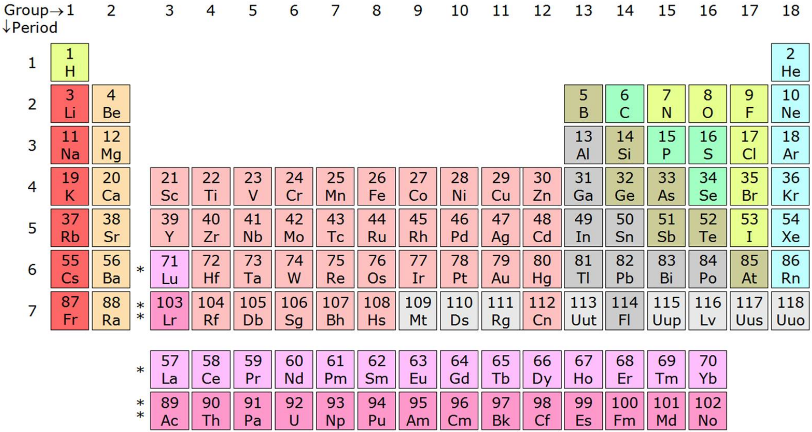
If G is a connected graph with n vertices and $n-1$ edges, then G is a tree.

Proof: induct on n

- Base case: $n = 1$
- Assume proposition is true for all graphs with $n-1$ vertices
- Since G is connected, it has no vertices of degree 0
- Use handshaking to show G must have a vertex v of degree 1
- Delete v and the edge next to it to get a new graph G'
- G' is a tree, so G must have been as well

Chemistry

Chemical formulas encode degree sequences



Atom	C	N	O	H
Degree	4	3	2	1

Shortcuts around Carbon and Hydrogen

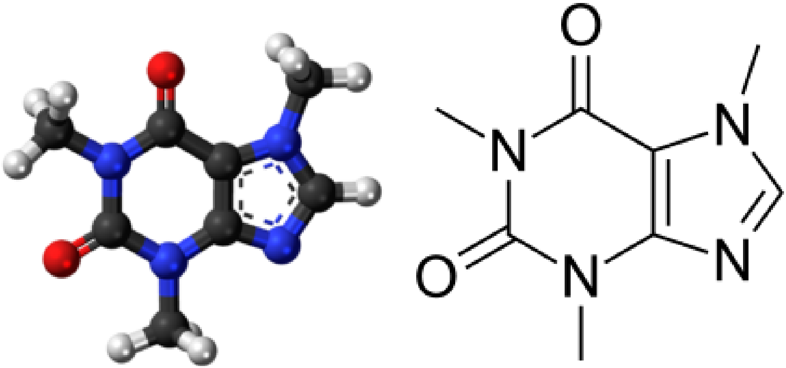


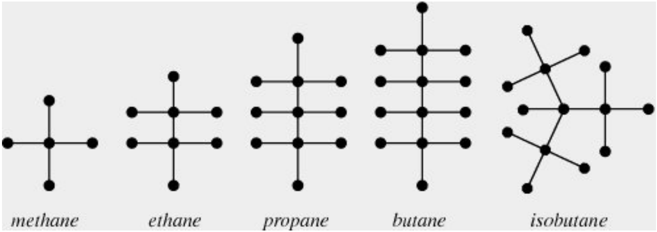
Figure: Two pictures of Caffeine

- Unlabelled vertices are Carbon
- Hydrogen not drawn; inferred to make degrees correct

Isomers are graphs with the same degree sequence

Definition

An *Alkane* is a molecule with formula $C_n H_{2n+2}$



Definition (Isomer)

Two different molecules are *isomers* if they have the same chemical formula.

Lemma: Any alkane is a tree.

Proof: Handshaking.

Question: How many isomers does $C_5 H_{12}$ have?