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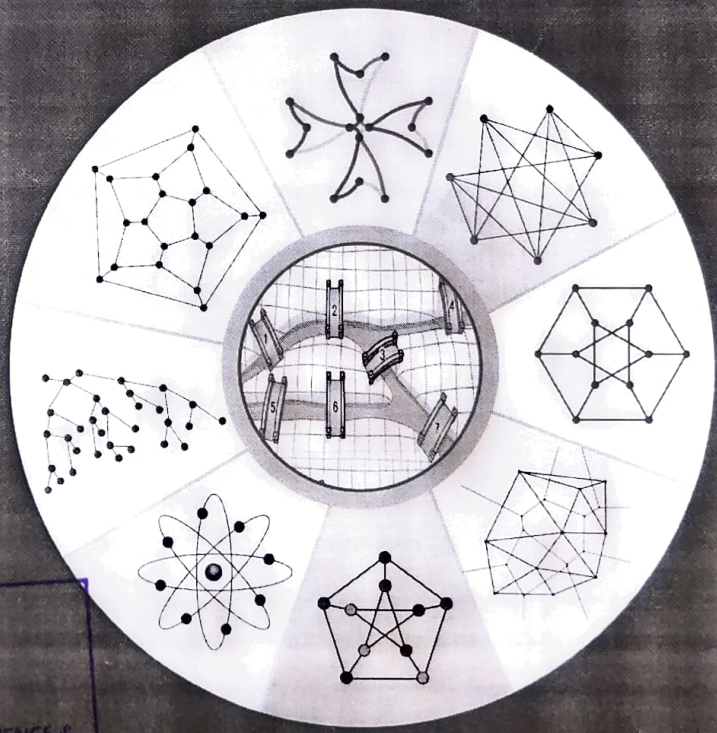

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Applications of Spectral Graph Theory

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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 applications of spectral graph theory, including the fields of chemistry, biology, and graph colouring. 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 colouring 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. 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.

Introduction:

A **graph** $G = (V, E)$ is a pair of vertices V and a set of edges$E$, assumed finite i.e. $|V| = n$ and $|E| = m$. 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 a **complete graph** if each pair of vertices is joined by an edge. In the example graph below,

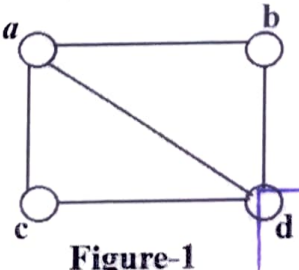


Figure-1

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

A 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 **order of G** is the cardinality of the vertex set $V(G)$. It is denote by $p(G)$ or p. The size of G is the cardinality of the edge set $E(G)$. It is denoted by $q(G)$ or q. A graph G can be denoted as a G(p, q) graph.

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. In Figure-1, a walk from b to c would be bdc. The graph is **connected** if each pair of vertices in a graph is joined by a walk. 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 b to c is 2. The **diameter** of the graph G is the maximum distance between all of the pairs of vertices of a graph. It is denoted by diam(G). In Figure-1, the distance between any two vertices is either 1 or 2, making diam(G) = 2. The vertices and edges may have certain attributes such as colour or weight. When the edges are given direction we have a **digraph** or **directed graph**. Digraphs can be used to model road maps. The vertices represent landmarks, while the edges represent one-way or two-way streets.

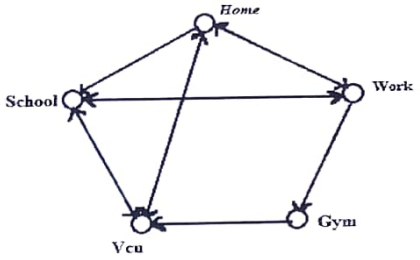


Figure-2

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.

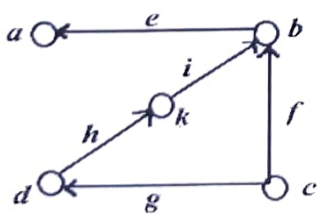


Figure-3

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

A graph is called as **multi-graph** if two vertices are joined by more than one edge.

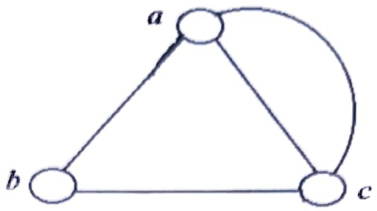


Figure-4

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 *aa* is joining a pair of non-distinct vertices. Therefore, there is a self-loop at vertex *a*.

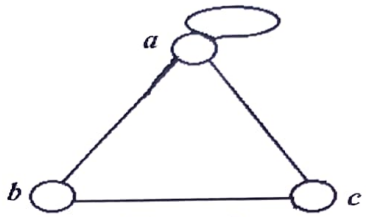


Figure-5

Graphs *G* and *H* are **isomorphic** if there is a vertex bijection $f: V(G) \rightarrow V(H)$ such that for all $u, v \in V(G)$, *u* and *v* adjacent in $G \leftrightarrow f(u)$ and f(*v*) are adjacent in H.

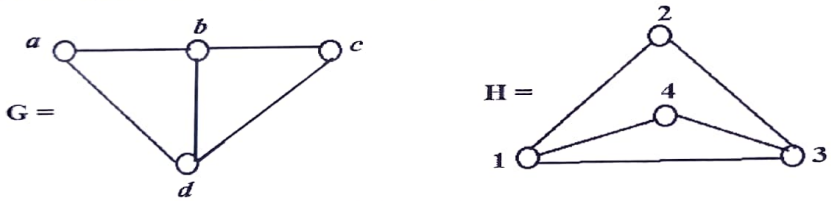


Figure-6

Graphs *G* and *H* are isomorphic, because a vertex bijection between them is: *f*(*a*) = 2, *f*(*b*) = 3, *f*(*c*) = 4, and *f*(*d*) = 1.

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**. 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,

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

For example,

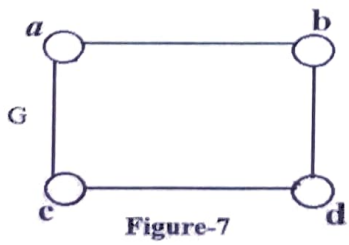


Figure-7

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

Note 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 *tr*(**A**) is 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, $a_{ij} = a_{ij}$.

Result-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.

For example,

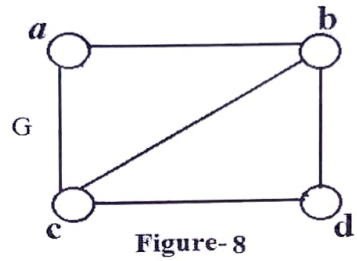


Figure- 8

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

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

$$A^2 = \begin{array}{c} \\ a \\ b \\ c \\ d \end{array} \begin{array}{c} \begin{array}{cccc} a & b & c & d \end{array} \\ \begin{bmatrix} 2 & 1 & 1 & 2 \\ 1 & 3 & 2 & 1 \\ 1 & 2 & 3 & 1 \\ 2 & 1 & 1 & 2 \end{bmatrix} \end{array}$$

Therefore if we look at element (*b*, *d*) = element (*d*, *b*) = 1. There isone walk from *b* to *d* of length 2. That walk is *bcd*.

Result-2: The trace of A^2 is twice the number of edges in the graph.

In our example in Figure 8, the trace of A^2 is 10 and the number of edges is 5.

Result-3: The trace of A^3 is six times the number of triangles in the graph.

In our example in Figure 8,

$$A^3 = \begin{bmatrix} 2 & 5 & 5 & 2 \\ 4 & 4 & 5 & 5 \\ 5 & 4 & 4 & 4 \\ 2 & 5 & 5 & 2 \end{bmatrix}$$

The trace of A^3 is 12 and the number of triangles in the figure is 2.

The **characteristic polynomial** of a graph G of order n is the determinant$det(A - \lambda I)$, where I is the $n \times n$ identity matrix and $A$is adjacency matrix of graph G.The general form of any characteristic polynomial is$\lambda^n + c_1\lambda^{n-1} + c_2\lambda^{n-2} + \cdots \ldots + c_n$.

Result-3: The coefficients of the characteristic polynomial that coincide with matrix$A$ of a graph G have the following characteristics:

i) $c_1 = 0$
ii) $-c_2$is the number of edges of G
iii) $-c_3$is twice the number of triangles in G.

In our example in **Figure 8**, the characteristic polynomial is $det(A-\lambda I) = \lambda^4 - 5\lambda^2 - 4\lambda$

i) There is no λ^3, so$c_1 = 0$
ii) The number of edges of G is 5 because $-c_2 = 5$
iii) The number of triangles in G is 2 because$-c_3 = 4$, so

The roots of a characteristic polynomial are called the **eigenvalues**. Setting thecharacteristic polynomial$det(A-\lambda I) = \lambda^4 - 5\lambda^2 - 4\lambda$equal to zero and solving we get the eigenvalues $\{-1, -1, 2\}$.

Result-4: The sum of the eigenvalues of a matrix equals its trace.

The **algebraic multiplicity** of an eigenvalue is the number of times that the valueoccurs as a root of the characteristic polynomial. The **geometric multiplicity** is the dimension of the **eigenspace** or the subspace spanned byall of the eigenvectors.

Result-5: If a matrix is real symmetric, then each eigenvalue of the graph relating tothat matrix is real.

Result-6: The geometric and algebraic multiplicities of each eigenvalue of a realsymmetric matrix are equal.

Result-7: The eigenvectors that correspond to the distinct eigenvalues areorthogonal.

Note that when $u$and $v$are two orthogonal eigenvectors of Aassociated with two distincteigenvalues $\lambda$and μ then the unit vectors $\frac{u}{||u||}$ and $\frac{v}{||v||}$are orthonormal eigenvectors associated with$\lambda$and μrespectively.

Result-8: If a graph is connected, the largest eigenvalue has multiplicity of 1.

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. Originally, spectral graph theory analyzed the adjacency matrix of a graph, especially its eigenvalues.

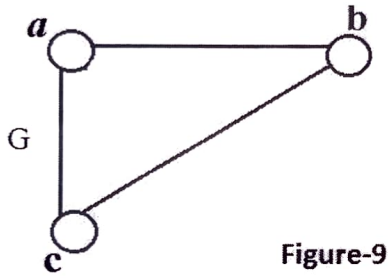
The **spectrum** of a graph G is the set of eigenvalues of G, together with their **algebraic multiplicities**, or the number of times that they occur.

Result-9: A graph with n vertices has n eigenvalues.

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

$$Spec(G) = \begin{pmatrix} \lambda_1 & \lambda_2 & \cdots & \lambda_k \\ m(\lambda_1) & m(\lambda_2) & \cdots & m(\lambda_k) \end{pmatrix} \text{where} \sum_{i=0}^{k} \lambda_i = n.$$

For example,



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

Figure-9

The characteristic polynomial is$\lambda^3 - 3\lambda - 2$with eigenvalues $\{-1, -1, 2\}$. Our graph has two distinct eigenvalues: -1 and 2, hence the spectrum of the graph G is given by

$$Spec(G) = \begin{pmatrix} -1 & 2 \\ 2 & 1 \end{pmatrix}$$

A graph is **connected** if for everypair of vertices u and v, there is a walk from $u$to v. 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 $\lambda_1$is less than or equal to the largest degree ofthe graph. Also, $\lambda_1$increases with graphs that contain vertices of higher degree. Inaddition, the degrees of the vertices adjacent to the vertex with the largest degree affectvalue of λ_1.

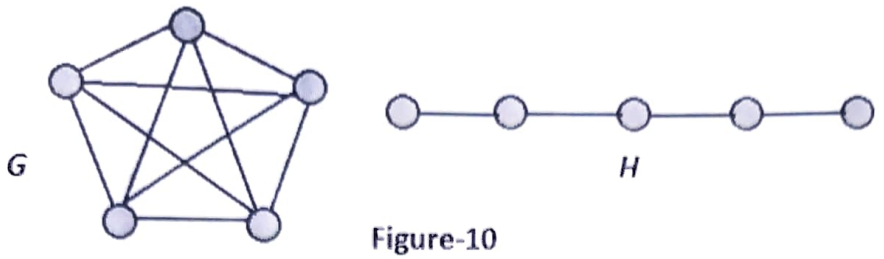


Figure-10

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

A **bipartite graph** G is one whose vertex-set V can be partitioned into twosubsets U and W such that each edge of G has one endpoint in U and one in W. The pairU, W is called the **bipartitionof** G, and U and W are called the **bipartition subsets.**

Result-10: Agraph is bipartite if and only if it contains no odd cycles.

Result-11: If G is bipartite graph and λ is an eigenvalue then – λ is also aneigenvalue.

Result-12: The spectrum of a bipartite graph is symmetric around 0.

Result-13: If G is a bipartite graph then $c_{2k-1} = 0$ for $n \geq 1$.

A **minimal polynomial** of a graph G is the monic polynomial $q(x)$ of smallest degree such that $q(G) = 0$.

Result-14: The degree of the minimal polynomial is larger that the diameter.

Result-15: If a graph G has diameter $d$and has $m$distinct eigenvalues then $m > d + 1$.

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

Result-16: The complete graph is the only connected graph with exactly two distincteigenvalues.

Result-17: The complete graph $K_p$is determined by its spectrum.

The **Laplacian L**of a graph is the square matrix that corresponds to the vertices of a graph. The main diagonal of the matrix represents the degreeof the vertex while the other entries are as follows:

$$A_{ij} = \begin{cases} -1 & \text{if } v_i \text{ and } v_j \text{ are adjacent} \\ 0 & \text{otherwise} \end{cases}$$

The Laplacian can also be derived from $D - A$, where $D$is the diagonal matrixwhose entries represent the degrees of the vertices and $A$is the adjacency matrix.

For example,

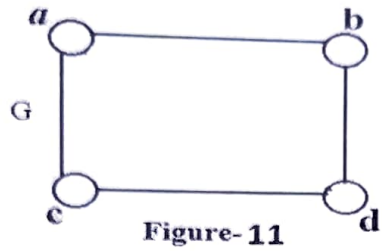


Figure-11

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

The Laplacian of a connected graph has eigenvalues $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$. Thealgebraic connectivity is defined to be λ_2, the second smallest eigenvalue. The name isa result of its connection to the vertex connectivity and the edge connectivity of a graph.

The Laplacian concerns the number of spanning trees of a graph. 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 nextsection.

A **positive semidefinite matrix** is one that is Hermitian, and whose eigenvaluesare all non-negative. A Hermitian matrix is one which equals its conjugate transpose.This is usually written:$A^H = \overline{A^T} = A$.

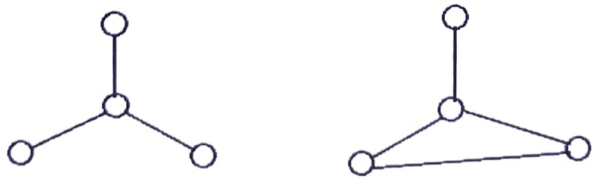
The **characteristic function** is the function for which every subset N of X, has avalue of 1 at points of N, and 0 at points of $X - N$. In other words, it takes the value of 1 for numbers in the set and 0 for numbers not in the set.

Result-18: The smallest eigenvalue of $L$is 0.

Result-19: The multiplicity of 0 as an eigenvalue of L is the number of connectedcomponents in the graph.

Result-20: The algebraic connectivity is positive if and only if the graph isconnected.

A **tree** isa connected graph that has no cycles.



A tree Not a tree

Figure-12

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.Somesubgraphs of the tree above are

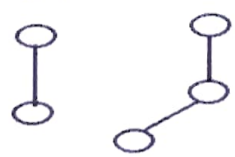
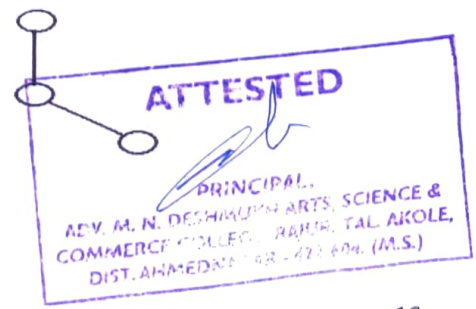


Figure-13



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

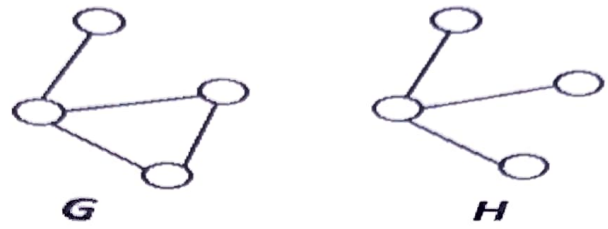

Figure-14

Result-21(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 thevalue of any cofactor of the matrix $C - A$.

Result-22(Cayley's Tree Formula): The number of different trees on $n$labeled vertices isn^{n-2}.

Chemical Applications:

A chemical tree is a tree where no vertex has a degree higher than 4. Chemicaltrees 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 aremethane, ethane, propane, and butane. After that, the alkanes are named based on Greeknumbers. 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-15, which represents methane.

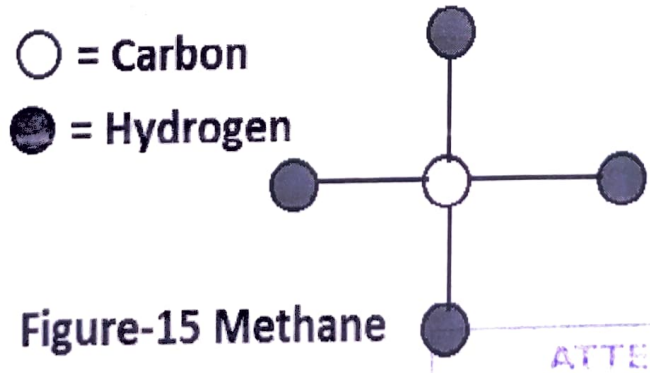

Figure-15 Methane

Figure-15 shows us butane, which is C_4H_{10}.

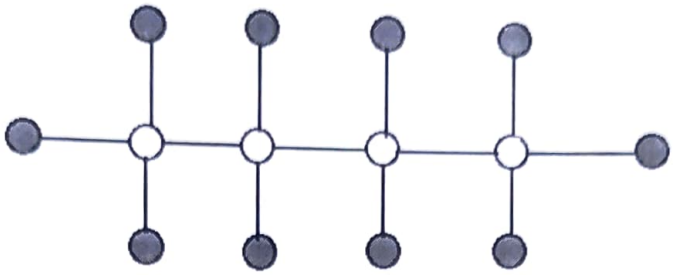

Figure-16 Butane

Compounds that have the same formula, but different structures, are called**isomers**. When$C_4H_{10}$is restructured as in Figure-17, we have isobutane or 2-Methylpropane. Butane and 2-Methylpropane are isomers.

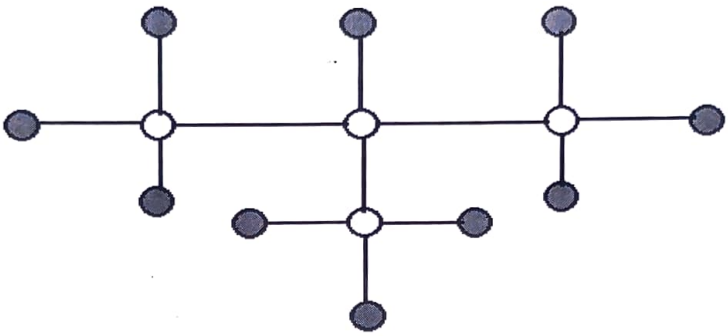

Figure-17 Isobutane or 2-Methylpropane

Compounds with four carbons have 2 isomers, while those with five carbons have3 isomers. The growth, however, is not linear. The chart below compares the number ofcarbons 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
$C_{15}H_{32}$	4347

When a carbon has four carbons bonded to it, we have a **quarternary** carbon. An example is below in Figure-18, which is called a 2,2-Dimetylpropane. It is isomeric toPentane.

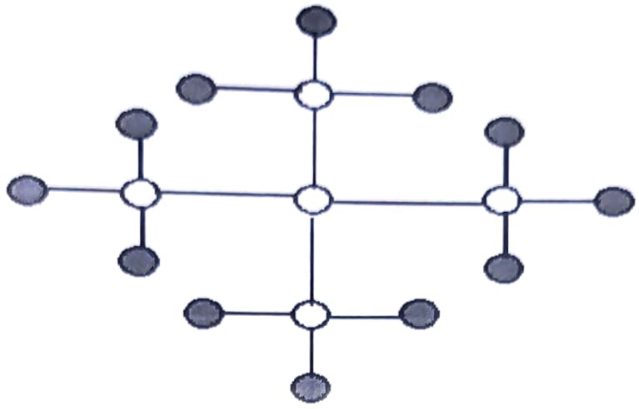

Figure-18 2,2-Dimetylpropane

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

Study was done on the eigenvalues of molecular graphs and in particular λ_1(thelargest eigenvalue of a graph). When the isomeric alkanes are ordered according to theirλ_1 values, regularity is observed.

LetΔ denote the maximum degree of a graph. The chemical trees that pertain tothe 18 isomeric octanes C_8H_{18} follow a pattern with respect to their largest eigenvalue λ_1.The isomer with the smallest $\lambda_1(3.8478)$ value is the straight-chain octane in Figure-19,that $has\ \Delta = 2$.

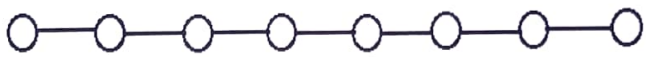

Figure-19

The next 10 isomers have various extensions of branching, but none possess aquaternary carbon atom. All of them have $\Delta = 3$and their λ_1's are greater than that ofthe 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-20.

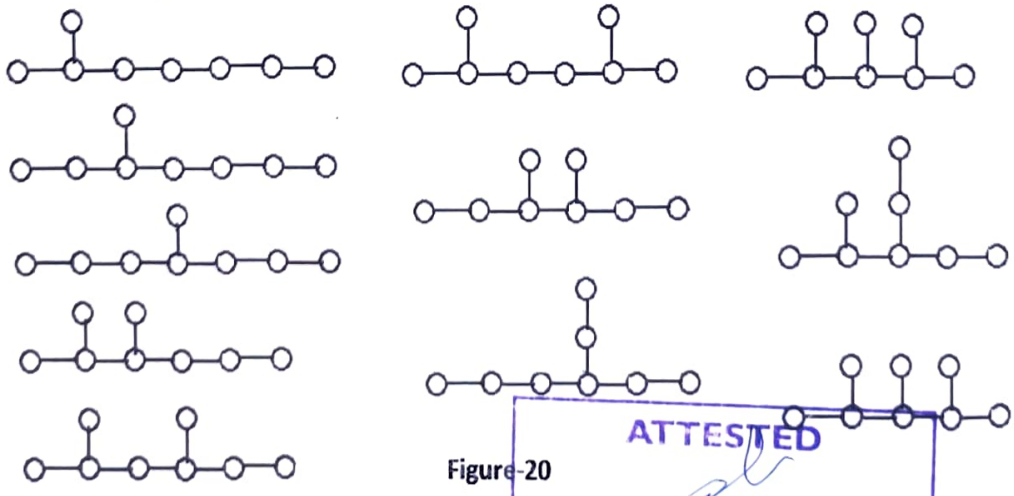

Figure-20

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 $\lambda_1 = 5.6458$ and is the last tree shown below in Figure-21.

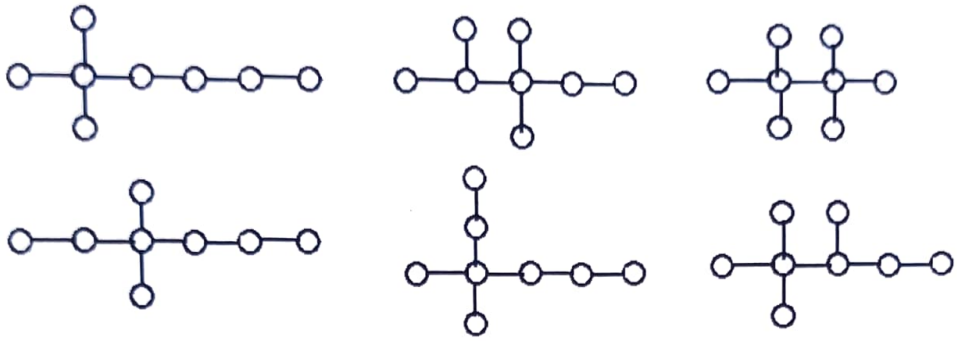

Figure-21

This same regularity occurs with isomeric alkanes with *n* carbon atoms, discussedabove. The normal alkane with Δ = 2 has the smallest λ1. All alkanes with Δ = 3 have λ1greater than the alkanes with Δ = 2, and smaller than any isomer with Δ = 4. We cantherefore draw theconclusion that Δ, which tells us whether or not there is a quaternary41carbon atom, is the main molecular structure descriptor affecting the value λ1, the largestLaplacian eigenvalue of an alkane. It has been discovered that λ1 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, λ1 can be estimatedby

$$\lambda_1 \approx \Delta + 1 + \gamma\Delta - 1,$$

where γ depends on both $n$and Δ. For alkanes, it has been discovered through numericaltesting that $\gamma \approx 0.2$. It is possible to establish the alkane isomers with $\Delta = 3$ or $\Delta = 4$ that have theminimal 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 $\Delta = 4$.

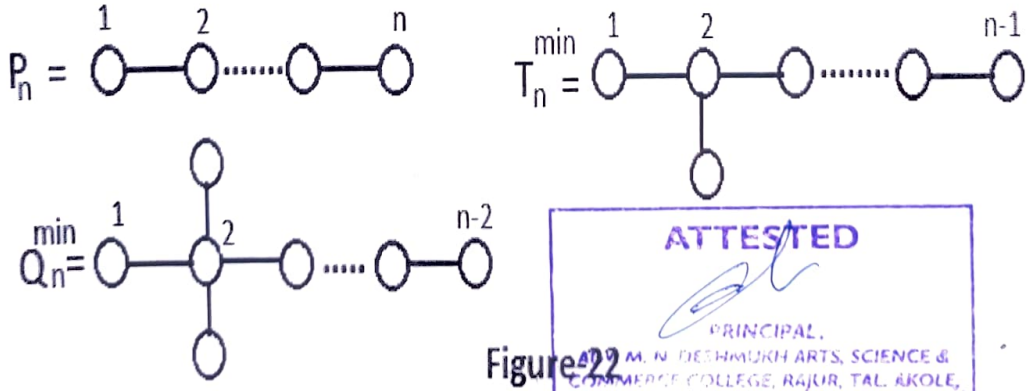

Figure-22

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 maximalλ_1 and minimal W, where W represents the Wiener topological index of alkanes andconforms to the formula $W = \lambda$. The exact characterizations of these trees are complex and will not be covered here.

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