

MA859: SELECTED TOPICS IN GRAPH THEORY

LECTURE: 18

Some applications of Laplacian Matrix

Chemical Applications

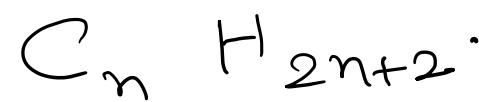
Recall that the eigenvalues of $L(G)$, the Laplacian Matrix of a graph G are $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$, where $\lambda_n = 0$ and $\lambda_{n-1} > 0$

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 greater than 4. The chemical trees are molecular graphs representing constitutional isomers of alkanes.

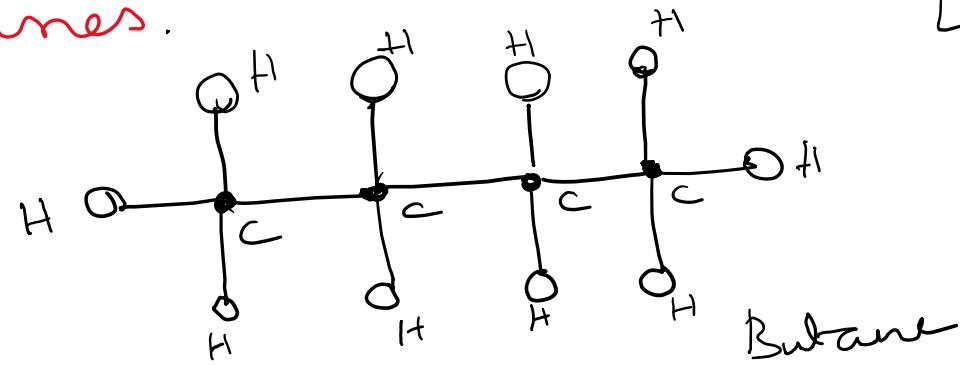
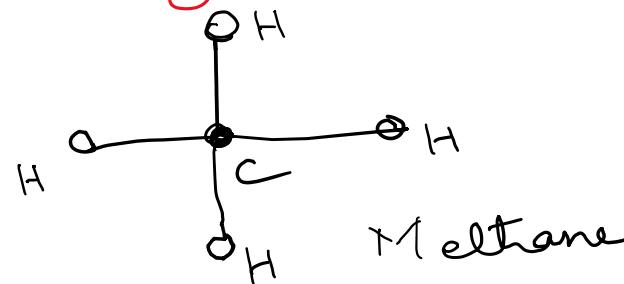
If there are n vertices, each chemical tree represents a particular isomer of



The first four are methane, ethane, propane and butane. After that the alkanes are named based on Greek numbers.

For example $C_5 H_{12}$ is pentane.

Compounds whose carbons are all linked in a row, like the two below, are called straight-chain alkanes.

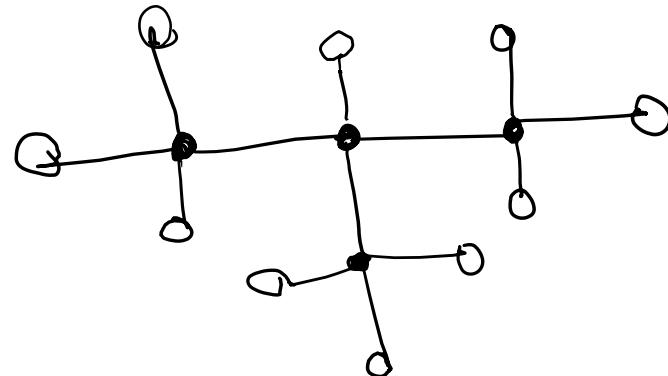


[Hard dots - Carbon
Hollow dots - Hydrogen]

Compounds that have the same formula, but different structures, are called **isomers**.

When C_4H_{10} is restructured as in the figure below, we have isobutane or 2-Methylpropane.

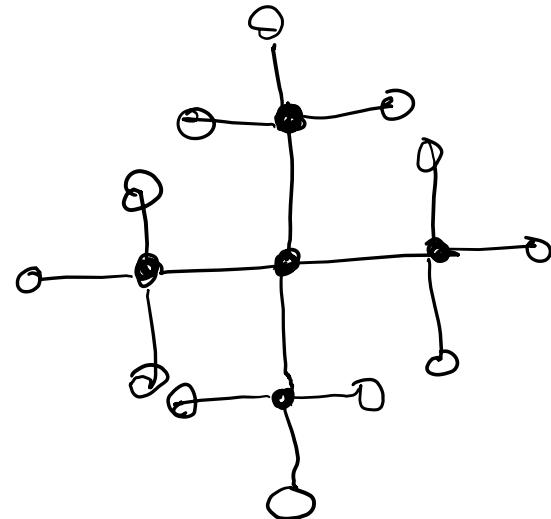
Butane and 2-Methylpropane
are isomers



Compounds with 4 carbons have 2 isomers, while those with 5 carbons have 3 isomers. The growth, however, is not linear. The chart below compares the no. of carbons with the no. of isomers.

Formula	Number of Isomers
$C_6 H_{14}$	5
$C_7 H_{16}$	9
$C_8 H_{18}$	18
$C_9 H_{20}$	35
$C_{10} H_{22}$	75
$C_{15} H_{32}$	4347
$C_{20} H_{42}$	366319

When a carbon has four carbons bonded to it, we have a **quaternary** carbon. An example below is a 2,2-Dimethylpropane. It is isometric to Pentane



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

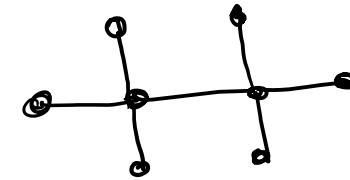
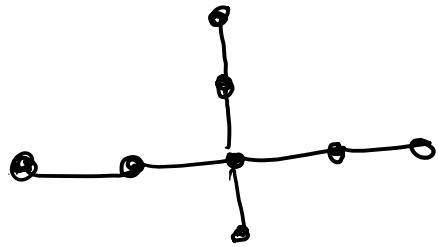
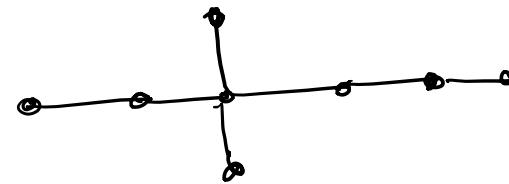
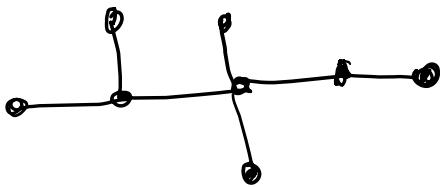
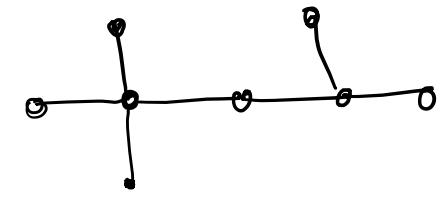
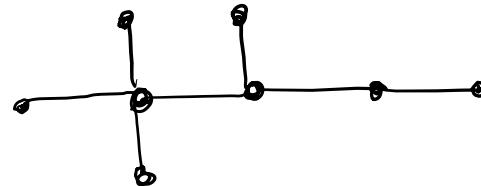
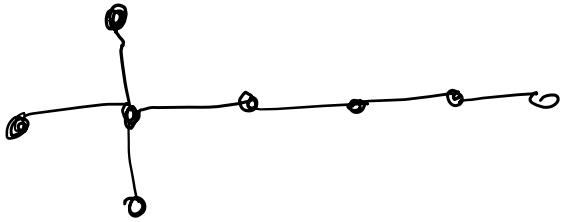
Study was done on the eigenvalues of the molecular graphs, and in particular, λ_1 , the largest eigenvalue of a graph. When isometric alkanes are ordered according to their λ_1 values, regularity is observed.

Let Δ denote the maximum degree of a graph. The chemical trees that pertain to the 18 isometric 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 as in the figure below.



$$\Delta = 2$$

The next 10 isomers have various extensions of branching; but none possesses a quaternary carbon atom. All of them have $\Delta = 3$, and their Δ_i 's are greater than that of the straight-chain graph (as in the figure on the previous slide), where $\Delta = 2$, and less than the following seven, who have $\Delta = 4$.



The 12th through the 18th octanes contain a quaternary carbon atom, they all have $\Delta = 4$, and they have the largest γ_1 . The largest one has $\gamma_1 = 5.6458$.

This same regularity occurs with isometric alkanes with n carbon atoms. The normal alkane with $\Delta = 2$ has the smallest γ_1 . All alkanes with $\Delta = 3$, have γ_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 of λ_1 , the largest Laplacian eigenvalue of an alkane. It is found that

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

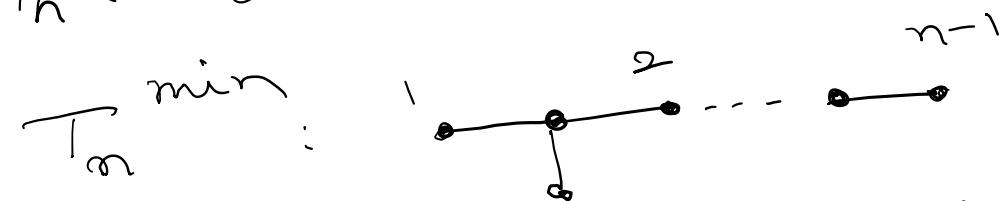
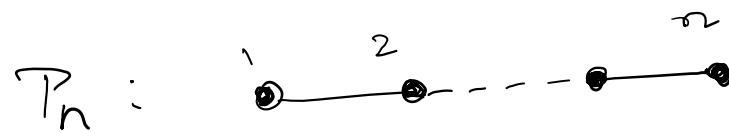
Also, by using a linear combination of the lower and the upper bounds, λ_1 can be estimated

by $\lambda_1 \approx \Delta + 1 + \gamma \sqrt{\Delta - 1}$, where γ depends on both n and Δ .

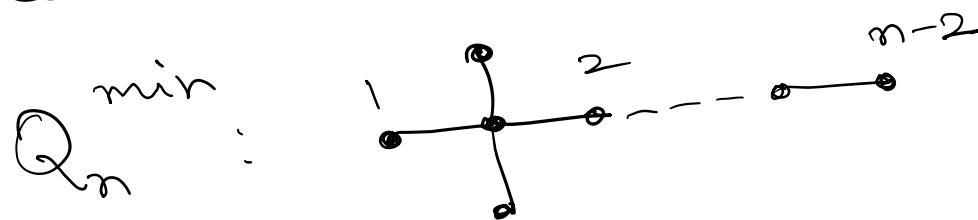
For alkanes, it has been determined through the numerical techniques that $\gamma \approx 0.2$.

It is possible to establish the alkane isomers with $\Delta = 3$ and $\Delta = 4$ that have the minimal λ_1 .

Given P_n ,



the minimal τ_1 for $D=3$.



the minimal τ_1 for $D=4$.

is the tree that establishes

$D=3$.

is the tree that establishes

$D=4$.

The structure of trees that represent the maximal π_1 are more complex.

The T_m^{\max} and Q_n^{\max} coincide with the chemical trees that have the same Δ and n , having maximal π_1 and minimal W , where W is the

Wiener Topological Index of alkanes, and conforms to the formula $W = n \sum_{i=1}^{n-1} \frac{1}{\pi_i}$.

The exact characterizations of these trees are very complex, and will not be covered here.

Graph Coloring

One of the classical problems in graph theory
is vertex coloring, where no two adjacent vertices
receive the same color.

The proper coloring of a graph also forms a
natural partition of the vertex set.
The Chromatic Number $\chi(G)$ is the least number
of colors required for such a partition.

A graph G is ℓ -critical if $\chi(G) = \ell$ and for all proper induced subgraphs $G' \neq G$, we have $\chi(G') < \ell$.

The spectrum of a graph gives us insight into the Chromatic number.

Theorem: Given a graph G with $\chi(G) = \ell \geq 2$, there exists a proper subgraph G' of G such that $\chi(G') = \ell$ and every vertex of G' has degree $\geq \ell$ in G' .

Proof: The set of all induced subgraphs of G is non-empty and contains some graph whose chromatic number is l (including G). Also, it contains some subgraphs whose chromatic number is not l (for example, the trivial subgraph).

Let G' be a subgraph of G such that $\chi(G') = l$. Let G' be a subgraph of G such that $\chi(G') = l$. Also, let $\chi(G')$ is minimal with respect to the number of vertices. So, G' is l -critical.

If v is any vertex of G' , then $\langle V(G') - v \rangle$ has a vertex coloring with $l-1$ colors.

If $\deg v < \lambda - 1$ in G' , then we could extend this vertex coloring to G' , which is a contradiction to the fact that $\chi(G') = \lambda$. Hence $\deg v \geq \lambda - 1$. //

Theorem 2 For any graph G , $\chi(G) \leq 1 + \lambda_1$, where λ_1 is the largest eigenvalue of $A(G)$.

Proof: In view of theorem 1, there exists an induced subgraph G' of G such that $\chi(G) = \chi(G')$ and $\delta(G') \geq \chi(G) - 1$. Thus, we have $\chi(G) \leq 1 + \delta(G') \leq 1 + \lambda_1(G') \leq 1 + \lambda_1(G)$. //

$\chi(G) \leq n$, the no. of vertices. If $\lambda_1 < n-1$,
then $\chi(G) < n$.

Theorem 3 $1 + \frac{\lambda_1}{\lambda_{\min}} \leq \chi(G)$.

Proof: The vertex set $V(G)$ can be partitioned
into $\chi(G)$ coloring classes. So, $\Lambda(G)$ can be
partitioned into χ^2 submatrices. (verify!)

In this case, the diagonal submatrices A_{ii} consist
entirely of zeroes; so, $\chi_1(A_{ii}) = 0$.

There is a known result that

$$\lambda_1(A) + (t-1)\lambda_{\min}(A) \leq \sum_{i=1}^t \lambda_{\max}(A_{ii})$$

Hence, we have

$$\lambda_1(A) + (\chi(G)-1)\lambda_{\min}(A) \leq 0.$$

But if G has at least one edge, then

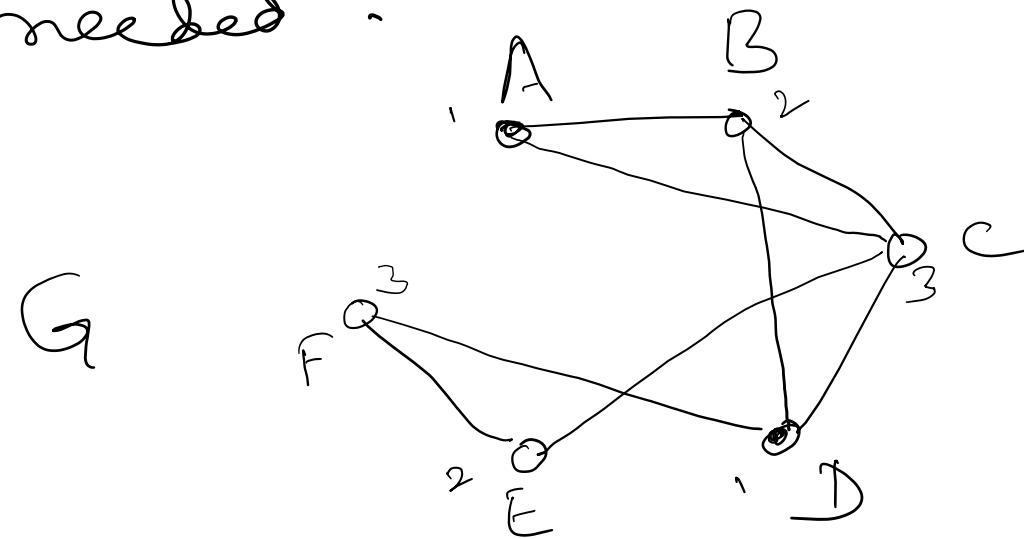
$$\lambda_{\min}(A) = \lambda_1(G) < 0. //$$

Another application to graph coloring is a sorting problem.

Ex Some fish can be in the same tank together; while other fish can not. Say, there are 6 types of fish A, B, C, D, E & F. They can be put into tanks as below:

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

When we set up a graph such that each fish is a vertex and edges are drawn between those that can not be in a tank together, the chromatic number tells us how many tanks are needed :



The adjacency matrix

$$A(G) = \begin{bmatrix} 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 & 0 \end{bmatrix}$$

$$\lambda_1(G) = 2.853 \quad \text{and} \quad \lambda_{\min} = -2.158$$

Using Theorem 3, $\chi(G) \geq 1 + \frac{\lambda_1}{-\lambda_{\min}}$

$$\Rightarrow \chi(G) \geq 2.322$$

\Rightarrow at least 3 colors are necessary,
(which can be easily verified).

One tank will hold A & D

Second tank will hold B & E

Third tank will hold C & F. //

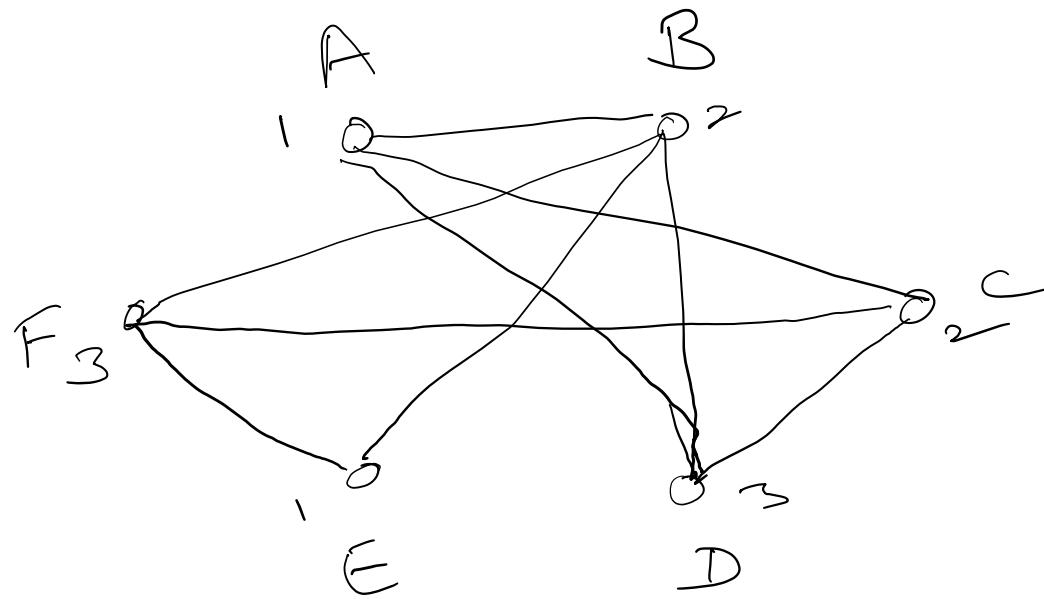
A more recent application of graph coloring
is in setting up frequencies of radio stations
(cellphone towers etc.)

In order to keep radio stations from interfering
with each other, stations within 150 kms of
one another must be of different frequencies.

An example below, gives the table of 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 radio stations & edges connect those which are less than 150 kms apart.



$$A(G) =$$

$$\begin{bmatrix} 0 & 1 & 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 & 1 & 0 \end{bmatrix}$$

$$\lambda_1 = 3.087 \quad \lambda_{\min} = -2.179 \quad \chi(G) \geq 2.417$$

\Rightarrow 3 colors are needed. So, we need at most three frequencies. Stations A & E can have the same frequency; so have F & D and B & C.

Miscellaneous Applications

- * Identifying clusters is an important aspect in electrical networks. Graph spectral method is extremely useful here 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 between i and j .
The goal is to find the location of ' n ' vertices that minimizes the weighted sum of squared

distances between the vertices. We don't discuss the full process here. The key point of interest is that the second smallest eigenvalue of the Laplacian matrix, \mathcal{L} , 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 DNA studies.
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 in accordance with 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 zeroes 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 BFS works in this situation. However, 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. This is a rather involved process (that will not be fully covered here).

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.

// End of lecture //