V. GRAPH THEORY (The Book, chapter 10)

To this point, we have considered various sets, just as collections of elements. We now consider sets with specified relations between the elements.

25. Basic ideas about graphs — There are many ways to define a graph.

Definition 25.1. *A graph is a pair* $\Gamma = (V, E)$*, where* V *is a set, and* E *is a collection of two-element subsets of* V*.*

We will always assume V is finite. A graph Γ may be drawn as a collection of vertices V with edges between vertices. Note that our definition allows at most one edge between vertices, and no edges from a vertex to itself (loops). Some people like their graphs to have multiple edges and loops and maybe arrows on the vertices. They would call our graphs, as defined above, "simple graphs". At one point, we will encounter graphs with multiple edges between vertices, and we will call these "multigraphs".

For example, the complete graph K_n has $V = \{1, \ldots, n\}$ and an edge between every pair of vertices. So $E = \binom{V}{2}$, the set of all two element subsets of V, and K_n has $\binom{n}{2}$ edges, each edge connected to $n-1$ other edges. Every graph with n vertices is a **subgraph** of K_n. That is, it has all the vertices of K_n and just some of the edges of K_n.

Other interesting examples: n-cycle, polyhedra, hypercubes, bipartite $K_{p,q}$.

One can also describe a graph in terms of its **adjacency matrix**. If $V = \{v_1, \ldots, v_n\}$ then the adjacency matrix A is $n \times n$ with entry in row i column j equal to 1 if $\{v_i, v_j\} \in E$, and equal to 0 if $\{v_i, v_j\} \notin E$. This formulation is how a computer prefers to think of a graph.

Yet another description is in terms of functions. Let $\Gamma = (V, E)$ be a graph. As before, let $\binom{V}{2}$ denote the set of two element subsets of V. Define

$$f : \binom{V}{2} \longrightarrow \{0, 1\}$$

by $f(u, v) = 1$ if $\{u, v\} \in E$, and $f(u, v) = 0$ if $\{u, v\} \notin E$. Thus, Γ is obtained from K_n by erasing those edges with f-value zero, and keeping those edges with f-value 1. This formulation is useful for counting graphs.

The first theorem in graph theory is a relation between edges and vertices. The **degree** of a vertex v is the number $d(v)$ of edges connected to it.

25.1 Theorem. *Let* $\Gamma = (V, E)$*, and let* $e = |E|$ *be the number of edges in* Γ*. Then*

$$2e = \sum_{v \in V} d(v).$$

Proof. We use induction on the number of edges. If there are no edges, then the degree of every vertexi is zero, so 25.1 holds. Assume 25.1 holds for all graphs with $e-1$ edges, and let Γ be a graph with e edges. Remove an edge $\{u, v\}$ from Γ, while keeping these two vertices. The resulting graph has $e-1$ edges, and the same vertices. All vertices except u, v have their degrees unchanged, but the degrees of u, v have been reduced by one. By the induction hypothesis,

$$2(e-1) = \sum_{\substack{x \in V \\ u \neq x \neq v}} d(x) + d(u) - 1 + d(v) - 1 = -2 + \sum_{x \in V} d(x).$$

So $2e = \sum_{x \in V} d(x)$. $\square$

26. Isomorphisms and Automorphisms — There are many ways to draw a given graph, depending on where you place the vertices, and how you draw the edges. For example K_4 can be drawn as a square with a cross or as a triangle with a center. Also, the vertex sets of two graphs could be different, but having corresponding edge relations. We want a precise definition of when two graphs are "the same".

An **isomorphism** between two graphs $\Gamma = (V, E)$ and $\Gamma' = (V', E')$ is a bijection $f : V \longrightarrow V'$ such that $\{u, v\} \in E$ if and only if $\{f(u), f(v)\} \in E'$.

In other words, if u, v are adjacent in Γ, then $f(u)$, $f(v)$ must be adjacent in Γ', and conversely. So an isomorphism of graphs is a bijection from V to V' which induces a bijection from E to E'. This is called "preserving the graph structure". Many (all?) mathematical objects are sets with additional structure, such as graphs, groups, vector spaces, etc. An isomorphism between two objects of the same type is always a bijection which preserves the structure of the objects.

An **automorphism** of a graph Γ is an isomorphism from Γ to itself. The set of automorphisms forms a group under composition, denoted $\mathrm{Aut}(\Gamma)$.

An automorphism is therefore a permutation of the vertices that sends edges to edges. The size of $\mathrm{Aut}(\Gamma)$ is an indication of the amount of symmetry of Γ. The most symmetric graph is K_n. Since every vertex in K_n is connected to every other vertex, any permutation of $\{1, \ldots, n\}$ will be a graph automorphism. Therefore

$$\mathrm{Aut}(K_n) = \mathcal{S}_n$$

is the symmetric group on $\{1, \ldots, n\}$.

For an arbitrary graph Γ with n-vertices, the group $\mathrm{Aut}(\Gamma)$ is a subgroup of $\mathcal{S}_n$. For the octahedron graph O, the group $\mathrm{Aut}(O)$ is the subgroup of $\mathcal{S}_6$ consisting of the permutations commuting with the antipodal automorphism

$$\alpha = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 \\ 2 & 1 & 4 & 3 & 6 & 5 \end{pmatrix}.$$

Here we view O as K_6 with the edges $\{1,2\}, \{3,4\}, \{5,6\}$ erased. For any $\sigma \in \mathrm{Aut}(O)$, there are 6 choices for $\sigma(1)$, 4 choices for $\sigma(3)$, 2 choices for $\sigma(5)$, and these choices determine the effect of σ on the remaining vertices. Hence $|\mathrm{Aut}(O)| = 6 \cdot 4 \cdot 2 = 48$.

27. Trees — A connected graph without cycles is called a **tree**. In other words, a tree is a graph in which there is a unique path of edges between any pair of distinct vertices. In still other words, a tree is a connected graph which becomes disconnected when any edge is removed. A **leaf** on a tree, or any graph, is a vertex of degree one. The basic fact about trees is

27.1 Theorem. *Trees have leaves.*

Proof. Suppose there is a tree without leaves. Then every vertex has degree ≥ 2. Pick a vertex v_1, and walk to an adjacent vertex v_2. Exit v_2 on an edge other than $\{v_1, v_2\}$, arriving at v_3. Exit v_3 on an edge other than $\{v_2, v_3\}$, arriving at v_4, etc. In this way, we form a list of vertices $v_1, v_2, v_3, \ldots$. But there are only finitely many vertices, so we must have $v_i = v_j$ for some $i < j$. The path $(v_i, v_{i+1}, \dots, v_j)$ is therefore a cycle in our tree. This is a contradiction. □

Note that the finiteness of the vertex set is used in the proof. There are infinite trees without leaves, but we will not consider these.

27.2 Corollary. *Let T be a tree with n vertices and e edges. Then $e = n - 1$.*

Proof. Remove a leaf, and use induction on the number of vertices. □

Suppose you have a connected graph Γ, which is not a tree. Then Γ contains a cycle. Remove an edge from this cycle, and call the new graph Γ'. Note that Γ' has the same vertices as Γ, and Γ' is still connected, since the removed edge belonged to a cycle. If Γ' is not a tree, then we can remove an edge from a cycle in Γ', resulting in Γ'', etc. Eventually we arrive at a tree T which is a subgraph of Γ, and contains all the vertices of Γ. Such a tree is called a **spanning tree** of Γ. We have just proved that every connected graph has a spanning tree. Often one can use facts about trees to prove facts about general graphs, using spanning trees.

Here is an example. Suppose we want to color the vertices of a Γ with two colors, red and blue, such that adjacent vertices have different colors. We call this "2-coloring". It amounts to partitioning the vertices into two subsets, such that vertices in the same set are not adjacent. When can we do this? Clearly it can be done for a square, but not a triangle. Also, it is easy to see, using induction and 26.1 that any tree can be 2-colored.

27.3 Theorem. *A graph can be 2-colored if and only if it has no odd cycles.*

Proof. An odd cycle cannot be 2-colored, so any graph containing an odd cycle cannot be 2-colored. Suppose, conversely, that Γ has no odd cycles. Choose a spanning tree T for Γ, and a 2-coloring of T. We claim this is also a 2-coloring of Γ. If it were not, there would be and edge $\{u, v\}$ in Γ such that u, v have the same color. Consider the path in T from u to v. Say the vertices on the path are $u = v_1,\ v_2, \dots,\ v_k = v$. The colors alternate along the path, since each edge of the path is in T. Since v_1 and v_k have the same color, we must have k odd. Replacing the edge $\{u, v\}$ we find an odd cycle in Γ. This is a contradiction. □

There are many ways to draw a given graph, depending on where you place the vertices, and how you draw the edges. For example K_4 can be drawn as a square with a cross or as a triangle with a center. Also, the vertex sets of two graphs could be different, but having corresponding edge relations. We want a precise definition of when two graphs are "the same".

28. Euler's formula — A graph is **planar** (not planer or plainer) if it can be drawn in the plane so that no edges cross. A **face** of a planar graph is a connected component of the plane with the graph removed. A planar graph looks like a map; the faces are the countries, and the surrounding sea. For example, the sea is the only face of a tree.

A planar graph Γ has a **dual multigraph** Γ^*, obtained as follows. The vertices of Γ^* are the faces of Γ, and there is an edge between two vertices u^*, v^* in Γ^* for every edge in Γ shared by u^*, v^*, viewed as faces in Γ. You draw Γ^* by placing one Γ^*-vertex in each face of Γ and drawing one edge between two Γ^* vertices u^*, v^* across each Γ-edge shared by the regions containing u^*, v^*. The multigraph Γ^* is also planar, and every face of Γ^* contains exactly one vertex of Γ. Hence, if Γ has

n vertices, e edges and f faces, then Γ^* has f vertices, e edges and n faces. If you take the dual of Γ^*, you get back to the original Γ. That is, Γ^{**} is isomorphic to Γ.

28.1 Lemma. *Suppose Γ is connected and planar, with dual multigraph Γ^*. Let T be a spanning tree for Γ, and let T^* be the subgraph of Γ^* consisting of the edges in Γ^* which do not cross edges in T. Then T^* is a spanning tree for Γ^*.*

Proof. The exterior and interior of any cycle in Γ^* is a union of faces of Γ^*, each of which contains a vertex of Γ. Hence there are vertices u, v in Γ connected by a path in T which cuts across the cycle. Since the edges of T and T^* do not cross, this cycle cannot be contained in T^*. Hence T^* contains no cycles.

If T^* is not connected, any component of T^* not connected to the outside face must be surrounded by a cycle in T. Since T has no cycles, it follows that T^* is connected.

Similarly, T^* missed a vertex of Γ^*, that vertex would be in a region of Γ surrounded by a cycle in T.

This proves that T^* is a spanning tree of Γ^*. □

28.2 Theorem. *If Γ is a connected planar graph with n vertices, e edges, and f faces, then*

$$n - e + f = 2. \qquad \textit{Euler's Formula}$$

Proof. It is easy, but not so interesting, to prove this by induction on the number of edges (see exercises). We use instead the spanning trees T, T^*. Note that 26.2 is Euler's formula for trees. So

$$e_T = n - 1, \quad e_{T^*} = f - 1.$$

Since every edge of Γ is either in T or T^*, we have $e = e_T + e_{T^*}$. Hence $e = n - 1 + f - 1$. □

A planar graph cannot have too many edges, or they will be forced to cross. Euler's Formula leads to more precise numerical restrictions. To see this, we have to be more careful in our counting. Let n_i be the number of vertices of degree i. So

$$n = n_1 + n_2 + \cdots,$$

and the sum of degrees is

$$2e = n_1 + 2n_2 + 3n_3 + \cdots.$$

Define the degree of a face to be the number of edge sides that it meets. The smallest possible degree is 3. A face can meet an edge on two sides, so this edge contributes 2 to the degree of the face. In fact every edge contributes 2 to the sum of face degrees, so if f_i denotes the number of faces of degree i, then we have

$$f = f_3 + f_4 + \cdots,$$

and

$$2e = 3f_3 + 4f_4 + 5f_5 + \cdots.$$

Hence $2e - 3f = f_4 + 2f_5 \geq 0$.

28.3 Corollary. *If Γ is a connected planar graph with n vertices, e edges and f faces, then*

(1) $e \leq 3n - 6$.
(2) *Some vertex in Γ has degree ≤ 5.*

Proof. By Euler's formula, $f = 2 - n + e$, so

$$0 \leq 2e - 3f = 2e - 3(2 - n + e) = 3n - 6 - e,$$

which proves (1). For (2), assume all vertices have degree ≥ 6. Then

$$2e - 6n = n_7 + 2n_8 + \cdots$$

so

$$0 \leq (2e - 6n) + 2(2e - 3f) = -6(n - e + f) = -12,$$

a contradiction. □

A similar proof is of recent importance in chemistry. A **Fullerene graph** is a planar graph with all vertices of degree 3, and faces either hexagons or pentagons. The vertices represent carbon atoms, and the edges are bonds between carbon atoms. These isotopes of carbon were discovered in 1985 and chemists have since written hundreds of papers about them. The smallest is C_{60} with 60 vertices, and has the pattern of a soccer ball. Geometers (who knew about the graph of C_{60} for centuries before the molecule was discovered in nature) call it the "truncated icosahedron" since you can make it by slicing off each vertex from an icosahedron. Other known Fullerenes have 70, 72 and 84 vertices. The most basic fact about Fullerenes is the following consequence of Euler's formula.

28.4 Corollary. *A Fullerene has exactly 12 pentagons.*

Proof. Since every vertex has degree 3, we have $2e = 3n$. From Euler's formula, we get

$$4 = 2n - 2e + 2f = 2f - n.$$

On the other hand, the only face degrees are 5 and 6, so

$$f = f_5 + f_6, \qquad \text{and } 2e = 5f_5 + 6f_6.$$

So $f_5 = 6f - 2e = 6f - 3n = 3(2f - n) = 3 \cdot 4 = 12$. □

Chemists believe that for a Fullerene graph Γ to exist as a molecule in nature, no two pentagons in Γ can share a common vertex.