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Properties and Recent Applications in Spectral Graph Theory

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By

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To: David, Mom, Dad and Shannon. Thank you for all of you support and encouragement. I couldn't have done it without you.

To: Nikki and Will. Through determination and perseverance, you can achieve anything.

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Abstract

There are numerous applications of mathematics, specifically spectral graph theory, within the sciences and many other fields. This paper is an exploration of recent applications of spectral graph theory, including the fields of chemistry, biology, and graph coloring. Topics such as the isomers of alkanes, the importance of eigenvalues in protein structures, and the aid that the spectra of a graph provides when coloring a graph are covered, as well as others.

The key definitions and properties of graph theory are introduced. Important aspects of graphs, such as the walks and the adjacency matrix are explored. In addition, bipartite graphs are discussed along with properties that apply strictly to bipartite graphs.

The main focus is on the characteristic polynomial and the eigenvalues that it produces, because most of the applications involve specific eigenvalues. For example, if isomers are organized according to their eigenvalues, a pattern comes to light. There is a parallel between the size of the eigenvalue (in comparison to the other eigenvalues) and the maximum degree of the graph. The maximum degree of the graph tells us the most carbon atoms attached to any given carbon atom within the structure.

The Laplacian matrix and many of its properties are discussed at length, including the classical Matrix Tree Theorem and Cayley's Tree Theorem. Also, an alternative approach to defining the Laplacian is explored and compared to the traditional Laplacian.

CHAPTER 1: GRAPH THEORY

SECTION 1.1: INTRODUCTION TO GRAPH THEORY

A **graph** G is a finite nonempty set of points called **vertices**, together with a set of unordered pairs of distinct vertices called **edges**. The set of edges may be empty. The **degree** of a vertex *v*, deg(*v*), is the number of edges incident on *v*. A graph is **regular** if all vertices have equal degrees. A graph is considered a **complete graph** if each pair of vertices is joined by an edge.

In the example graph below, the set of vertices is V(G) = {a, b, c, d} while the set of edges is E(G) = {ab, ac, bc, bd, cd}. The graph is not complete because vertices *a* and *d* are not joined by an edge. deg(*a*) = 2 = deg(*d*), deg(*b*) = 3 = deg(*c*). Two vertices are **adjacent** if there is an edge that connects them. In Figure 1-1, vertices *a* and *c* are adjacent, while vertices *a* and *d* are not.

Graph G

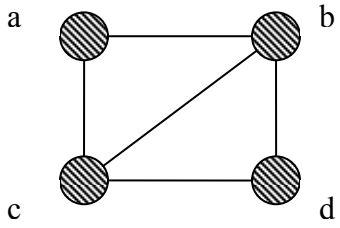


Figure 1-1

A wide variety of real world applications can be modeled using vertices and edges of a graph. Examples include electrical nodes and the wires that connect them, the stops and rails of a subway system and communication systems between cities. The cardinality of the vertex set V(G) is called the **order of G** and is denoted by *p*(G), or simply *p* when the context makes it clear. The cardinality of the edge set E(G) is called the **size of G**, and is usually denoted by *q*(G) or *q*. A graph G can be denoted as a G(p, q) graph.

A v_iv_j **walk** in G is a finite sequence of adjacent vertices that begins at vertex v_i and ends at vertex v_j. In Figure 1-1, a walk from *a* to *d* would be *acd*. Another walk from *a* to *d* is *abcd*. If each pair of vertices in a graph is joined by a walk, the graph is said to be **connected**. The **distance** between any two vertices in a graph is the number of edges "traced" on the shortest walk between the two vertices. The distance from *a* to *d* is 2. The maximum distance between all of the pairs of vertices of a graph is the **diameter** of the graph. In Figure 1-1, the distance between any two vertices is either 1 or 2, making 2 the diameter of G, or diam(G) = 2.

The vertices and edges may have certain attributes, such as color or weight. Also, the edges may have direction. When the edges are given direction we have a **digraph**, or **directed graph**, as shown below in Figure 1-2. Digraphs can be used to model road maps. The vertices represent landmarks, while the edges represent one-way or two-way streets.

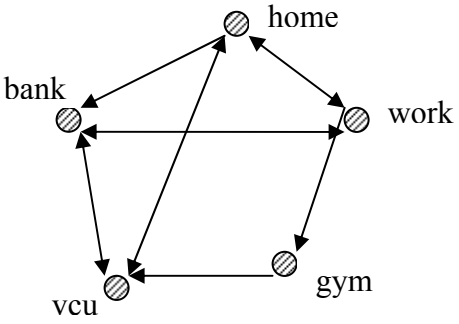
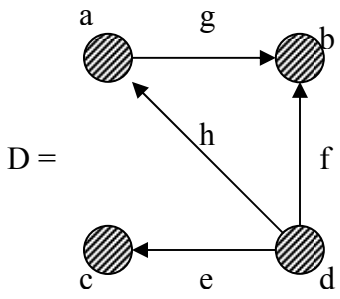


Figure 1-2

An **incidence matrix** associated with a digraph G is a $q \times p$ matrix whose rows represent the edges and columns represent the vertices. If an edge *k* starts at vertex *i* and ends at vertex *j*, then row *k* of the incidence matrix will have +1 in its (*k*, *i*) element, and –1 it its (*k*, *j*) element. All other elements are 0.



D =

$$I = \begin{array}{c} \\ e \\ f \\ g \\ h \end{array} \begin{array}{c} \begin{array}{cccc} a & b & c & d \end{array} \\ \begin{bmatrix} 0 & 0 & -1 & 1 \\ 0 & -1 & 0 & 1 \\ 1 & -1 & 0 & 0 \\ -1 & 0 & 0 & 1 \end{bmatrix} \end{array}$$

Figure 1-3

Example: A directed graph and its incidence matrix are shown above in Figure 1-3.

When two vertices are joined by more than one edge, like the example in Figure 1-4, it becomes a **multi-graph**.

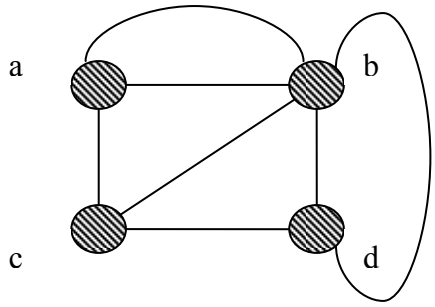


Figure 1-4

When a pair of vertices is not distinct, then there is a self-loop. A graph that admits multiple edges and loops is called a **pseudograph**. In the pseudograph below, edge *cc* is joining a pair of non-distinct vertices; therefore, there is a self-loop at vertex *c*.

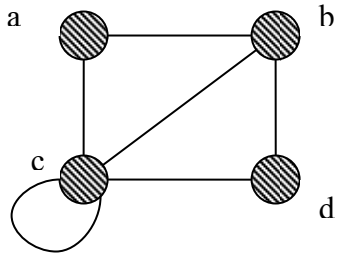


Figure 1-5

Graphs G and H are **isomorphic**, written G ≅ H, if there is a vertex bijection

f: V(G) → V(H) such that for all *u*, *v* ∈ V(G), *u* and *v* adjacent in G ⇔ f(*u*) and f(*v*) are adjacent in H. Likewise, *u* and *v* not adjacent in G ⇔ *f*(*u*) and *f*(*v*) are not adjacent in H.

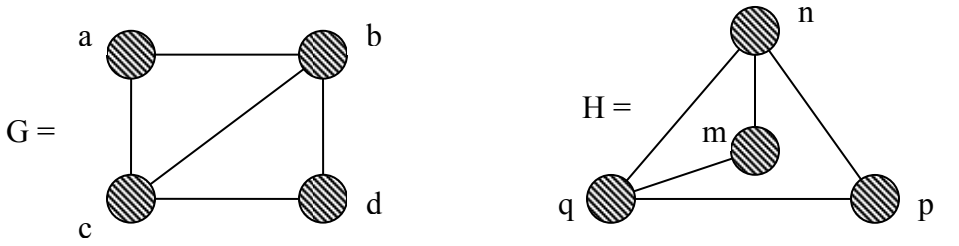


Figure 1-6

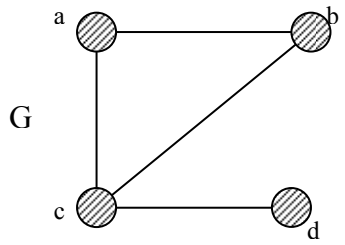
Graphs G and H are isomorphic, because a vertex bijection between them is: *f*(*a*) = *m*, *f*(*b*) = *n*, *f*(*c*) = *g*, and *f*(*d*) = *p*.

SECTION 1.2: ADJACENCY MATRICES

There is a great deal of importance and application to representing a graph in matrix form. One of the key ways to do this is through the **adjacency matrix**, **A**. The rows and columns of an adjacency matrix represent the vertices, and the elements tell whether or not there is an edge between any two vertices. Given any element, a_{ij},

$$a_{ij} = \begin{cases} 1 \text{ if } a_i \text{ and } a_j \text{ are connected} \\ 0 \text{ otherwise} \end{cases}$$

Example: A graph G with its adjacency matrix **A**.



$$A = \begin{array}{c} \\ a \\ b \\ c \\ d \end{array} \begin{array}{c} \begin{array}{cccc} a & b & c & d \end{array} \\ \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \end{array}$$

Figure 1-7

Notice that the diagonal of an adjacency matrix of a graph contains only zeros because there are no self-loops. Remember that our graphs have no multiple edges or loops. This causes the **trace** of the adjacency matrix, written $tr(\mathbf{A})$, the sum of its main diagonal, to be zero. Also, when A represents a graph, it is square, symmetric, and all of the elements are non-negative. In other words, $a_{ij} = a_{ji}$.

Property 1-1: The number of walks of length l from v_i to v_j in G is the element in position (i, j) of the matrix A^l [Bi, p9].

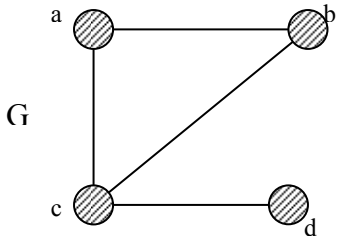
Proof: If $l = 0$, then the number of walks from v_i to v_j, $i \neq j$, is 0, making element

$(i, j) = 0$. The number of walks from any vertex to itself of length zero is 1, making element $(i, i) = 1$, giving us the identity matrix. $\mathbf{A}^0 = \mathbf{I}$, therefore it checks if $l = 0$. If $l = 1$, then $\mathbf{A}^1 = \mathbf{A}$, the adjacency matrix. Let Property 1-1 be true for $l = \mathrm{L}$. The set of walks of length L+1 from vertex v_i to vertex v_j is in bijective correspondence with the set of walks of length L from v_i to v_h adjacent to v_j. In other words, if there is a walk of length L from v_i to v_h, and v_h is adjacent to v_j, then there is a walk of length L+1 from v_i to v_j. The number of such walks is

$$\sum_{\{v_h, v_j\} \in E(G)} (A^L)_{ih} \;=\; \sum_{h=1}^{n} (A^L)_{ih}\, a_{hj} \;=\; (\mathbf{A}^{\mathrm{L+1}})_{\mathrm{ij}}$$

Therefore, the number of walks of length L+1 joining $\mathrm{v_i}$ to $\mathrm{v_j}$ is $(\mathbf{A}^{\mathrm{L+1}})_{ij}$. By induction, the property holds. □

Example: Look again at graph G and its adjacency matrix **A**:



$$A = \begin{array}{c} \\ a \\ b \\ c \\ d \end{array} \begin{array}{c} \begin{array}{cccc} a & b & c & d \end{array} \\ \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \end{array}$$

Figure 1-7

The number of walks from vertex *b* to vertex *d* of length 2 can be found by squaring matrix **A**.

$A^2 = \begin{bmatrix} 2 & 1 & 1 & 1 \\ 1 & 2 & 1 & 1 \\ 1 & 1 & 3 & 0 \\ 1 & 1 & 0 & 1 \end{bmatrix}$, therefore if we look at element (b, d) = element $(d, b) = 1$. There is one walk from *b* to *d* of length 2. That walk is *bcd*.

Likewise, $A^3 = \begin{bmatrix} 2 & 3 & 4 & 1 \\ 3 & 2 & 4 & 1 \\ 4 & 4 & 2 & 3 \\ 1 & 1 & 3 & 0 \end{bmatrix}$. Element (*a, c*) = element (*c, a*) = 4. Therefore, there are 4 walks of length 3 from vertex *a* to vertex *c*. These walks are: *acac, acdc, acbc, abac*.

Property 1-1 has two immediate corollaries. We list them as Property 1-2 and Property 1-3.

Property 1-2: The trace of $\mathbf{A}^2$ is twice the number of edges in the graph.

Proof: Let v_i be an arbitrary vertex of G. For every edge v_iv_j of G, by Property 1-1, we get a count of 1 towards the (i, j) position of $\mathbf{A}^2$. That is, the (i, j) position of $\mathbf{A}^2$ is equal to the degree of v_i, because every walk v_iv_i that involves only one v_iv_j edge will have a length of 2. This means: $tr(A^2) = \sum_{v_i \in V(G)} \deg(v_i) = 2q$. Recall, q equals the cardinality of the edge set of G. □

This can be seen in our example in Figure 1-7. $\mathbf{A}^2 = \begin{bmatrix} 2 & 1 & 1 & 1 \\ 1 & 2 & 1 & 1 \\ 1 & 1 & 3 & 0 \\ 1 & 1 & 0 & 1 \end{bmatrix}$. The trace of $\mathbf{A}^2$ is 8 and the number of edges is 4.

Property 1-3: The trace of $\mathbf{A}^3$ is six times the number of triangles in the graph.

Proof: Let v_i be an arbitrary vertex of G. For every 3-cycle v_iv_j of G, again by Property 1-1, we get a count of 1 towards the (i, j) position of $\mathbf{A}^3$. That is, the (i, j) position of $\mathbf{A}^3$ is equal to the number of 3-cycles that start and end at v_i. However, every 3-cycle $v_iv_jv_kv_i$ is counted six times because the vertices of the 3-cycle can be ordered in 6 ways. This means that $tr(\mathbf{A}^3) = 6$*(# of triangles)* in the graph. □

Again, let's test it with the graph from Figure 1-7. $\mathbf{A}^3 = \begin{bmatrix} 2 & 3 & 4 & 1 \\ 3 & 2 & 4 & 1 \\ 4 & 4 & 2 & 3 \\ 1 & 1 & 3 & 0 \end{bmatrix}$. The trace is 6 and the number of triangles in the figure is 1, illustrating Properties 1-2 and 1-3.

SECTION 1.3: THE CHARACTERISTIC POLYNOMIAL AND EIGENVALUES

The **characteristic polynomial**, Γ, of a graph of order *n* is the determinant $\det(\lambda\mathbf{I} - \mathbf{A})$, where **I** is the $n \times n$ identity matrix.

Example 1: given adjacency matrix

$$\mathbf{A} = \begin{array}{c} \\ a \\ b \\ c \end{array}\!\!\begin{array}{c} \begin{array}{ccc} a & b & c \end{array} \\ \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix} \end{array}$$

From graph G

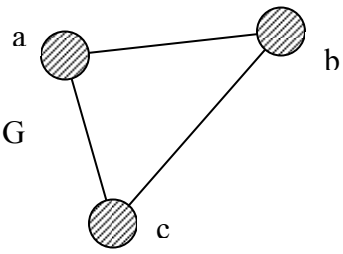


Figure 1-8

$$\Gamma = \det(\lambda I - A) = \det\left(\begin{bmatrix} \lambda & 0 & 0 \\ 0 & \lambda & 0 \\ 0 & 0 & \lambda \end{bmatrix} - \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix}\right) = \det\left(\begin{bmatrix} \lambda & -1 & -1 \\ -1 & \lambda & -1 \\ -1 & -1 & \lambda \end{bmatrix}\right) = \lambda^3 - 3\lambda - 2$$

The general form of any characteristic polynomial is

$$\lambda^n + c_1\lambda^{n-1} + c_2\lambda^{n-2} + \ldots + c_n \qquad \textbf{Equation 1}$$

Property 1-4: The coefficients of the characteristic polynomial that coincide with matrix A of a graph G have the following characteristics:

1) $c_1 = 0$
2) $-c_2$ is the number of edges of G
3) $-c_3$ is twice the number of triangles in G

Proof: For each $i \in \{1, 2, \ldots, n\}$, the number $(-1)^i c_i$ is the sum of those principal minors of **A** which have *i* rows and columns. So we can argue as follows:

1) Since the diagonal elements of **A** are all zero, $c_1 = 0$.

2) A principal minor with two rows and columns, and which has a non-zero entry, must be of the form $\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$. There is one such minor for each pair of adjacent vertices of the characteristic polynomial, and each has a value of – 1. Hence, $(-1)^2 c_2 = -|E(G)|$.

3) There are essentially three possibilities for non-trivial principal minors with three rows and columns: $\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix}$. Of these, the only non-zero one is the last one (whose value is two). This principal minor corresponds to three mutually adjacent vertices in Γ, and so we have the required description of c_3. [Bi, p8-9] □

Example: This can be seen from the characteristic polynomial of **A** above. $n = 4$

1) there is no λ^2, making $c_1 = 0$
2) $-c_2 = 3$. The number of edges of G is 4.
3) $-c_3 = 2$. The number of triangles in G is 1.

The characteristic polynomial is enormously important to spectral graph theory, because it is an algebraic construction that contains graphical information. It will be explored more in Chapter 2.

The roots of a characteristic polynomial are called the **eigenvalues**. Setting the characteristic polynomial $\lambda^3 - 3\lambda - 2$ from Example 1 equal to zero and solving gives us the eigenvalues $\{-1, -1, 2\}$. Eigenvalues are at the heart of understanding the properties and structure of a graph. We will also study them more in chapter 2.

Property 1-5: The sum of the eigenvalues of a matrix equals its trace.

Example: Let us consider a 2×2 adjacency matrix

$\mathbf{A} = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$. $\text{Det}(\mathbf{A} - \lambda\mathbf{I}) = \lambda^2 - (a + d)\lambda + (ad - bc)$. Applying the quadratic equation and setting b = c, we get $\lambda_1 = \frac{(a+d)+\sqrt{(a-d)^2+4b^2}}{2}$ and $\lambda_2 = \frac{(a+d)-\sqrt{(a-d)^2+4b^2}}{2}$. Adding the eigenvalues gives us $\lambda_1 + \lambda_2 = \frac{2a+2d}{2} = a + d =$ the sum of the diagonal, or *tr*(A). Similar computations can be applied to any adjacency matrix, regardless of the dimensions. □

The **algebraic multiplicity** of an eigenvalue is the number of times that the value occurs as a root of the characteristic polynomial. In example 1, the eigenvalue -1 has a multiplicity of 2 and the eigenvalue of 2 has a multiplicity of 1.

The eigenvectors that correspond to the eigenvalues are $\begin{bmatrix} -1 \\ -1 \\ 2 \end{bmatrix}, \begin{bmatrix} -1 & -1 & 1 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{bmatrix}$. The **geometric multiplicity** is the dimension of the **eigenspace**, or the subspace spanned by all of the eigenvectors.

Property 1-6: If a matrix is real symmetric, then each eigenvalue of the graph relating to that matrix is real.

Proof: The proof follows from the Spectral Theorem from Linear Algebra: Let **A** be a real, symmetric matrix. Then there exists an orthogonal matrix **Q** such that

$\mathbf{A} = \mathbf{Q}\,\mathbf{\Lambda}\,\mathbf{Q}^{-1} = \mathbf{Q}\,\mathbf{\Lambda}\,\mathbf{Q}^{T}$, where $\mathbf{\Lambda}$ is a real diagonal matrix. The eigenvalues of **A** appear on the diagonal of $\mathbf{\Lambda}$, while the columns of **Q** are the corresponding orthonormal eigenvectors. The entries of an adjacency matrix are real and the adjacency matrix is symmetric. Therefore, all of the eigenvalues of an adjacency matrix are real.

[Ol, p419] □

Property 1-7: The geometric and algebraic multiplicities of each eigenvalue of a real symmetric matrix are equal.

Property 1-8: The eigenvectors that correspond to the distinct eigenvalues are orthogonal (mutually perpendicular).

Note: When u and v are two orthogonal eigenvectors of **A** associated with two distinct eigenvalues λ and μ in that order, then the unit vectors $\frac{u}{\|u\|}$ and $\frac{v}{\|v\|}$ are orthonormal eigenvectors associated with λ and μ respectively.

Property 1-9: If a graph is connected, the largest eigenvalue has multiplicity of 1.

Let's check these properties with Example 1 from above:

$$\mathbf{A} = \begin{array}{c} \\ a \\ b \\ c \end{array} \begin{array}{c} \begin{array}{ccc} a & b & c \end{array} \\ \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix} \end{array}$$

From graph G

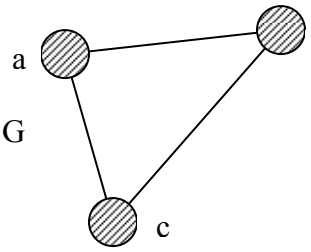


Figure 1-8

The eigenvalues are {– 1, – 1, 2}. All are real, demonstrating Property 1-6. The algebraic multiplicity of – 1 is two, and the algebraic multiplicity of 2 is one. The eigenvector that corresponds to the eigenvalue -1 is the linear combination of the vectors $\begin{bmatrix} -1 \\ 0 \\ 1 \end{bmatrix}, \begin{bmatrix} -1 \\ 1 \\ 0 \end{bmatrix}$. We can easily show that the two vectors are independent. This means the dimension of the subspace they span is 2. Thus the geometric multiplicity is also 2.

The eigenvector that corresponds to the eigenvalue 2 is $\begin{bmatrix}1\\1\\1\end{bmatrix}$. It spans a subspace of dimension one, giving geometric multiplicity of one. Thus, Property 1-7 holds.

To see if Property 1-8 maintains, we need to calculate whether or not the vectors corresponding to distinct eigenvalues are orthogonal.

Let $v_1 = \begin{bmatrix}-1\\0\\1\end{bmatrix}, v_2 = \begin{bmatrix}-1\\1\\0\end{bmatrix}$ and $v_3 = \begin{bmatrix}1\\1\\1\end{bmatrix}$. $\langle v_1, v_3\rangle = -1(1) + 0(1) + 1(1) = 0$ and $\langle v_2, v_3\rangle = -1(1) + 1(1) + 0(1) = 0$. Therefore, the vectors corresponding to the distinct eigenvalues are orthogonal. Using the Gram-Schmidt process we can get the orthonormal basis $u_1 = \begin{bmatrix}-\frac{\sqrt{2}}{2}\\ \frac{\sqrt{2}}{2}\\ 0\end{bmatrix}$, $u_2 = \begin{bmatrix}-\frac{\sqrt{6}}{6}\\ -\frac{\sqrt{6}}{6}\\ \frac{\sqrt{6}}{3}\end{bmatrix}$ spanning the same subspace spanned by v_1 and v_2. If we let $u_3 = \frac{v_3}{\|v_3\|} = \begin{bmatrix}\frac{\sqrt{3}}{3}\\ \frac{\sqrt{3}}{3}\\ \frac{\sqrt{3}}{3}\end{bmatrix}$ then we see that we have an orthonormal set. Property 1-9 applies because the largest eigenvalue is 2, and it has a multiplicity of one.

CHAPTER 2: SPECTRAL GRAPH THEORY

SECTION 2.1: INTRODUCTION

Spectral graph theory is a study of the relationship between the topological properties of a graph with the spectral (algebraic) properties of the matrices associated with the graph. The most common matrix that is studied within spectral graph theory is the adjacency matrix. L. Collatz and U. Sinogowitz first began the exploration of this topic in 1957 with their paper, Spektren Endlicher Grafen [Sp].

Originally, spectral graph theory analyzed the adjacency matrix of a graph, especially its eigenvalues. For the last 25 years, many developments have been leaning more toward the geometric aspects, such as random walks and rapidly moving Markov chains [Chu, p1].

A central goal of graph theory is to deduce the main properties and the structure of a graph from its invariants. The eigenvalues are strongly connected to almost all key invariants of a graph. They hold a wealth of information about graphs. This is what spectral graph theory concentrates on.

Remember, our definition of a graph from Chapter 1 does not admit self-loops or multi-edges.

SECTION 2.2: THE SPECTRUM OF A GRAPH

The **spectrum** of a graph G is the set of eigenvalues of G, together with their **algebraic multiplicities**, or the number of times that they occur.

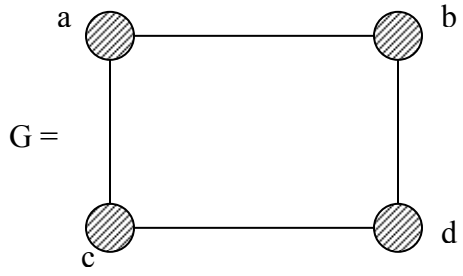
Property 2-1: A graph with *n* vertices has *n* eigenvalues.

Proof: This is a direct result of the Fundamental Theorem of Algebra. The characteristic polynomial of G with *n* vertices is a polynomial of degree *n*, and the Fundamental Theorem of Algebra states that every polynomial of degree *n* has exactly *n* roots, counting multiplicity, in the field of complex numbers.

If a graph has *k* distinct eigenvalues $\lambda_1 > \lambda_2 > \ldots > \lambda_k$ with multiplicities $m(\lambda_1), m(\lambda_2), \ldots m(\lambda_k)$, then the spectrum of G is written

$\text{Spec(G)} = \begin{pmatrix} \lambda_1 & \lambda_2 & \ldots & \lambda_n \\ m(\lambda_1) & m(\lambda_2) & \ldots & m(\lambda_n) \end{pmatrix}$, where $\sum_{i=0}^{k} \lambda_i = n$ [Bi, p8] □

Example:



$$M = \begin{array}{c} \\ a \\ b \\ c \\ d \end{array} \begin{array}{c} \begin{array}{cccc} a & b & c & d \end{array} \\ \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix} \end{array}$$

Figure 2-1

The characteristic polynomial is $4\lambda^4 - 4\lambda^2$ with eigenvalues $\{0, 0, 2, -2\}$. Our graph has three distinct eigenvalues: -2, 0, and 2, hence the spectrum of the graph G is given by $\text{Spec(G)} = \begin{pmatrix} -2 & 0 & 2 \\ 1 & 2 & 1 \end{pmatrix}$.

One consistent question in graph theory is: when is a graph characterized by its spectrum? [Do, p568] Properties that cannot be determined spectrally can be determined by comparing two nonisomorphic graphs with the same spectrum. Below are two graphs with the same spectrum.

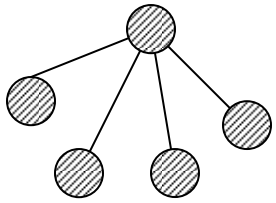
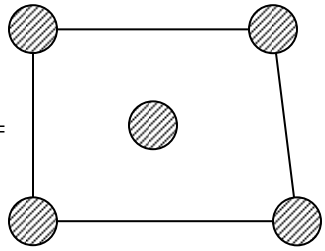
G =  H = 

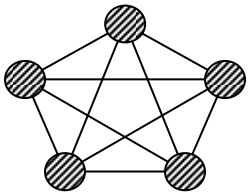
Figure 2-2

It is clear that the two graphs are structurally different, with different adjacency matrices, and yet they have the same spectrum, which is $\begin{pmatrix} -2 & 0 & 2 \\ 1 & 3 & 1 \end{pmatrix}$. We know that graphs with the same spectrum have the same number of triangles. The example above shows that both graphs have no triangles, but it also shows that graphs with the same spectrum do not necessarily have the same number of rectangles. While the first has no rectangle, the second one has one rectangle. Our example also shows that graphs with the same spectrum do not necessarily have the same **degree sequence** (the sequence formed by arranging the vertex degrees in non-increasing order). The degree sequence of graph G is <4, 1, 1, 1, 1> while that of H is <2, 2, 2, 2, 0>. Finally, our example also shows that connectivity cannot be determined by the spectrum. A graph is **connected** if for every pair of vertices *u* and *v*, there is a walk from *u* to *v*. Here the graph G is connected while graph H is not.

There is a correlation between the degree of the vertices of a graph and the largest eigenvalue, λ_1. When we have a *k*-regular graph (all vertices have degree *k*), then $\lambda_1 = k$.

When we have a complete graph (all vertices are adjacent to one another) with *n* vertices, $\lambda_1 = n - 1$. If G is a connected graph, then λ_1 is less than or equal to the largest degree of the graph. Also, λ_1 increases with graphs that contain vertices of higher degree. In addition, the degrees of the vertices adjacent to the vertex with the largest degree affect value of λ_1.

Example: Look at graphs G and H below.



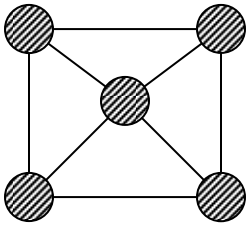
G

H

Figure 2-3

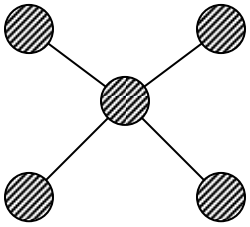
Both have 5 vertices. The degree of each vertex in G is 4; in other words, G is a complete graph, so $\lambda_1(G) = 4$. The second graph, H, is a path; the degrees of the vertices of H are 1 and 2, much smaller than that of G: $\lambda_1(H) = \sqrt{3} \approx 1.732$.

Example: Compare graphs G and H below, and their respective λ_1's. In each graph, the vertex with the highest degree has degree 4, but the adjacent vertices in G have degree 3, while in H they have degree 1. This illustrates how the degrees of the vertices adjacent to the vertex with the largest degree affect the value of λ_1.



G

$\lambda_1 = 1 + \sqrt{5} \approx 3.236$



H

$\lambda_1 = 2$

SECTION 2.3: BIPARTITE GRAPHS

A **bipartite graph** G is one whose vertex-set V can be partitioned into two subsets U and W such that each edge of G has one endpoint in U and one in W. The pair U, W is called the **bipartition** of G, and U and W are called the **bipartition subsets**. Bipartite graphs are also characterized as follows:

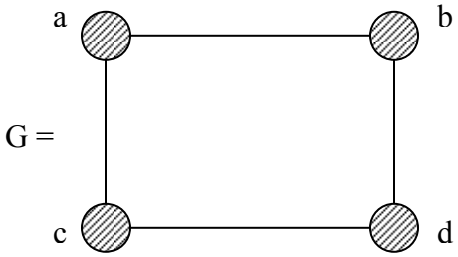
Property 2-2: A graph is bipartite if and only if it contains no odd cycles.

Proof: $\Rightarrow$ Let $v_1\ v_{2\ldots}\ v_k\ v_1$ be a cycle in a bipartite graph G; let's also assume, without loss of generality, that $v_1 \in$ U. Then, by definition of a bipartite graph, $v_2 \in$ W, $v_3 \in$ U, $v_4 \in$ W, . . . $v_k \in$ W, and k must be even. Therefore, the walk from v_1 to v_k is odd, and the cycle v_1 to v_1 is even.

$\Leftarrow$ Let's assume G is connected and without odd cycles. The case of G disconnected would follow from this special case. Consider a fixed vertex $v_0 \in$ V(G). Let V_i be the set of all vertices that are at distance i from v_0, that is

$V_i = \{ u \in V(G) | d(u, v_0) = i\}$, i = 0, 1, …, $t\}$, where t is the length of the longest path in G. Clearly t is finite since G is connected, and $V_0, V_1, \ldots, V_t$ provides a partition of the vertices of G. Let's observe that no two vertices in V_1 are adjacent, otherwise there will be a 3-cycle in G. Similarly, no two vertices in V_2 are adjacent because we do not have a 3-cycle or a 5-cycle. In fact every edge of G is of the form uv, where $u \in V_i$ and $v \in V_{i+1}$ for some i = 0, …, $t - 1$. Let $U = V_0 \cup V_2 \cup V_4 \cup \ldots \cup V_{2j}$, the union of all the even subscripted sets and $W = V_1 \cup V_3 \cup V_5 \cup \ldots \cup V_{2r+1}$, the union of all the odd subscripted sets. This shows that G is bipartite. □

Example: Graph G from Figure 2-1 below is a bipartite graph. The vertex subsets are U = {*a, d*}, W = {*b, c*}. Its characteristic polynomial is $\lambda^4 - 4\lambda$ and its eigenvalues are {-2, 0, 0, 2}.



$$M = \begin{array}{c} \\ a \\ b \\ c \\ d \end{array} \begin{array}{c} \begin{array}{cccc} a & b & c & d \end{array} \\ \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix} \end{array}$$

Figure 2-1

Example: Take also a look at the bipartite graph P_7, the path on 7 vertices.

Figure 2-4

It has the spectrum:

$$\left(-\sqrt{2+\sqrt{2}}, -\sqrt{2}, -\sqrt{2-\sqrt{2}}, 0, \sqrt{2-\sqrt{2}}, \sqrt{2}, \sqrt{2+\sqrt{2}}\right)$$

The eigenvalues of bipartite graphs have special properties.

Property 2-3: If G is bipartite graph and λ is an eigenvalue, then – λ is also an eigenvalue.

Proof: Let G be a bipartite graph. Let U = {u_1, u_2, . . . u_n} and W = {w_1, w_2, . . . w_n}, where U and W are the partite sets of V(G). Then all edges are of the form $u_i w_j$ where $u_i \in$ U and $w_j \in$ W. Also, there are no edges that go from u_i to u_j or from w_i to w_j for any *i, j*. This makes the adjacency matrix of G $\mathbf{A} = \begin{bmatrix} 0 & B \\ B^T & 0 \end{bmatrix}$, where **B** is an $n \times m$ matrix.

Because λ is an eigenvalue, we know $\mathbf{A}v = \lambda v$. So $\begin{bmatrix} 0 & B \\ B^T & 0 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \lambda \begin{bmatrix} x \\ y \end{bmatrix}$. Using simple

matrix multiplication, we get $\mathbf{By} = \lambda\mathbf{x}$. Multiplying both sides by negative one gives us $\mathbf{B}(-\mathbf{y}) = -\lambda\mathbf{x}$. The second equation that results from the matrix multiplication is $\mathbf{B^T x} = \lambda\mathbf{y}$, and $\lambda\mathbf{y} = (-\lambda)(-\mathbf{y})$. Therefore, $\mathbf{B^T x} = (-\lambda)(-\mathbf{y})$. This gives us the matrix equation

$$\begin{bmatrix} 0 & B \\ B^T & 0 \end{bmatrix}\begin{bmatrix} x \\ -y \end{bmatrix} = -\lambda\begin{bmatrix} x \\ -y \end{bmatrix}$$

giving us the eigenvalue $-\lambda$. □

Corollary 2-3-1: The spectrum of a bipartite graph is symmetric around 0. [Do, p558]. This logically follows from the theorem. The eigenvalues of a bipartite graph occur in pairs of additive inverses.

Recall from chapter one the general form of a characteristic polynomial is

$$\lambda^n + c_1\lambda^{n-1} + c_2\lambda^{n-2} + \ldots + c_n$$

Property 2-4: If G is a bipartite graph then $c_{2k-1} = 0$ for $n \geq 1$.

Proof: Since G is bipartite, by Property 2-2, there are no odd cycles in G. Thus, $c_{2n-1} = 0$ for $n \geq 1$. □

Let's check this with another bipartite graph.

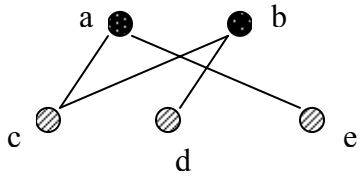
G = 

Figure 2-5

Its adjacency matrix is $\begin{bmatrix} 0&0&1&0&1 \\ 0&0&1&1&0 \\ 1&1&0&0&0 \\ 0&1&0&0&0 \\ 1&0&0&0&0 \end{bmatrix}$; with characteristic polynomial $\lambda^5 - 4\lambda^3 + 3\lambda$ and eigenvalues $\{-\sqrt{3}, -1, 0, 1, \sqrt{3}\}$. For every eigenvalue λ, $-\lambda$ is also an eigenvalue, as

stated in Theorem 2-2, and the eigenvalues are symmetric around zero. Looking at the characteristic polynomial, c_1 and c_3 are both zero as stated in Property 2-4.

SECTION 2.4: WALKS AND THE SPECTRUM

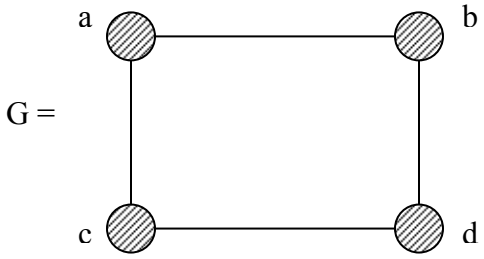
Recall that a $v_i v_j$ **walk** in G is a finite sequence of adjacent vertices that begins at vertex v_i and ends at vertex v_j. Also recall that $\mathbf{A}^k_{i,j}$ represents the number of walks of length k from vertex v_i to vertex v_j. This means, given vertices v_i and v_j with dist(v_i, v_j) = t in G, a graph with adjacency matrix **A**, we have $A^k_{i,j} = 0$, for $0 \leq k < t$, and $A^k_{i,j} \neq 0$.

A **minimal polynomial** of a graph G is the monic polynomial $q(x)$ of smallest degree, such that $q(G) = 0$. For example, if $f(x) = x^3(x - 5)^2(x + 4)^4$, the minimal polynomial for $f(x) = x(x - 5)(x + 4)$.

Property 2-5: The degree of the minimal polynomial is larger that the diameter.

Proof: Since **A** is symmetric, the minimum polynomial is given by $q(G{:}\lambda) = \prod(\lambda - \lambda_k)$, $1 \leq k \leq m$, where the λ_k's are all distinct. If we have m distinct eigenvalues, then the degree of the minimum polynomial is m. Suppose $m \leq d$, where d is the diameter of G and suppose i and j are two vertices of G whose distance is equal to m, then the (i, j) entry of $\mathbf{A}^m$ is positive while the (i, j) entry of $\mathbf{A}^k$ is 0 for all $k < m$. This means $q(G{:}A) \neq 0$, which is a contradiction, thus $m > d$. □

Example: Using the graph from Figure 2-1, we can see that the diameter of graph G is 2.



We found the characteristic polynomial is $4\lambda^4 - 4\lambda^2 = 4\lambda^2(\lambda^2 - 1)$. The minimal polynomial $4\lambda(\lambda^2 - 1)$ has degree 3, which is larger than the diameter of 2.

Property 2-6: If a graph G has diameter *d* and has *m* distinct eigenvalues, then $m > d + 1$.

Proof: This follows from Property 2-5. □

Example: Let's look at this with Example 1 from Chapter 1, below. We have already established that the diameter of this graph is 2, because the distance between any two vertices is either one or two.

Graph G

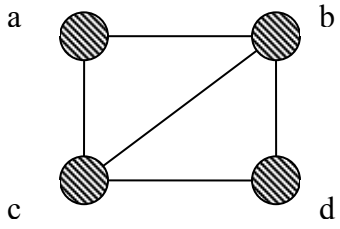


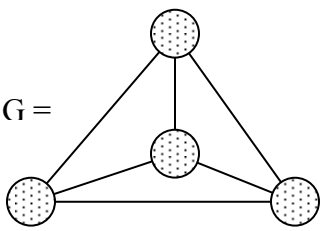
Figure 2-6

The adjacency matrix for G is $\mathbf{A} = \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix}$, giving us the characteristic polynomial $\lambda^4 - 5\lambda^2 - 4\lambda$ with the 4 eigenvalues {-1.56, -1, 0, 2.56}. There are 4 distinct eigenvalues, giving us $m = 4$. The diameter is 2. Therefore, $m > d + 1$.

A **complete graph** is one in which every pair of vertices is joined by an edge. A complete graph with *n* vertices is denoted by K_n.

Example: Two isomorphic K_4 graphs are

G =



H=

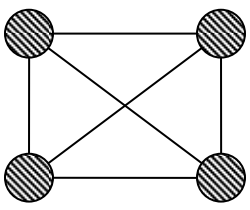


Figure 2-7

Property 2-7: The complete graph is the only connected graph with exactly two distinct eigenvalues.

Proof: If a graph has exactly 2 distinct eigenvalues, then its diameter has to be 1 or 0. Remember that two distinct eigenvalues means we have a minimal polynomial of degree 2. Also, the degree must be greater than the diameter. If the diameter is 0, then the graph is K_1. Otherwise, the graph is K_p for $p > 1$. □

Furthermore, the degree of the characteristic polynomial of a complete graph is p (giving us p eigenvalues). Using matrix algebra one can show that the characteristic polynomial for K_p is $(\lambda+1)^{p-1}(\lambda-p+1)$; then – 1 is a root of the characteristic polynomial with multiplicity p – 1 and the other root, which occurs once, is p – 1 [Sc, Wednesday AM].

In the example below, the matrix of the complete graph yields a characteristic polynomial of degree four. Note that – 1 occurs as a root 3 times, and 3 = 4 – 1 occurs once.

Example: The adjacency matrix from Graph G in figure 2-5 is $\mathbf{A} = \begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{bmatrix}$. G is a complete graph, and its characteristic polynomial is $\lambda^4 - 6\lambda^2 - 8\lambda - 3$ with eigenvalues {-1, 3} where -1 is a triple root and 3 is a single root. The graph has 4 vertices, 4 roots, and exactly two distinct roots.

Property 2-8: The complete graph K_p is determined by its spectrum.

Proof: This comes from Properties 2-1 and 2-7. If there are exactly two eigenvalues in the spectrum, then we know that the graph is a complete graph, and we know how many vertices the graph has based on the multiplicities of the eigenvalues. □

Example: Given Spec G = $\begin{pmatrix} 2 & -1 \\ 1 & 2 \end{pmatrix}$, we know that the graph is complete with three vertices, giving us the graph G in Figure 2-8.

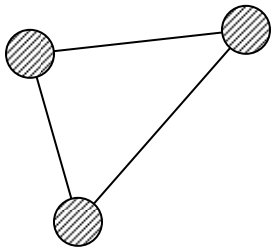
G = 

Figure 2-8

CHAPTER 3: THE LAPLACIAN

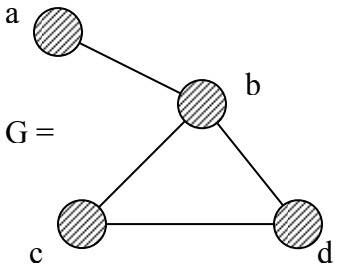
SECTION 3.1: INTRODUCTION

The Laplacian is an alternative to the adjacency matrix for describing the adjacent vertices of a graph. The **Laplacian, L,** of a graph is the square matrix that corresponds to the vertices of a graph [Do, p570]. The main diagonal of the matrix represents the degree of the vertex while the other entries are as follows:

$$\mathbf{A}_{ij} = \begin{cases} \text{-1 if } v_i \text{ and } v_j \text{ are adjacent} \\ 0 \quad \text{otherwise} \end{cases}$$

The Laplacian can also be derived from **D** – **A**, where **D** is the diagonal matrix whose entries represent the degrees of the vertices, and **A** is the adjacency matrix.

Example:



$$L = \begin{array}{c} \\ a \\ b \\ c \\ d \end{array} \begin{array}{c} \begin{array}{cccc} a & b & c & d \end{array} \\ \begin{bmatrix} 1 & -1 & 0 & 0 \\ -1 & 3 & -1 & -1 \\ 0 & -1 & 2 & -1 \\ 0 & -1 & -1 & 2 \end{bmatrix} \end{array}$$

Figure 3-1

The Laplacian of a connected graph has eigenvalues $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$. The **algebraic connectivity** is defined to be λ_2, the second smallest eigenvalue. The name is a result of its connection to the vertex connectivity and the edge connectivity of a graph. It is the most important information contained within the spectrum of a graph [Mo 2, p14] and will be discussed more in Chapter 4.

The oldest result about the Laplacian concerns the number of spanning trees of a graph [Do, p570]. The Matrix Tree Theorem is one of the most significant applications of the Laplacian, and is usually contributed to Kirchhoff. It is discussed in the next section.

A **positive semidefinite matrix** is one that is Hermitian, and whose eigenvalues are all non-negative. A Hermitian matrix is one which equals its conjugate transpose. This is usually written:

$$\mathbf{A}^{\mathrm{H}} = \overline{A^T} = \mathbf{A}.$$

Example: $B = \begin{bmatrix} 1 & 2+4i \\ 2-4i & 3 \end{bmatrix}$, then $\mathbf{B}^H = \mathbf{B}$. This means **B** is Hermitian. Here **B** is Hermitian but it is not symmetric. On the other hand, $\mathbf{C} = \begin{bmatrix} 1 & 2+4i \\ 2+4i & 3 \end{bmatrix}$, is symmetric but not Hermitian. On the other hand, a real matrix is symmetric if and only if it is Hermitian. This is because the every real number is its own conjugate. Here **A** is the real symmetric matrix $\mathbf{A} = \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$. If we look at each element, $a_{ij} = \overline{a_{ji}}$; its eigenvalues are $\{0, 2\}$.

The **characteristic function** is the function for which every subset N of X, has a value of 1 at points of N, and 0 at points of X – N. In other words, it takes the value of 1 for numbers in the set, and 0 for numbers not in the set.

Property 3-1: The smallest eigenvalue of **L** is 0.

Proof: This is a direct result of the Laplacian matrix being a positive semidefinite matrix. It will have *n* real Laplace eigenvalues: $0 = \lambda_1 \leq \lambda_2 \leq \ldots \lambda_n$. □

Property 3-2: The multiplicity of 0 as an eigenvalue of **L** is the number of connected components in the graph.

Proof: Let H be a connected component of graph G. Denote by $f^H \in R^V$ the characteristic function of V(H). Then, **L**(G) $f^H = 0$. Since the characteristic functions of different connected components are linearly independent, the multiplicity of the eigenvalue 0 is at least the number of connected components of G.

Conversely, let $f \in R^V$ be a function from the kernel of **L**(G). Then $\langle f, \mathbf{L}f \rangle = 0$, implying that f is constant on each connected component of G. Therefore f is a linear combination of the characteristic functions of connected components of G. [Mo 2, p6] □

Property 3-3: The algebraic connectivity is positive if and only if the graph is connected.

Proof: $\Rightarrow$ If $\lambda_2 > 0$ and $\lambda_1 = 0$, then G must be connected, because, as mentioned above, the eigenvalues of the Laplacian are $0 = \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$.

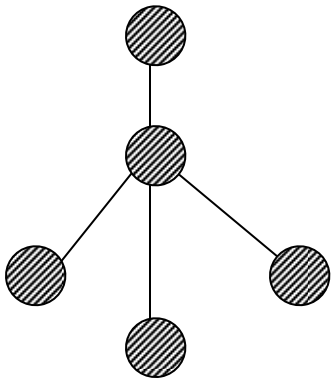
$\Leftarrow$ This is a direct result of Property 3-1. If G is connected, then zero is the smallest eigenvalue. λ_2 must be greater than zero, and therefore positive. □

When we have a k-regular graph, a graph whose vertices all have degree k, there is a linear relationship between the eigenvalues of the Laplacian and the eigenvalues of the adjacency matrix **A**. If $\theta_1 \leq \theta_2 \leq \ldots \leq \theta_n$ are the eigenvalues of **L** (Laplacian eigenvalues of G) and $\lambda_1, \lambda_2, \ldots \lambda_n$ are the eigenvalues of A (the adjacency matrix of G), then $\theta_i = k - \lambda_i$. This is a result of the graph being a regular graph, giving us the relationship $L = k\mathbf{I} - \mathbf{A}$ between the Laplacian and the adjacency matrix. No such relationship exists between the eigenvalues of the Laplacian and adjacency matrix of a non-regular graph.

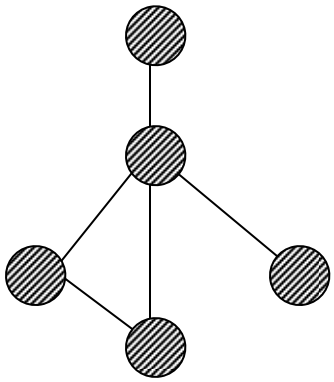
SECTION 3.2: SPANING TREES

In order to discuss spanning trees, we must first cover a few definitions. A **tree** is a connected graph that has no cycles.

Example:



A tree



Not a tree

Figure 3-2

A **subgraph** H of a graph G is a graph whose vertex and edge sets are subset of V(G) and E(G) in that order. A few subgraphs of the tree above are:

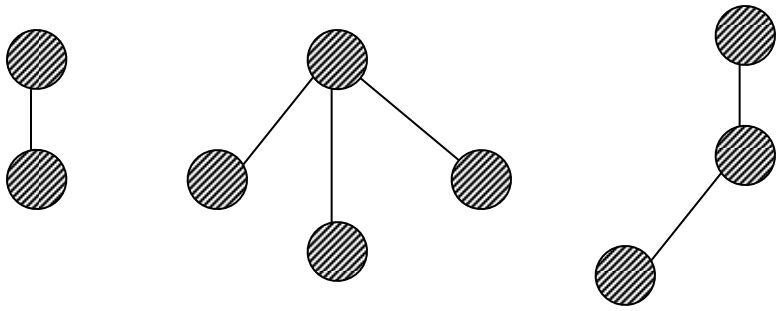
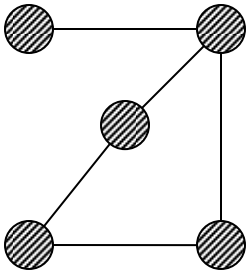
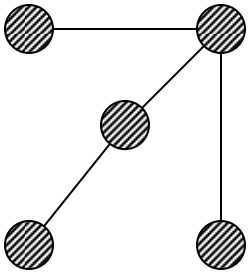


Figure 3-3

A subgraph H is said to **span** a graph G if V(H) = V(G). A **spanning tree** of a graph is a spanning subgraph that is a tree. Given graph G below, graph H is a spanning tree of G.



Graph G



Graph H

Figure 3-4

Before we go into the next few properties, we need to understand a cofactor of a matrix, which begins with the minor of a matrix. A **minor** $\mathbf{M}_{ij}$ of a matrix **B** is determined by removing row *i* and column *j* from **B**, and then calculating the determinant of the resulting matrix. The **cofactor** of a matrix is $(-1)^{i+j}\mathbf{M}_{ij}$.

Example: $\mathbf{B} = \begin{bmatrix} b_{11} & b_{12} & b_{13} & b_{14} \\ b_{21} & b_{22} & b_{23} & b_{24} \\ b_{31} & b_{32} & b_{33} & b_{34} \\ b_{41} & b_{42} & b_{43} & b_{44} \end{bmatrix}$. Minor $\mathbf{M}_{23}$ comes from deleting row 2 and column 3, and then calculating the determinant of the resulting matrix, $\begin{bmatrix} b_{11} & b_{12} & b_{14} \\ b_{31} & b_{32} & b_{34} \\ b_{41} & b_{42} & b_{44} \end{bmatrix}$.

$\mathbf{M}_{23} = b_{11}b_{32}b_{44} + b_{12}b_{34}b_{41} + b_{14}b_{42}b_{31} - b_{14}b_{32}b_{41} - b_{34}b_{42}b_{11} - b_{44}b_{31}b_{12}$.

Cofactor $\mathbf{C}_{23} = (-1)^{2+3}\mathbf{M}_{23}$

$= -b_{11}b_{32}b_{44} - b_{12}b_{34}b_{41} - b_{14}b_{42}b_{31} + b_{14}b_{32}b_{41} + b_{34}b_{42}b_{11} + b_{44}b_{31}b_{12}$

Also, given an $n \times n$ matrix **B**,

$\det(\mathbf{B}) = a_{1j}\mathbf{C}_{1j} + a_{2j}\mathbf{C}_{2j} + \ldots + a_{nj}\mathbf{C}_{nj} = a_{i1}\mathbf{C}_{i1} + a_{i2}\mathbf{C}_{i2} + \ldots + a_{in}\mathbf{C}_{in}$

= the sum of the cofactors multiplied by the entries that generated them.

Property 3-4, The Matrix Tree Theorem: Given a graph G, its adjacency matrix **A**, and its degree matrix **C**, the number of nonidentical spanning trees of G is equal to the value of any cofactor of the matrix **C – A**.

Proof: Let $\mathbf{D} = \mathbf{C} - \mathbf{A}$. The sum of the elements of any row i or any column i of $\mathbf{A}$ is the degree of vertex v_i. Therefore, the sum of any row i or column i of matrix $\mathbf{D}$ is zero. It is a result of matrix theory that all cofactors of $\mathbf{D}$ have the same value.

Let G be a disconnected matrix of order p. Let G_n be a subgraph of G whose vertex set is $\{v_1, v_2, \ldots, v_n\}$. Let $\mathbf{D}'$ be the $(p-1) \times (p-1)$ matrix that results from deleting row p and column p from matrix $\mathbf{D}$. Since the sum of the first n rows of $\mathbf{D}'$ is the zero vector with $p-1$ entries, the rows of $\mathbf{D}'$ are linearly dependent, implying that $\det(\mathbf{D}') = 0$. Hence, one cofactor of $\mathbf{D}$ has value zero. Zero is also the number of spanning trees of G, since G is disconnected.

Now let G be a connected (p, q) graph where $q \geq p - 1$. Let $\mathbf{B}$ denote the incidence matrix of G and in each column of $\mathbf{B}$, replace one of the two nonzero entries by -1. Denote the resulting matrix by $\mathbf{M} = [m_{ij}]$. We now show that the product of $\mathbf{M}$ and its transpose $\mathbf{M}^T$ is $\mathbf{D}$. The (i, j) entry of $\mathbf{M}\mathbf{M}^T$ is $\sum_{k=1}^{q} m_{ik} m_{jk}$, which has the value deg v_i if $i = j$, the value -1 if $v_i v_j \in E(G)$, and 0 otherwise. Therefore, $\mathbf{M}\mathbf{M}^T = \mathbf{D}$.

Consider a spanning subgraph H of G containing $p - 1$ edges. Let $\mathbf{M}'$ be the $(p-1) \times (p-1)$ submatrix of $\mathbf{M}$ determined by the columns associated with the edges of H and by all rows of $\mathbf{M}$ with one exception, say row k.

We now need to determine the determinant of $\mathbf{M}'$. If H is not connected, then H has a component, H*, not containing v_k. The sum of the row vectors of $\mathbf{M}'$ corresponding to the vertices of H* is the zero vector with $p - 1$ entries. Hence, $\det \mathbf{M}' = 0$. Now assume H is connected. H is then a spanning tree of G. Let $h_1 \neq v_k$ be an end-vertex of H, and e_1 the edge incident with it. Also, let $h_2 \neq v_k$ be an end-vertex of the tree

H – h_1 and e_2 the edge of H – e_1 incident with e_2. We continue this process until finally only v_k remains. A matrix $\mathbf{M}'' = [\, m''_{ij} \,]$ can now be obtained by a permutation of the rows and columns of **M** such that $|\, m''_{ij} \,| = 1$ if and only if u_i and e_i are incident. From the manner in which $\mathbf{M}''$ was defined, any vertex u_i is incident only with edges e_j, where $j \leq i$. This, however, implies that $\mathbf{M}''$ is lower triangular, and since $|\, m''_{ij} \,| = 1$ for all i, we conclude that $\det(\mathbf{M}'') = 1$. However, the permutation of rows and columns of a matrix affects only the sign of its determinant, implying that $\det(\mathbf{M}') = \det(\mathbf{M}'') = 1$.

Since every cofactor of **D** has the same value, we evaluate only the i^{th} principal cofactor. That is, the determinant of the matrix obtained by deleting from **D** row i so that the aforementioned cofactor equals $\det(\mathbf{M}_i\mathbf{M}_i^{\mathrm{T}})$, which implies that this number is the sum of the products of the corresponding major determinants of $\mathbf{M}_i$ and $\mathbf{M}_i^{\mathrm{T}}$. However, corresponding major determinants have the same value and their product is 1 if the defining columns correspond to a spanning tree of G and is 0 otherwise. [Cha, p66] □

A key result to the Matrix Tree Theorem is Cayley's Tree Formula.

Corollary 3-4-1, Cayley's Tree Formula: The number of different trees on n labeled vertices is n^{n-2}.

Proof: Start with the matrix (**D** – **A**) of a complete graph; we get an $n \times n$ matrix **M** with $m_{ij} = \begin{cases} n-1, & i = j \\ -1, & otherwise \end{cases}$. Calculating the determinant of a cofactor of **M** gives us n^{n-2}. From the Matrix Tree Theorem this number is the number of spanning trees. □

SECTION 3.3: AN ALTERNATIVE APPROACH

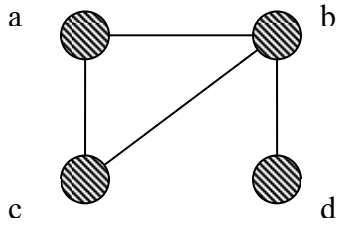
There is an alternative way of defining eigenvalues. We can define them in their "normalized" form. One advantage to this definition is that it is consistent with eigenvalues in spectral geometry and in stochastic processes [Chu, p2]. It also allows results which were only known for regular graphs to be generalized to all graphs. We will use **NL** to represent the Laplacian calculated using this definition.

In a graph where d_v represents the degree of vertex v, the Laplacian would be defined to be the matrix

$$\mathbf{NL}(u, v) \begin{cases} 1 & \text{if } u = v \text{ and } d_v \neq 0 \\ \dfrac{-1}{\sqrt{d_u d_v}} & \text{if } u \text{ and } v \text{ and adjacent} \\ 0 & \text{otherwise} \end{cases}$$

Example:

Graph G



$$\mathbf{NL} = \begin{bmatrix} 1 & \frac{-1}{\sqrt{6}} & \frac{-1}{2} & 0 \\ \frac{-1}{\sqrt{6}} & 1 & \frac{-1}{\sqrt{6}} & \frac{-1}{\sqrt{3}} \\ \frac{-1}{2} & \frac{-1}{\sqrt{6}} & 1 & 0 \\ 0 & \frac{-1}{\sqrt{3}} & 0 & 1 \end{bmatrix}$$

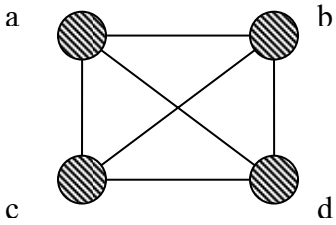
Figure 3-5

When graph G is a k-regular graph, it is easy to see that $\mathbf{NL} = \mathbf{I} - \frac{1}{k}\mathbf{A}$. The degree of each vertex is k, so $\sqrt{d_u d_v} = k$. Every entry of **A** that has a 1 will become $\frac{1}{k}\mathbf{A}$, and when we subtract that from **I**, we get $\frac{-1}{k}$ for all vertices that are adjacent. The non-adjacent

elements will be 0 for both **I** and **A**. The diagonal entries of **I** are 1, and the diagonals of **A** (and therefore $\frac{-1}{k}\mathbf{A}$) are 0, giving us 1 when we subtract $\mathbf{I} - \frac{-1}{k}\mathbf{A}$.

Example:

Graph G



$$\mathbf{NL} = \begin{bmatrix} 1 & \frac{-1}{3} & \frac{-1}{3} & \frac{-1}{3} \\ \frac{-1}{3} & 1 & \frac{-1}{3} & \frac{-1}{3} \\ \frac{-1}{3} & \frac{-1}{3} & 1 & \frac{-1}{3} \\ \frac{-1}{3} & \frac{-1}{3} & \frac{-1}{3} & 1 \end{bmatrix} = \mathbf{I} - \frac{1}{3}\mathbf{A}$$

Figure 3-6

Let **S** be a matrix whose rows represent the vertices of a graph G and whose columns represent the edges of G. Each column corresponding to an edge $e = uv$ has an entry of $\frac{1}{\sqrt{d_u}}$ in the row corresponding to vertex u and an entry of $\frac{-1}{\sqrt{d_v}}$ in the row corresponding to vertex v. All other entries in the column will be zero.

Property 3-5: $\mathbf{NL} = \mathbf{S}\,\mathbf{S}^{\mathrm{T}}$.

Proof: This is a direct result of their definitions. When we multiply an element u of **S** by an element v of $\mathbf{S}^{\mathrm{T}}$, and there exists an edge uv, then we are multiplying $\frac{1}{\sqrt{d_u}} \times \frac{-1}{\sqrt{d_v}} = \frac{-1}{\sqrt{d_u d_v}} =$ corresponding element in **NL**. If there is no edge uv, then the entries in **S**, $\mathbf{S}^{\mathrm{T}}$, and **NL** are zero. □

Example:

G =

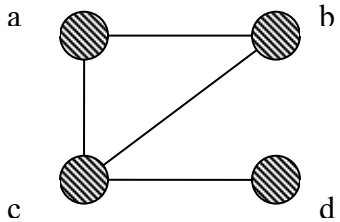


Figure 3-7

$$\mathbf{NL} = \begin{bmatrix} 1 & \frac{-1}{2} & \frac{-1}{\sqrt{6}} & 0 \\ \frac{-1}{2} & 1 & \frac{-1}{\sqrt{6}} & 0 \\ \frac{-1}{\sqrt{6}} & \frac{-1}{\sqrt{6}} & 1 & \frac{-1}{\sqrt{3}} \\ 0 & 0 & \frac{-1}{\sqrt{3}} & 1 \end{bmatrix} \cdot \mathbf{S} = \begin{array}{c} \\ a \\ b \\ c \\ d \end{array} \begin{array}{c} \begin{array}{cccc} ab & ac & bc & cd \end{array} \\ \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 \\ \frac{-1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{-1}{\sqrt{3}} & \frac{-1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \\ 0 & 0 & 0 & 1 \end{bmatrix} \end{array}$$

$$\mathbf{S} \times \mathbf{S}^{\mathrm{T}} = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 \\ \frac{-1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{-1}{\sqrt{3}} & \frac{-1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \\ 0 & 0 & 0 & 1 \end{bmatrix} \times \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} & 0 & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{-1}{\sqrt{3}} & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{3}} & 0 \\ 0 & 0 & \frac{1}{\sqrt{3}} & 1 \end{bmatrix} = \begin{bmatrix} 1 & \frac{-1}{2} & \frac{-1}{\sqrt{6}} & 0 \\ \frac{-1}{2} & 1 & \frac{-1}{\sqrt{6}} & 0 \\ \frac{-1}{\sqrt{6}} & \frac{-1}{\sqrt{6}} & 1 & \frac{-1}{\sqrt{3}} \\ 0 & 0 & \frac{-1}{\sqrt{3}} & 1 \end{bmatrix} = \mathbf{NL}$$

Property 3-6: 0 is an eigenvalue of **NL**.

Proof: Let g denote an arbitrary function which assigns to each vertex v of G a real value $g(v)$. We can view g as a column vector. Then $\frac{\langle g, Lg\rangle}{\langle g, g\rangle} = \frac{\langle g, T^{-1/2}LT^{-1/2}g\rangle}{\langle g, g\rangle}$ where **T** = the diagonal matrix where the entries are the degrees of the vertices, and **L** is the "regular" Laplacian. $g = \mathbf{T}^{1/2}f$ and $\sum_{u\sim v}$ = the sum over all unordered pairs $\{u, v\}$ for which u and v are adjacent. $\sum_x f(x)g(x)$ denotes the standard inner product in $\Re^n$. Then

$$\frac{\langle g, Lg\rangle}{\langle g, g\rangle} = \frac{\langle g, T^{-1/2}LT^{-1/2}g\rangle}{\langle g, g\rangle} = \frac{\langle f, Lf\rangle}{\langle T^{1/2}f, T^{1/2}f\rangle} = \frac{\sum_{u\sim v}(f(u)-f(v))^2}{\sum_v f(v)^2 d_v}$$ [Chu, p 4],

which = 0 when f(u) = f(v). This also shows us how all eigenvalues are nonnegative. Therefore the spectrum of **NL** is the set of eigenvalues $0 = \lambda_0 \le \lambda_1 \le \ldots \le \lambda_{n-1}$. □

When we use this normalized definition of the Laplacian for a graph with n vertices and no isolated vertices, a few properties unfold.

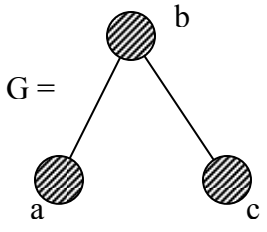
Property 3-7: $\sum_i \lambda_i \le n$

Proof: $\sum_i \lambda_i = tr(\mathbf{NL})$, the trace of **NL**. If the graph is connected, then $tr(\mathbf{NL}) = n$, because each element of the diagonal is 1, and we have an $n \times n$ matrix. If the graph is disconnected, then one or more elements of the diagonal will be zero, causing the sum of the diagonals to be less than n, and giving us a $tr(\mathbf{NL}) < n$. □

Property 3-8: For $n \ge 2$, $\lambda_1 \le \frac{n}{n-1}$ and $\lambda_{n-1} \ge \frac{n}{n-1}$

Proof: Assume that $\lambda_1 > \frac{n}{n-1}$; since all the remaining n -2 eigenvalue in the spectrum are at least as large as λ_1 their sum $\sum_i \lambda_i > n$. This contradicts Property 3.7; thus $\lambda_1 \le \frac{n}{n-1}$. Similarly assume that $\lambda_{n-1} < \frac{n}{n-1}$; since this eigenvalue is the largest in the spectrum, and λ_0 is established to be 0, the sum of the n eigenvalues $\sum_i \lambda_i < n$. This again contradicts Property 3.7 and therefore $\lambda_{n-1} \ge \frac{n}{n-1}$. □

Let's look at Figure 3-8, a very simple example, and apply these properties.

G = 

NL = $\begin{bmatrix} 1 & \frac{-1}{\sqrt{2}} & 0 \\ \frac{-1}{\sqrt{2}} & 1 & \frac{-1}{\sqrt{2}} \\ 0 & \frac{-1}{\sqrt{2}} & 1 \end{bmatrix}$

Figure 3-8

The characteristic polynomial is $\lambda^3 - 3\lambda^2 + 2\lambda$, yielding eigenvalues {0, 1, 2}. Property 3-6 holds, since 0 is an eigenvalue. The sum of the eigenvalues is 3, so property 3-7 holds, and $\lambda_2 = 2 \geq \frac{3}{2}$, which demonstrates Property 3-8.

CHAPTER 4: APPLICATIONS

SECTION 4.1: CHEMICAL APPLICATIONS

Recall that the eigenvalues of **L**(G), the Laplacian matrix of graph G are $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$ where $\lambda_n = 0$ and $\lambda_{n-1} > 0$ if and only if G is connected. Also recall that a tree is a connected acyclic graph.

A chemical tree is a tree where no vertex has a degree higher than 4. Chemical trees are molecular graphs representing constitutional isomers of alkanes. If there are *n* vertices, each chemical tree represents a particular isomer of C_nH_{2n+2}. The first four are methane, ethane, propane, and butane. After that, the alkanes are named based on Greek numbers. For example, C_5H_{12} is pentane. Compounds whose carbons are all linked in a row, like the two below, are called **straight-chain alkanes**. For example, if $n = 1$, we have the graph in Figure 4-1, which represents methane.

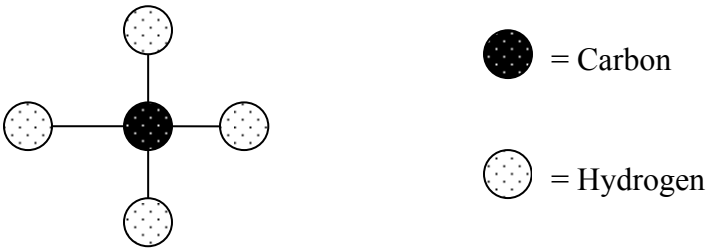


Figure 4-1
Methane

Figure 4-2 shows us butane, which is C_4H_{10}.

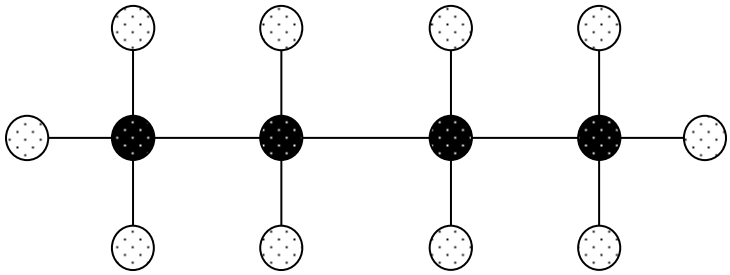


Figure 4-2
Butane

Compounds that have the same formula, but different structures, are called **isomers**. When C_4H_{10} is restructured as in Figure 4-3, we have isobutane, or 2-Methylpropane. Butane and 2-Methylpropane are isomers.

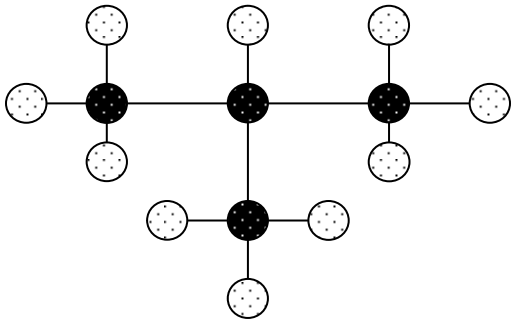


Figure 4-3
Isobutane or
2-Methylpropane

Compounds with four carbons have 2 isomers, while those with five carbons have 3 isomers. The growth, however, is not linear. The chart below compares the number of carbons with the number of isomers.

Formula	Number of Isomers
C_6H_{14}	5
C_7H_{16}	9
C_8H_{18}	18
C_9H_{20}	35
$C_{10}H_{22}$	75
$C_{15}H_{32}$	4,347
$C_{20}H_{42}$	366,319

[Mc, p76]

When a carbon has four carbons bonded to it, we have a **quarternary** carbon. An example is below in Figure 4-4, which is called a 2,2-Dimetylpropane. It is isomeric to Pentane.

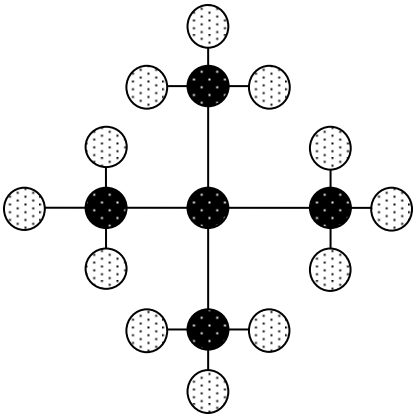


Figure 4-4

For simplicities sake, we will just draw the carbon atoms from this point on, with the understanding that there are enough hydrogen atoms attached to each carbon to give that carbon atom a degree of 4.

Study was done on the eigenvalues of molecular graphs, and in particular, λ_1, the largest eigenvalue of a graph. When the isomeric alkanes are ordered according to their λ_1 values, regularity is observed. [Gu, p 408]

Let Δ denote the maximum degree of a graph. The chemical trees that pertain to the 18 isomeric octanes C_8H_{18} follow a pattern with respect to their largest eigenvalue, λ_1. The isomer with the smallest λ_1 (3.8478) value is the straight-chain octane in Figure 4-5, that has $\Delta = 2$.

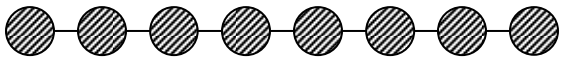


Figure 4-5

The next 10 isomers have various extensions of branching, but none possess a quaternary carbon atom. All of them have $\Delta = 3$, and their λ_1's are greater than that of the straight-chain graph in Figure 4-5, where $\Delta = 2$, and less than the following seven, who have $\Delta = 4$. They are shown below in Figure 4-6.

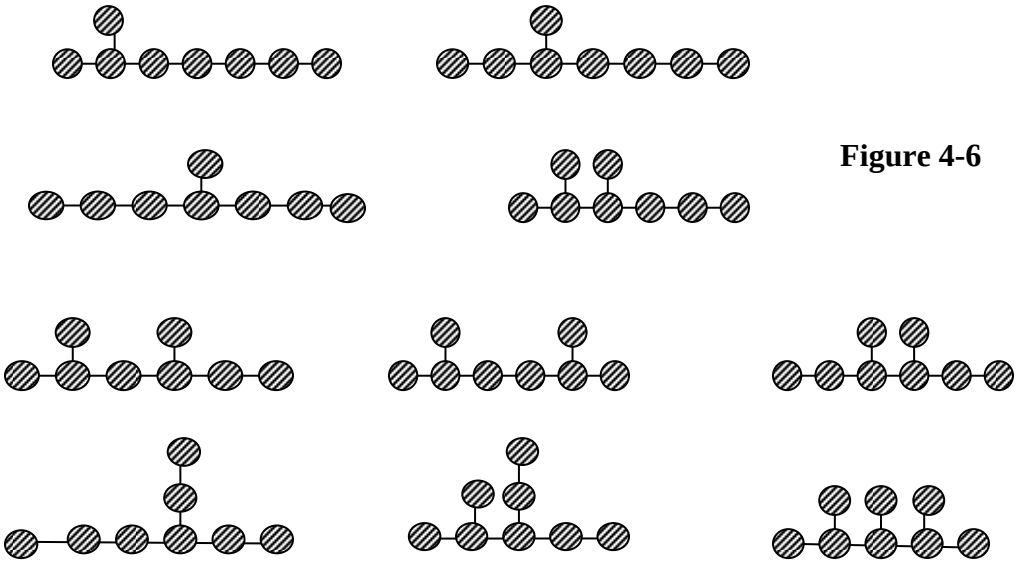


Figure 4-6

The 12th through the 18th octanes contain a quaternary carbon atom, they all have $\Delta = 4$, and they have the largest λ_1. The largest one has $\lambda_1 = 5.6458$ and is the last tree shown below in Figure 4-7.

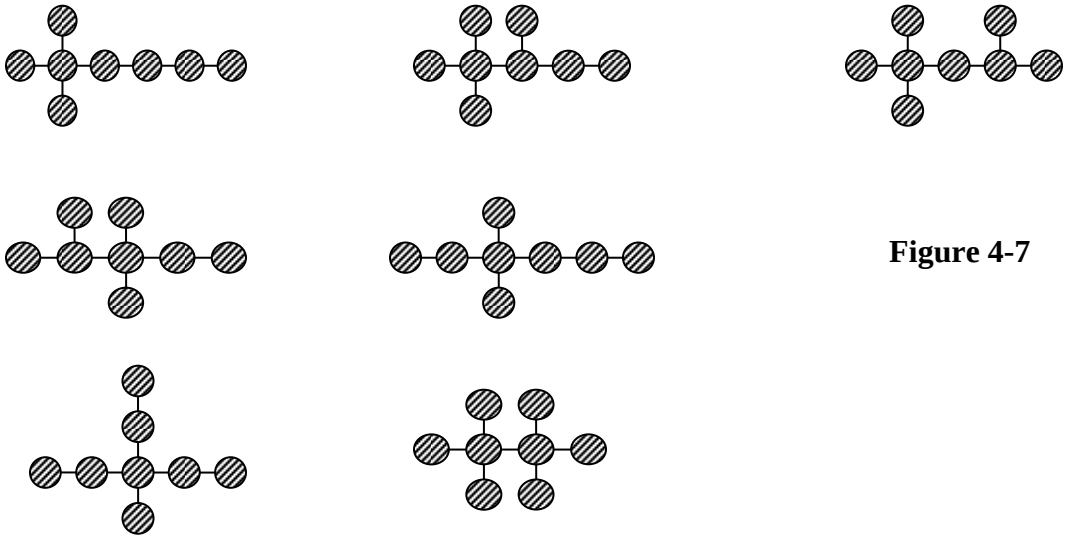


Figure 4-7

This same regularity occurs with isomeric alkanes with *n* carbon atoms, discussed above. The normal alkane with $\Delta = 2$ has the smallest λ_1. All alkanes with $\Delta = 3$ have λ_1 greater than the alkanes with $\Delta = 2$, and smaller than any isomer with $\Delta = 4$. We can therefore draw the conclusion that Δ, which tells us whether or not there is a quaternary

carbon atom, is the main molecular structure descriptor affecting the value λ_1, the largest Laplacian eigenvalue of an alkane. It has been discovered that λ_1 can be bounded by

$$\Delta + 1 < \lambda_1 < \Delta + 1 + 2\sqrt{\Delta - 1}$$

Also, by using a linear combination of the lower and upper bounds, λ_1 can be estimated by

$$\lambda_1 \approx \Delta + 1 + \gamma\sqrt{\Delta - 1},$$

where γ depends on both n and Δ. For alkanes, it has been discovered through numerical testing that $\gamma \approx 0.2$. [Gu p 410]

It is possible to establish the alkane isomers with $\Delta = 3$ or $\Delta = 4$ that have the minimal λ_1. Give P_n, below, T_n^{min} is the tree that establishes the minimal λ_1 for $\Delta = 3$, and Q_n^{min} is the tree that establishes the minimal λ_1 for $\Delta = 4$.

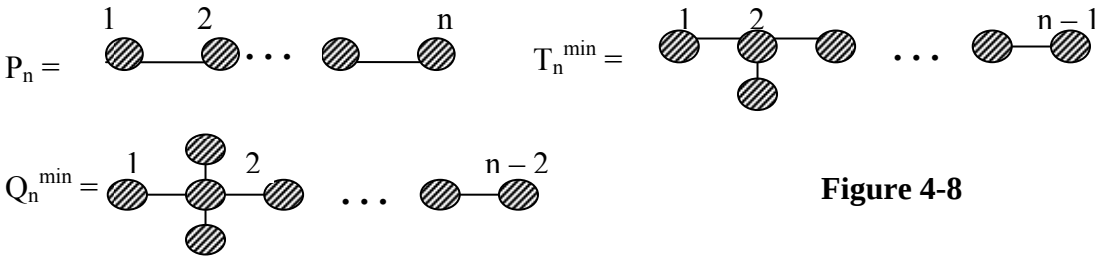


Figure 4-8

The structure trees that represent the maximal λ_1 are more complex. The T_n^{max} and Q_n^{max} coincide with the chemical trees that have the same Δ and n, having maximal λ_1 and minimal W, where W represents the Wiener topological index of alkanes, and conforms to the formula $W = n\sum_{i=1}^{n-1}\frac{1}{\lambda_i}$. The exact characterizations of these trees are complex, and will not be covered here.

SECTION 4.2: PROTEIN STRUCTURES

The three dimensional structure of proteins is the key to understanding their function and evolution [Vi, p10]. There are an enormous number of proteins in nature, but a limited number of three-dimensional structures that represent them. A protein is formed by the sequential joining of amino acids, end-to-end, to form a long chain-like molecule, or polymer. These polymers are referred to as polypeptides. There are four major protein classes, shown below in Figure 4-9. [Vi, p13] The cylinders represent helices (plural for helix) and the arrows represent strands. A helix is a spiral molecule formed from benzene rings. Two of the current challenges are identifying the fold adopted by the polypeptide chain, and identifying similarities in protein structures.

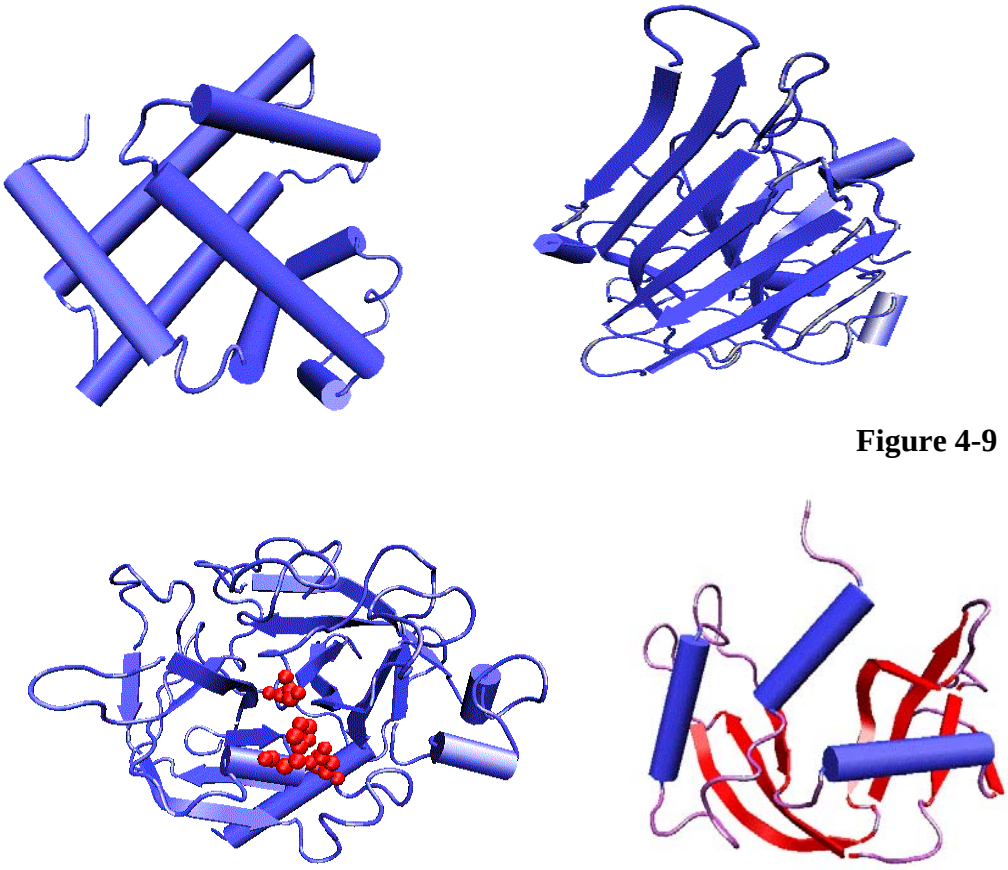


Figure 4-9

Analysis of stable folded three-dimensional structures provides insights into protein structures for amino acid sequences and drug design studies. The geometry of a protein structure is the composition of the protein backbone and side-chains. Protein structures can have the same gross shape, but have different geometries. Graphs have helped represent the topology of protein structures, no matter how complex. The main problem is to define the vertices and edges. Below are a few simple examples of proteins with their graphs below them.

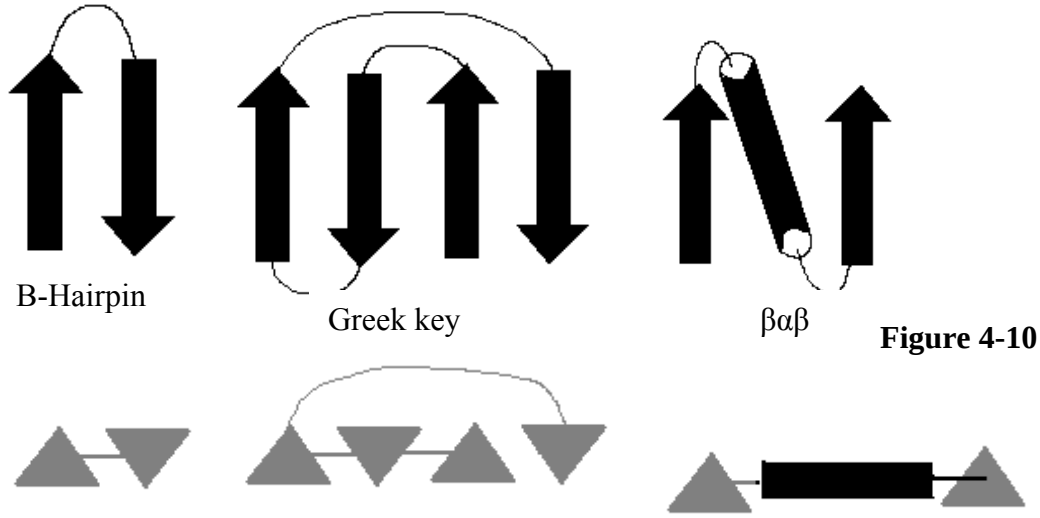


Figure 4-10

Properties of graphs and their graph spectral give information about protein structure, depending on how the vertices and edges are defined. The basic unit of a protein is its amino acid residue. To study cluster identification, the amino acids represent the vertices and the three-dimensional connectivity between them is represented by the edges. To study fold and pattern identification and the folding rules of proteins, α-helixes and β-strands are used for vertices and spatially closed structures are used for edges. To identify proteins with similar folds, the backbones are the vertices and the spatial neighbors within a certain radius are the edges.

Mathematical graphs are used to represent β structures, which is much more advantageous that drawing three-dimensional figures. The vertices represent the single β-strands and the two edge sets represent the sequential and hydrogen bond connections.

Connected graphs are used to represent α-helical structures. The vertices represent secondary structures and the edges represent contacts between helices. The main reason for setting the structures up this way was to gain information about the folding process of protein structures and understand better the organization and patterns within these structures. It is also used to compare protein structures. The protein connectivity is determined by identifying the main chain atoms, which is found due to the closeness within a prescribed distance. This comes from identifying clusters.

Two protein graphs can be compared to see if they have common features, and thus provide insight into structural overlaps of proteins. One way is a tree searching algorithm, which is a series of matrix permutations. Through it, subgraph isomorphisms are detected to determine the largest subgraph that is common in a pair of graphs. This can highlight areas of structural overlap & therefore show structural and functional commonalities not found through other methods. Unfortunately, this method requires a very high number of computations, but a few heuristic methods have been discovered to reduce the time and cost of the computations.

Structural biologists are continuously finding promising applications of graph theory with optimism that this field of mathematics will continually contribute substantially to the understanding of protein structure, folding stability, function and dynamics. Certainly, there is more to come.

SECTION 4.3: GRAPH COLORING

One of the classic problems in graph theory is vertex-coloring, which is the assignment of colors to the vertices of a graph in such a way that no two adjacent vertices have the same color. The object is to use as few colors as possible. The proper coloring of a graph also forms a natural partition of the vertex set of a graph. The **chromatic number,** χ(G), is the least number of colors required for such a partition. A graph G is ***l*-critical** if χ (G) = l and for all induced subgraphs $\Lambda \neq$ G we have χ (Λ) < l. The spectrum of a graph gives us insight into the chromatic number. Before we can understand the property that provides an upper-bound for χ(G), we must first establish Property 4-1.

Property 4-1: Given a graph G with χ (G) = $l \geq 2$, there exists a subgraph of G, $\Lambda \neq$ G, such that χ (Λ) = l, and every vertex of Λ has degree $\geq l$ in Λ.

Proof: The set of all induced subgraphs of G is non-empty and contains some graph whose chromatic number is l (including G itself). The set also contains some subgraphs whose chromatic number is not l. An example would be a graph with one vertex. Let Λ be a subgraph such that χ (Λ) = l, and χ (G) is minimal with respect to the number of vertices. Then Λ is l-critical. If v is any vertex of Λ, then $\langle V(\Lambda) \setminus v \rangle$ is an induced subgraph of Λ and has a vertex-coloring with $l - 1$ colors. If the degree of v in Λ were less than $l - 1$, then we could extend this vertex coloring to Λ, contradicting the fact that χ (Λ) = l. Thus the degree of v is at least $l - 1$. □

Property 4-2: For any graph G, χ (G) $\leq 1 + \lambda_1$, where λ_1 is the largest eigenvalue of the adjacency matrix of G.

Proof: From Property 4-1, there is an induced subgraph Λ of G such that $\chi(G) = \chi(\Lambda)$ and $d_{min}(\Lambda) \geq \chi(G) - 1$, where $d_{min}(\Lambda)$ is the least degree of the vertices of Λ. Thus we have $\chi(G) \leq 1 + d_{min}(\Lambda) \leq 1 + \lambda_1(\Lambda) \leq 1 + \lambda_1(G)$. [Bi, p55] □

Of course, the absolute largest value of $\chi(G)$ is n, the number of vertices. If $\lambda_1 < n - 1$, then we will have a smaller maximum than n.

Property 4-3: The lower bound of the chromatic number is $\chi(G) \geq 1 + \frac{\lambda_1}{-\lambda_{min}}$.

Proof: The vertex set V(G) can be partitioned into $\chi(G)$ coloring classes. Thus, the adjacency matrix **A** of G can be partitioned into χ^2 submatrices. This was seen in Chapter 2. In this case, the diagonal submatrices $\mathbf{A_{ii}}$ $(1 \leq i \leq v)$ consists entirely of zeros, and so $\lambda_1(A_{ii}) = 0$. . It is known that $\lambda_1(A) + (t-1)\lambda_{min}(A) \leq \sum_{i=1}^{t} \lambda_{max}(A_{ii})$. Therefore, we have $\lambda_1(A) + (\chi(G) - 1)\lambda_{min}(A) \leq 0$. But, if G has at least one edge, then $\lambda_{min}(A) = \lambda_1(G) < 0$. [Bi, p57] □

A classical application of vertex coloring is the coloring of a map. To make the process as inexpensive as possible, we want to use a few colors as possible. In the graph, the countries are represented by vertices with edges drawn between those countries that are adjacent. Determining the chromatic number of the graph gives us the fewest colors necessary to color the map.

Another application to graph coloring is a sorting problem, such as sorting fish in a pet store. Some fish can be in the same tank together, while other fish cannot. Say we have fish types A, B, C, D, E and F. They can be put into tanks according to the chart below

Type of Fish	A	B	C	D	E	F
Cannot be with fish type(s)	B, C	A, C, D	A, B, D, E	B, C, F	C, F	D, E

If the graph is set up such that the fish are the vertices and edges are drawn between those that cannot be in a tank together, the chromatic number will tell us how many tanks we need.

G =

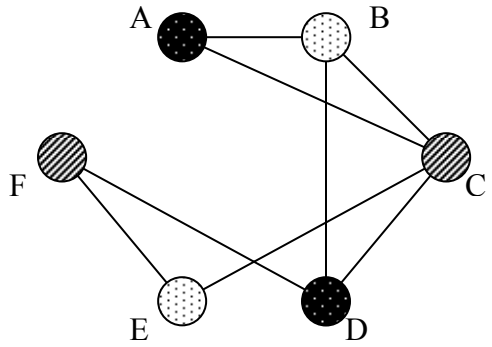


Figure 4-11

The adjacency matrix for G is $\mathbf{A} = \begin{bmatrix} 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 & 0 \end{bmatrix}$ which has $\lambda_1 = 2.853$ and $\lambda_{min} = -2.158$. Substituting these into the formula from Property 4-3, $\chi(G) \geq 1 + \frac{\lambda_1}{-\lambda_{min}}$, we get $\chi(G) \geq 2.322$. This tells us that we need at least three colors for our graph. This will save us time by preventing us from attempting to color it with fewer than 3 colors. In this case, we will need 3 tanks, as shown above in Figure 4-11. One tank will hold fish A and D, the second tank will hold fish B and E, and the third tank will hold fish C and F.

A more recent application of graph coloring is used by the Federal Communications Commission to set up the frequencies of radio stations. In order to keep

radio stations from interfering with each other, stations within 150 miles of one another must be on different frequencies. Below is the table of the distances between six radio stations.

Radio Station	A	B	C	D	E	F
A		35	108	90	215	188
B	35		192	50	62	14
C	108	192		55	175	87
D	90	50	55		209	158
E	215	62	175	209		48
F	188	14	87	158	48	

The vertices are the radio stations, with edges connecting those who are less than 150 miles apart. When we apply edge coloring, we will get the minimum number of frequencies required for all radio stations to operate without interfering with one another.

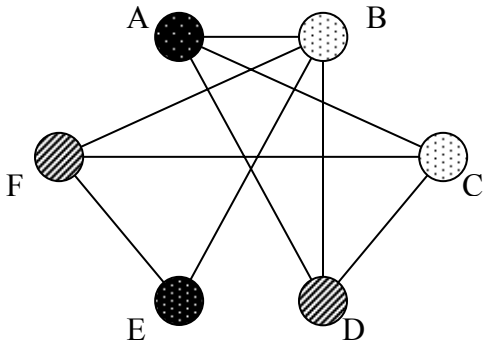


Figure 4-12

$\mathbf{A} = \begin{bmatrix} 0 & 1 & 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 & 1 & 0 \end{bmatrix}$ with $\lambda_1 = 3.087$, $\lambda_{min} = -2.179$, and $\chi(G) = 2.417$. Therefore, we need at least three colors. The colored graph in Figure 4-12 shows us that we need at most 3 frequencies. Stations A and E can have the same frequency, as can F and D, and B and C.

An even more recent application of this type of problem is with the signals of cell phone towers. Cell phone providers want as few towers as possible, so they want to avoid overlapping the tower coverage areas. Also, customers do not want "dead areas." They can apply the same type of chart above to determine the minimum number of towers necessary in a given area.

There are many applications of graph coloring, and the spectral of the graph gives us insight to the chromatic number, which is at the heart of graph coloring.

SECTION 4.4: MISCELLANEOUS APPLICATIONS

Identifying clusters is an important aspect in the field of electrical network connections [Vi, p9]. Graph spectral method is extremely helpful in this, and can find the needed results with minimal computations. An adjacency matrix is used, but edge weights are used as entries. The weights are $\frac{1}{d_{ij}}$, where d_{ij} represents the distance from vertices i and j. The goal is to find the location of "n" vertices that minimizes the weighted sum of the squared distances between the vertices. The full process will not be discussed here, but the key point of interest is that the second smallest eigenvalue of the Laplacian matrix, λ_2, and its vector component gives the clustering points in the graph. The vertices that are clustered have the same value for the second smallest eigenvalue. Also, the largest eigenvalue contains information regarding only one of the clusters. The vertex with the largest vector component is the vertex with the highest degree.

Spectral graph theory is used in the study of DNA. A molecule of DNA is a very long string consisting of a unique sequence using four amino acids. The goal is to determine this sequence for a given molecule of DNA. In general, the molecule is broken up into shorter fragments, which are separated according to their amino acid sequences. Once the sequence of the fragments is determined, the original DNA can be represented as a sequence of these fragments in some order. To use this method, each fragment F is allowed to bond to the DNA at a point P (called a probe) where the amino acid sequences match. The data of these matches is recorded into a matrix whose rows represent the fragments and columns represent the probes. A one is entered at the (F, P) positions, and zeros elsewhere. So, a one represents a match of fragment F to the DNA at probe P.

The DNA sequencing problem is to find the ordering of the rows and the ordering of the columns of the matrix, because this tells the order that the fragments occur along the DNA. Normally, a breadth first search works in this situation. Unfortunately, the procedure of matching the probes and fragments is error prone, so other more complex methods are employed. These methods employ spectral ordering involving the Laplacian and permuted matrices. It is a rather involved process that will not be covered fully here, but the process relies on spectral graph mathematics.

The Laplacian eigenvalues determine the kinematic behavior of a liquid flowing through a system of communicating pipes. In this situation, the vertices of graph G are beads, and the edges are mutual interactions between the beads. The basic behavior of the flow (periodic, aperiodic, etc) is determined by λ_2, the algebraic connectivity, or the second smallest Laplacian eigenvalue. [Ma, p35]

The algebraic connectivity derived its name from its relationship to the connectivity parameters of a graph – the vertex connectivity and the edge connectivity. λ_2 imposes reasonably good bounds on several properties of graphs which can be very difficult to compute.

Graphs with high connectivity properties are concentrators and expanders. They are used in the construction of switching networks that exhibit high connectivity as well as the construction of superconcentrators which are used in theoretical computer science. The Laplacian spectrum of a graph, particularly λ_2, appears naturally in the study of expanding properties of graphs. In a rather complex formula, it gives a lower bound on the number of neighbors a subset of the vertex set can have.

λ_2 is the main ingredient of the formula for an isoperimetric number of a graph, i(G). The isoperimetric number is used by geometers to investigate the spectral properties of Riemann surfaces. If $\lambda_2 = 2$, then we know that $i(G) \geq 1$. Also, the diameter of a graph holds a relationship with λ_2, which is diam(G) $\geq \frac{4}{n\lambda_2}$. There is also a more complex formula for the upper bound of the diameter involving the algebraic connectivity.

The applications of linear algebra, graph theory, and the spectral of a graph continue on and on through the various sciences and other fields. As we know, mathematics is found everywhere, and is required in many many situations in order to evaluate, process, and better understand the world around us.

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