Molecular Walks

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Dedication

Acknowledgments

Contents

Abstract

Write stuff here

Notation

$W_G^i(n)$ = the number of closed walks of length n at vertex i

$W_G(n)$ = the number of closed walks of length n for graph G

$G_{i,j}$ = the molecular graph of C_iH_j

Chapter 1

Background Information

1.1 Linear Algebra

Linear Algebra is the study of vectors and linear transformations. Transformations in this section will be matrices. A matrix is the result of organizing information related to linear transformations. Matrices of the same size can be added together and matrices that are not of the same size can be multiplied together. Moreover, we can evaluate matrices when they are in "reduced row echleon form."

Throughout this research we use something called the determinant. The determinant takes a square matrix (an $n \times n$ matrix) and makes it into a single number. It is denoted as $\det(A)$ where A is the matrix. If $\det(A) \neq 0$ then the matrix is invertible. For our purposes, we want the matrix to not equal zero. To find the total number of closed walks within our graph we

must be able to find the determinant of the eigenvalues.

1.1.1 Linear Algebra Definitions

There are many definitions that can give background to the research conducted when evaluating combinatorics and the different graphs studied. There are many connections that mathematics contains for this field of work. These parts of mathematics that help explain the work done includes: Linear Algebra, which is defined before, Graph Theory, and Combinatorics. Each field will contain different aspects that will be useful in the research done.

Definition 1.1.1 (Linear Transformation)**.** Let V, W be vector spaces over a field, $\mathbb{F}$. The map

$$T : V \to W$$

is a linear transformation if

$$T(\alpha v + \beta w) = \alpha Tv + \beta Tw.$$

For all $v, w \in V$ & $\alpha, \beta \in \mathbb{F}$.

Example 1.1.1. Let the mapping

$$T : \mathbb{R}^1 \to \mathbb{R}^1$$

be defined by

$$T(x) = 3x.$$

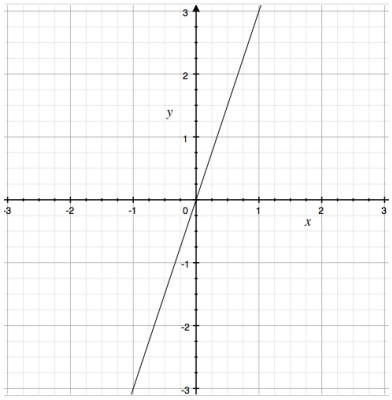


Figure 1.1: A graphical representation of T(x)= 3x

Let us evaluate the example:

$$T(\alpha v + \beta w) = 3(\alpha v + \beta w).$$

$$\alpha T(v) + \beta T(w) = 3v + \alpha 3v + \beta 3w = 3(\alpha v + \beta w).$$

They are equal! It's worth noting that this example works for all lines through the origin.

Example 1.1.2. We can also view T as a matrix. Let the matrix T have the mapping

$$\mathbb{R}^2 \to \mathbb{R}^2$$

and be represented by:

$$\begin{bmatrix} 1 & 2 \\ 0 & 4 \end{bmatrix}$$

where

$$v = \begin{bmatrix} v_1 \\ v_2 \end{bmatrix}$$

,

$$w = \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}$$

$$\alpha, \beta \in \mathbb{R}$$

$$\begin{bmatrix} 1 & 2 \\ 0 & 4 \end{bmatrix} \times \alpha \left(\begin{bmatrix} v_1 \\ v_2 \end{bmatrix} \right) + \left(\beta \begin{bmatrix} w_1 \\ w_2 \end{bmatrix} \right) = \begin{bmatrix} 1 & 2 \\ 0 & 4 \end{bmatrix} \begin{bmatrix} \alpha(v_1) + \beta(w_1) \\ \alpha(v_2) + \beta(w_2) \end{bmatrix} =$$

$$\begin{bmatrix} (\alpha(v_1) + \beta(w_1)) + 2(\alpha(v_2 + \beta(w_2)) \\ 4(\alpha(v_2 + \beta(W_2)) \end{bmatrix} =$$

$$\alpha \left(\begin{bmatrix} 1 & 2 \\ 0 & 4 \end{bmatrix} \right) \begin{bmatrix} v_1 \\ v_2 \end{bmatrix} + \beta \left(\begin{bmatrix} 1 & 2 \\ 0 & 4 \end{bmatrix} \right) \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}$$

Definition 1.1.2 (Determinant 2×2)**.** The determinant of a 2×2 matrix is given by

$$\det \begin{bmatrix} a & b \\ c & d \end{bmatrix} = ad - cd.$$

Example 1.1.3. Let us find the determinant of the matrix below:

$$\det \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} = 4 - 6 = -2.$$

Here we performed the operation of multiplication with 1×4 and subtracted this answer with 2×3. This resulted in the answer -2. Thus, the determinant of the matrix is -2.

We can generalize this to $n \times n$ matrices recursively. But we need certain tools first.

Definition 1.1.3 (Minors)**.** A minor of an $n \times n$ matrix M is the determinant of any square matrix obtained from M by deleting one row and one column. In other words, any entry m^i_j of a square matrix M is associated to a minor obtained by deleting the ith row and the jth column of M. Minors are represented by $M_{i,j}$

Definition 1.1.4 (Cofactors)**.** A cofactors is represented as $m_{i,j}$. The co-

factor of M corresponding to the entry m_j^i of M is the product of the minor associated to m_j^i and $(-1)^{i+j}$.

Therefore, we can evaluate matrices that are greater than 2×2.

Definition 1.1.5 (Determinant of an $n \times n$)**.** The determinant of an $n \times n$ matrix M is shown by

$$\det(M) = \Sigma(c_{i,j} \times M_{i,j})$$

When evaluating the answer for the given matrix, the signs of the equation should be folliowed. These signs are represented from the matrix below.

$$\begin{bmatrix} + & - & + \\ - & + & - \\ + & - & \ddots \end{bmatrix}$$

Definition 1.1.6 (Transpose)**.** The transpose of a column vector is the corresponding row vector and vice versa:

Example 1.1.4. Let $v =$

$$\begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}.$$

Then $v^T =$

$$\begin{pmatrix} 1\,2\,3 \end{pmatrix}$$

and $(v^T)^T = v$ This is because an operation performed twice does not affect the equation.

Proposition 1.0.1. *If M is a square matrix then* $\det M^T = \det M$

Proof. We know that the determinant can be computed by a cofactor expansion along any row or column.

Let us prove this by induction on n. For the base case $n = 1$ we have $A = A^T$, thus

$$\det A = \det A^T$$

. This is what we wanted thus we can move to our inductive step. Let us assume the result is true for $n = k - 1$ and let A be a $k \times k$ matrix. Let the matrix $A =$

$$\begin{bmatrix} a_{11} & a_{12} & \dots & a_{1k} \\ a_{21} & a_{22} & \dots & a_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ a_{k1} & a_{k1} & \dots & a_{kk} \end{bmatrix}$$

so that $A^T =$

$$\begin{bmatrix} a_{11} & a_{21} & \dots & a_{k1} \\ a_{12} & a_{22} & \dots & a_{k2} \\ \vdots & \vdots & \ddots & \vdots \\ a_{1k} & a_{2k} & \dots & a_{kk} \end{bmatrix}$$

Using cofactor expansion along the first column of A we have

$\det A = a_{11} \det A_{11} - a_{21} \det A_{21} + ... + (-1)^{k+1} a_{k1} \det A_{k1}$, where $A_{i,j}$ is the matrix obtained from A by removing the ith row and the jth column. Using cofactor expansion along the first row of A^T we have:
$\det(A^T) = a_{11} \det(A^T)_{11} - a_{21} \det(A^T)_{12} + ... + (-1)^{k+1} a_{k1} \det(A^T)_{1k}$

We notice that $(A^T)_{ij} = (A_{ij})^T$. Since A_{ji} is a $(k-1) \times (k-1)$ matrix we can use the inductive hypothesis to see that
$\det(A^T)_{ij} = \det((A_{ij}^T) = \det A_{ij}$.

If we subsitute this to the above formula for $\det(A^T)$ we get
$\det(A^T) = \det A$.

□

There are some properties that we should consider that involve elementary row operations and determinants.

1. If B is the matrix obtained by permuting two rows of A, then
   $\det(B) = -\det(A)$

2. If B is the matrix obtained by multiplying one row of A by any scalar k, then
   $\det(B) = k \det(A)$

3. If B is the matrix obtained by adding a mutliple of any row of to a different row of A, then
   $\det(B) = \det(A)$

Let's take a look at a 4×4 matrix. Remember, when finding a determinant, a matrix must be a *squared* matrix, this means that there must be the same amount of rows and columns. Hence, when referring to a determinant we define it with an $n \times n$, where $n = n$.

Example 1.1.5.

$$\begin{bmatrix} 1 & 2 & 0 & 3 \\ 0 & 1 & 2 & 0 \\ 3 & 0 & 1 & 0 \\ 1 & 4 & 0 & 1 \end{bmatrix} = 3 \times \begin{vmatrix} 2 & 0 & 3 \\ 1 & 2 & 0 \\ 4 & 0 & 1 \end{vmatrix} - 0 + 1 \times \begin{vmatrix} 1 & 2 & 3 \\ 0 & 1 & 0 \\ 1 & 4 & 1 \end{vmatrix} - 0 =$$

$$(3 \times 2 \begin{vmatrix} 2 & 0 \\ 0 & 1 \end{vmatrix} - 0 + 3 \times \begin{vmatrix} 1 & 2 \\ 4 & 0 \end{vmatrix}) - 0 + (1 \times 0 - 1 \begin{vmatrix} 1 & 3 \\ 1 & 1 \end{vmatrix} + 0) =$$

$$[(3 \times 2 \times (2 - 0) + 3 \times (0 - 8)] - 0 + [1 \times 0 - 1 \times (1 - 3) + 0] = 242$$

need to wolfram alpha..

Definition 1.1.7. Invertible

An invertible matrix for M is symbolized as M^{-1}. It is only invertible if the reduced row echleon form of the matrix M^* is the identity matrix, I_n.

Proposition 1.0.2. $\det(M) \neq 0 \iff M^{-1}$ *exists*

put in own words!

Proof. Let M^* denote the reduced row echelon form of M. We know M is invertible if and only if $M^* = I_n$. Since M^* is obtained from M by performing a sequence of elementary row operations, then by the properties of the determinant (that are listed above) imply that $\det(M)$ is a nonzero multiple of $\det(M^*)$. If M is invertible, then $\det(M^*) = \det(I_n) = 1$, to ensure $\det(M)$ is nonzero.

Conversly, if $\det(M) \neq 0$ then $\det(M^*) \neq 0$, which implies that $M^* = I_n$. Thus, making M invertible. □

Definition 1.1.8. Trace

The trace of a $n \times n$ matrix is the sum of the diagonals

Example 1.1.6. We can show this through a given matrix, M a 4×4 we looked at earlier for the determinant

$$tr \begin{bmatrix} 1 & 2 & 0 & 3 \\ 0 & 1 & 2 & 0 \\ 3 & 0 & 1 & 0 \\ 1 & 4 & 0 & 1 \end{bmatrix}$$

The diagnonals of this matrix are: 1, 1, 1, 1. Let's add them! 1+1+1+1 = 4 Thus, the trace of this matrix is 4.

The trace is useful because we are able to do a lot of mathematical processes with the trace.

Proposition 1.0.3. *Given a $n \times n$ matrix A, B*

$tr(AB) = tr(BA)$

Proof.

$$tr(AB) = \Sigma_i(\Sigma_k A_{i,k} B_{i,k} = tr(BA)$$

$$tr(B) = tr(S^{-}1AS) = tr(ASS^{-}1) = tr(A)$$

□

Definition 1.1.9. Eigenvector/Eigenvalue

Given the Linear Transformation $L : V \to V$, The vector $v \in$?? scalar $\lambda \in F$ set. $Lv = \lambda v$ is called an eigenpair, v is an eigenvector, and λ is an eigenvalue.

An important theorem to consider:

Theorem 1.1. *Invertible Matrix Theorem*

The $n \times n$ matrix A is invertible if and only if 0 is an eigenvalue of A.

These are invertible because there is a pivot position in every column, thus there is only the trivial solution (0) within the matrix.

I DONT KNOW IF THIS ANSWERS THE QUESTION***

I NEED HELP DECIPHERING THIS PART**

Example 1.1.7. Eigenvector/Eigenvalue 1

$\frac{d}{dx}$ functions $\rightarrow$ functions $\frac{d}{dx}e^{cx} = ce^{cx}$, $v = e^x$ and $x = e$

Example 1.1.8. Eigenvector/Eigenvalue 2

Let us have a matrix, M and two vectors, v_1 and v_2

$$M = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}, v_1 = \begin{bmatrix} 1 \\ -1 \end{bmatrix} \lambda = 1, v_2 = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \lambda = 3$$

But how do we find the eigenvectors and eigenvalues?

Proposition 1.1.1. *Given an $n \times n$ matrix M. The roots of* $\det(M - \lambda\, I) = 0$ *are the eigenvalues of M.*

The equation of the characteristic polynomial is as follows:

$$\det(M - \lambda\, I) = 0 \tag{1.1}$$

The I represents the identity matrix and the A symbolizes the matrix that is being used. I DONT KNOW IF THIS COULD BE A PROOF OR IS JUST REALLY AN EXAMPLE***

Proof. Let's us assume we have an $n \times n$ matrix, M.

$$\begin{bmatrix} a_{11} & a_{21} \\ a_{12} & a_{22} \end{bmatrix}$$

We can say

$$M - \lambda I = \begin{bmatrix} a_{11} & a_{21} \\ a_{12} & a_{22} \end{bmatrix} - \begin{bmatrix} \lambda & 0 \\ 0 & \lambda \end{bmatrix} = \begin{bmatrix} -\lambda & a_{21} \\ a_{12} & a_{22} - \lambda \end{bmatrix}$$

Thus, we have the characteristic polynomial $\det(M - \lambda\ I) = -\lambda(a_{22} - \lambda) - (a_{12}(a_{21})) = 0$ Thus, we can find the roots of the equation from there and show the eigenvalues. □

Proposition 1.1.2. *The eigenvalues of a triangular matrix are the entries of the main diagonal*

Proof. By visualizing we can see that the determinant of a triangular matrix is the product of the main diagonal elements. Let

$$M = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ 0 & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & a_{nn} \end{bmatrix}$$

then the characteristic equation is

$$\det(M - \lambda\ I) = \begin{bmatrix} a_{11} - \lambda & a_{12} & \dots & a_{1n} \\ 0 & a_{22} - \lambda & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & a_{nn} - \lambda \end{bmatrix}$$

$$= (a_{11} - \lambda)(a_{22} - \lambda \ldots (a_{nn} - \lambda) = 0 \Rightarrow a_{11}, a_{22}, \ldots, a_{nn}$$

are the eigenvalues of M. □

But how to get v_λ? There are infinitely many of these v's! Because the $\det(M - \lambda\, I) = 0$ so does not exist in M^{-1}. Hence there is no unique solution to $Mv = 3v$.

Definition 1.1.10. We call the solution set of $Mv = \lambda v$ the eigenspace associated to λ.

Example 1.1.9. Let $Mv = 3v$ Let's find v.

$$\begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = 3 \begin{bmatrix} a \\ b \end{bmatrix} \begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \left[\begin{array}{cc|c} -1 & 1 & 0 \\ 1 & -1 & 0 \end{array}\right]$$

Let us add $R_1 + R_2 \to R_2$ in order to form a row of zeros and make the matrix in reduced row echelon form.

$$\left[\begin{array}{cc|c} -1 & 1 & 0 \\ 0 & 0 & 0 \end{array}\right]$$

$$-1a + b = 0$$

$$a = b$$

$$S = \left. \begin{pmatrix} a \\ a \end{pmatrix} \right| a \in R$$

$$v = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \in S$$

Example 1.1.10.

$$\det(\begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} - \lambda\, I) = \det(\begin{bmatrix} 2-\lambda & 1 \\ 1 & 2-\lambda \end{bmatrix}) = 3 - 4\lambda + \lambda^2 \Longleftrightarrow \lambda = 1, 3$$

Corollary 1.1.1. *The homogeneous $n \times n$ linear system $Ax = 0$ has an infinite number of solutions if and only if* $\det(A) = 0$*, and has only the trivial solution if and only if* $\det(A) \neq 0$*.*

Proof. The system $Ax = 0$ has the trivial solution $x = 0$ no matter what. This is the unique solution if and only if $\det(A)neq0$. The only other possibility for the equation is $\det(A) = 0$ which would mean that the system has infinitely many solutions. □

Proposition 1.1.3. ***Invertible***

A matrix is invertible if the simplest form of the matrix is an identity matrix.

Here is an example of the identity matrix:

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

1.2 Combinatorics

Combinatorics is an important concept in mathematics when analyzing graphs and different probabilities. For our research purposes, combinatorics evaluate graphs to find the total number of walks within a graph. Since we will be working with graphs throughout the research, it is important we understand the different theories that are a part of it. The most important aspects are most related to Graph Theory, which we will talk about later in this chapter.

1.2.1 Combinatoric Definitions

Definition 1.2.1. Combinatorial Trace Method

The combinatorial trace method is a technique for establishing equalities between combinatorial expressions and power sums. [[cite paper]]

The method relies on the principle: Given a finite graph G, the number of closed walks of length n equals the sum of the nth powers of the eigenvalues of any adjacency matrix of G.

An example normally given is the Fibonacci sequence. The sequence is recursive, therefore, starting with

$F_{-1} = 1, F_0 = 0, F_{n+2} = F_{n+1} + F_n$

Figure 1.2: An example of a graph.

(Definitions Jasmine and I found but need a credible source for- currently looking for a textbook)

Definition 1.2.2 (Combinatorial Expression)**.** A combinatorial expression is an expression with arithmetic operators as some terms

The Fibonacci and Lucas numbers are examples of this concept.

Definition 1.2.3 (Power Sum)**.** A power sum is a sum of the p^{th} powers on a set of n variables

1.3 Graph Theory

Graph Theory generalizes graphs and gives different theorems and concepts that can be used throughout our research. Understanding different parts of the graph, what they mean for the research and how we can utilize them accordingly. In addition, we will use the definitions, theorems, and proofs from Linear Algebra to help explain the Graph Theory used in the next chapter.

[2]

1.3.1 Graph Theory Definitions

Definition 1.3.1 (Graph)**.** A graph is a physical representation of vertices (nodes), edges, and loops.

Definition 1.3.2 (Vertex)**.** The vertex is the point on the graph. It is also known as a node.

Definition 1.3.3 (Edge)**.** An edge is a path between two vertices.

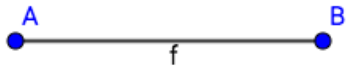


Figure 1.3: A and B represent vertices. f represents an edge.

Figure 2.2 demonstrate vertices and an edge. The vertices both have degree 1.

Definition 1.3.4 (Degree)**.** The degree of a vertex, v, is the number of edges incident with v, and is written deg(v). We can think of it as a number of roads at an intersection.

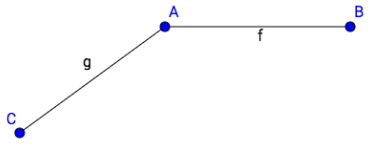


Figure 1.4: A has a degree of 2 and B and C have a degree of one.

As seen in figure 2.3, the degree of each vertex is different. A has a degree of 2 because it is connected to edges f and g.

Definition 1.3.5 (Loop)**.** A loop is an edge starting and ending at the same vertex.

A loop allows a vertex to have a closed walk of length one.

Definition 1.3.6 (Walk)**.** A walk is the path between one vertex to another vertex.

A walk is restricted to go from one node to another node. If it does not make it from one node to another it is not considered a walk.

Definition 1.3.7 (Path)**.** A path is a walk in which no vertex appears more than once.

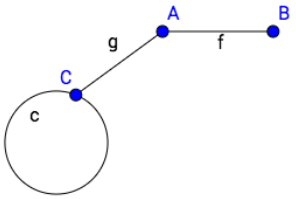
Definition 1.3.8 (Cycle)**.** A cycle is a walk begins at a particular vertex and ends that the same vertex.

add definition of connected

Definition 1.3.9 (Closed Walk)**.** A closed walk is a path that begins at one particular vertex and ends at the same vertex. (v_i to v_i).

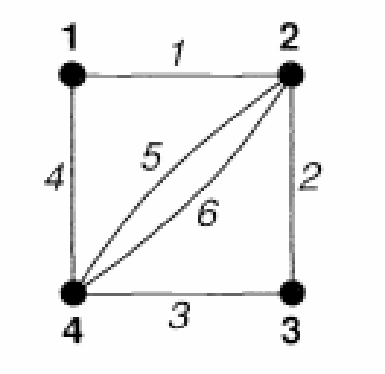
Here is an example of a loop.

Example 1.3.1. Here are words



Definition 1.3.10 (Adjacency matrix)**.** If G is a graph with vertices $1, 2, \ldots n$ its adjacency matrix A is the $n \times n$ matrix whose ijth entry is the number of edges joining vertex i and vertex j.

Example 1.3.2. Let us look at the figure below and determine its adjacency matrix.



$$A = \begin{bmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 2 \\ 0 & 1 & 0 & 1 \\ 1 & 2 & 1 & 0 \end{bmatrix}$$

Therefore, we can see that in the a_{11} entry we are looking at vertex 1 moving along an edge to get back to vertex 1. There is no such vertex therefore the entry is 0. Notice the diagonals are 0. This is because those entries represent the walk from a vertex back to itself. This does not exist so all those entries are 0.

As defined earlier, the trace is the sum of the diagonals in the matrix. If we add these entries up, we also know how many closed walks there are. Thus for a closed walk of length 1, there are no closed walks.

In the next chapter there will be examples to demonstrate these concepts. The three subjects will be linked together to demonstrate the research and how each subject is important.

Chapter 2

Combinatorics and Its Applications

The foundation of the research stems from the Combinatorial Trace Method and the Graph Theory used to further claims and understand concepts.

The **combinatorial trace method** is complex and therefore certain mathematical properties, operations, etc. need to be understood and defined before any further study. [1] Using these concepts we can take certain properties of graphs and apply it to the graphs explored throughout the research. Through these properties and observations we can review back and compare the graphs that are being explored and the general rules and properties it already has from the shape, the vertices, etc.

2.1 Applying the Definitions

Throughout the research, closed walks are explored for different graphs. Let us look at the closed walks in figure 2.1.

For example, the following matrix, A, is an adjacency matrix for the graph:

Figure 2.1: A graph of two vertices

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

This demonstrates a matrix that corresponds to the total number of walks of length one. This does not show the amount of closed walks.

The trace for the matrix A shown above would be equal to 1. The diagonal of the trace is from the top left to the bottom right entry. Here there are only two entries. Thus, the calculation would be:

$$0 + 1 = 1$$

Therefore, the trace is equal to 1. Thus, there is one closed walk of length n

for this graph.

Moreover, the eigenvalue and eigenvectors can be found from this matrix. The determinant equation will be used to find the eigenvalues.

Proposition 2.0.1. *The determinant of the eigenvalues of the adjacency matrix give the total number of closed walks within the graph of a given length.*

We can analyze this proposition:

$$det(A - \lambda\ I) = 0 \tag{2.1}$$

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

The eigenvalues evaluated to be

$$\lambda_1 = \frac{1+\sqrt{5}}{2}, \lambda_2 = \frac{1-\sqrt{5}}{2}$$

The eigenvalues and eigenvectors showcase the total number of closed walks. We can use these eigenvalues and put them to the power of n, length, and add them to find the total number of closed walks.
For example, the total number of walks within a graph of the given length is

represented below:

$$= \lambda_1^3 + \lambda_2^3$$
$$= (\frac{1+\sqrt{5}}{2})^3 + (\frac{1-\sqrt{5}}{2})^3 = 4$$

Thus, there are 4 total number of walks within the given length of 3 in this graph. We will explore this further in the next chapter.

Theorem 2.1. *Graphs without loops do not have a closed walk of length 1.*

Let us look at figure 2.3. We can look at the figure and contemplate

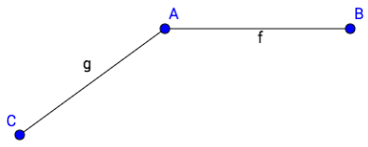


Figure 2.2: Figure 2.3 repeated

different walks we can take. For example, the walk from vertex C to vertex A exists, but the walk from vertex B to vertex C does not exist because there is no edge to connect them. Can we make any closed walks?
Yes, we can walk a walk of length 2 from vertex A to vertex B back to vertex A. Vertex A cannot return to itself with a length of one walk.

Let us assume there exists a closed walk of length 1. Since the only edges that exist within the graph are connected to the center vertex, A, that edge is counted twice. Therefore, the edge cannot be used. Thus, there are no walks without a loop, which connects a vertex to itself.

Proposition 2.1.1. *Graphs without a cycle do not have any total number of odd closed walks.*

The condition onto the graph, G, is that there are only a total number of closed walks of even length. The condition must be followed by all the subsets of G, and G itself.

Proof. For graphs with less than a cardinality of G edges ($|E(G)|$) the statement holds. Let us look at H as a subset of G. Therefore, the condition carries to H, that there cannot exist a total number of odd closed walks. Let there be closed even walks on v_j by the inductive hypothesis.

Let v_i take an edge to v_j, then v_j takes an edge that is not connected to v_i, thus v_j must make a closed walk that is even because there is no cycle within.

Base Case: Let us have a graph with 2 vertices, keep adding edges to the graph. Thus, the base case is satisfied because although adding edges, it is still a subset of G, which means the subset inherits the condition that there are no total number of odd closed walks.

IH: For graphs with less than ($|E(G)|$) edges, keep adding edges and assume it works for the small graph.

Then G can take any path and any vertex, but still has to encounter them twice because of the condition. Thus, let us remove an edge ad have it have 1 less edge. By the condition, v_j must have an even number of total closed

walks, because although only removed one edge, two walks along that edge were eliminated. Moreover, if the edge that was removed is added back, the edge will bring bacck a plus 2 number of walks. Therefore, it will force the condition back onto G. □

From this proof, we know that any subsets of the same symmetric graph hold the same condition, therefore, it is expected that the rest of the hydrocarbons do not have an odd total number of closed walks.

2.2 The Combinatorial Trace Method in Action

At the beginning of the research, the paper "The Combinatorial Trace Method in Action" was utilized and evaluated for further understanding of the world of combinatorics and how there can be different uses for the method.

If we look at the figure that was presented from the paper: *"The Combinatorial Trace Method in Action"*

Krebs and Martinez demonstrate the figure shown below.

Figure 2.3: The Combinatorial Trace Method in Action Example

The Combinatorial Trace Method in Action continues the idea stated

previously with eigenvalues, eigenvectors, adjacency matrices, etc. with the Fibonacci sequence and Lucas numbers.

The team used the Binet Formula

$$L_n = \phi^n + \phi^{-n}$$

This equation yielded

$$\phi = \frac{1+\sqrt{5}}{2}, \bar{\phi} = \frac{1-\sqrt{5}}{2}$$

The form of this equation-a combinatorial expression on the left and a power sum on the right-immediately suggests that the combinatorial trace method is applicable for an appropriate graph. This graph consists of two vertices a and b with an edge between them and a loop at b.

The walks that are ≥ 2 walks at b can either be back and forth along the edge or going around the loop. Hence the formula

$$B_n = B_{n-1} + B_{n-2}$$

By definition of the Fibonacci numbers, it can be said that $B_n = F_{n+1}$ Continuing this pattern, the number of closed walks of length 0 beginning at a is equal to 1 which is equal to F_{-1}. Moreover, the number of closed walks of length 1 is equal to 0, thus is equal to F_0. For all the closed walks ≥ 2,

consists of back and forth along the edge and around the loop at b with a closed walk of length $n-2$. Therefore, it gives the closed walks of length n to be equal to $B_{n-2} = F_{n-1}$.

The identity of the Lucas numbers is: $L_n = F_{n+1} + F_{n-1}$ it was found that the total number of closed walks in the graph of length n was $L_n = A_n + B_n$. This would include that the adjacency matrix would be the one given above and restated below.

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

with the eigenvalues stated previously. Therefore, this ensures a concrete path to finding a graph from an adjaceny matrix and its eigenvalues or vice versa, where the graph can help find the adjaceny matrix and the eigenvalues.

Let us think about our previous proposition:

Proposition 2.1.2. *The determinant of the eigenvalues of the adjacency matrix give the total number of walks within the graph of a given length.*

To further demonstrate this idea we can look at another example.

Let us evaluate the graph given previously.

We can create an adjacency matrix for the graph based on the number of vertices we have. Thus, the matrix will be a 2×2 matrix.

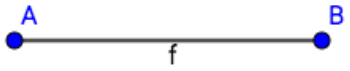


Figure 2.4: Another graph

$$\begin{bmatrix} w & x \\ y & z \end{bmatrix}$$

We will look for the total number of closed walks of length 1.

Looking at the first spot of the matrix, $a_{1,1}$, (denoted w), we evaluate whether there is a closed walk of length one from vertex A to itself. There does not exist such a walk therefore we will put a 0 in that spot.

$$\begin{bmatrix} 0 & x \\ y & z \end{bmatrix}$$

Moreover, the next spot x is a closed walk of length 1 from vertex A to vertex B. There is a walk that exists, thus, the number would be 1.

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

In addition, we can continue in this fashion and find:

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

Thus, this would be the resulting matrix.

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

$$\det \begin{bmatrix} -\lambda & 1 \\ 1 & -\lambda \end{bmatrix}$$

This would yield $\lambda^2 - 1$ which equals

$$(\lambda + 1)(\lambda - 1) = 0$$

$$\lambda = \pm 1$$

Thus, the eigenvalues were evaluated using the adjacency matrix and its determinant.

Chapter 3

Chemistry

3.1 A Chemical Background

Definition 3.1.1. Chemistry is the study of matter and the changes that material substances undergo.

There are different uses in chemistry that coincide directly with mathematics. Within chemistry, there are different visual representations utilized to symbolize different chemical structures. For example, there exists a form of illustration called the "Lewis Dot Structure."

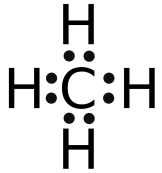


Figure 3.1: The Lewis Structure of a methane molecule.

The Lewis Structure of a molecule shows how the valence electrons are arranged among the atoms in the molecule. There exist rules which govern the formation of Lewis Structures for molecules. The most important rule for the formation requires the molecule to achieve noble gas configuration. (cite) An example of a Lewis Dot Structure can be seen in Figure 3.1. This means the molecule attains a total of eight valence electrons around the elements within the molecule.

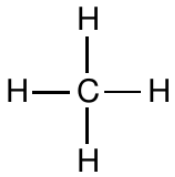


Figure 3.2: The molecular structure of methane.

The two dots represent a bond between the elements and can be replaced with a line. Figure 3.2 demonstrates this concept.

The illustration can translate to a mathematical graph that can be evaluated for the amount of walks that can be done throughout the structure. As mentioned before in the previous chapter, the graphs are used in combinatorics to count the number of closed walks. Thus, we can apply our knowledge of combinatorics to molecular structures and see if a pattern presents itself.

3.2 Combinatorics and Chemistry

Combinatorics can be used to explore chemical molecular structures. Similar to the mathematical graphs seen throughout previous chapters, there is a relationship that molecular bonds share that can be used within combinatorics. There are different types of structures that can represent a bond between elements.

Chapter 4

Application: Chemical Combinatorics

Combinatorics can be used to explore different areas of study. The chemical bonds represented by Lewis Structures can be evaluated for the total number of closed walks. Moreover, the closed walks may present a pattern that can be utlizied for the different molecular structures which may create a pattern. This pattern may be used to find a general equation to find the total number of closed walks, which can be applied to all the hydrocarbons being tested.

4.1 Methane

Methane is a molecule that is part of the alkane group. The representation of the molecular structure is presented in Figure 4.1.

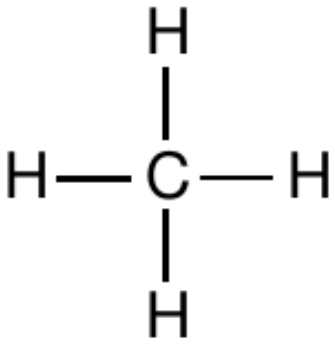


Figure 4.1: The molecular structure of methane.

This can be viewed as a graph to count the total number of walks throughout the structure.

Therefore, the graph contains 4 edges and 5 vertices represented by bonds (for edges) and the elemental symbol (for vertices.)
We can represent the structure as a mathematical graph we recognize.

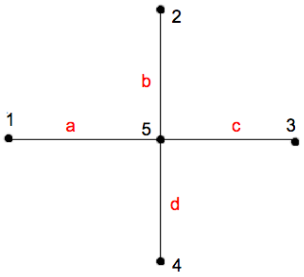


Figure 4.2: The graphical representation of the methane molecular structure.

Figure 4.2 illustrates the edges annoted as letters and the vertices annotated with numbers. To find the total number of walks, the adjacency matrix must

be calculated and its determinant found.

The adjacecy matrix shows how many walks from one vertex to another vertex has. Here the adjacency matrix is showing the total number of walks with length 1.
We can explore the number of walks throughout the molecule. From v_5 we notice that it has the most access over the other vertices. It can use all of the edges that are part of the molecule. The outlying vertices cannot reach each other without taking the edge to the center vertex first. Noticing this, we can make propositions about it.

Proposition 4.0.1. *Total number of closed walks of length 3 does not exist on the methane graph.*

Proof. We are given the methane graph and wish to prove that a closed walk of length 3 does not exist. We will do this via contradiction and assume that the closed walk of length 3 does exist.

Case 1: Outlying vertex Assuming the closed walk of length 3 exists, then I can take any vertex and have it make that closed walk. Let us take vertex v_n. We leave v_n via edge e_i. Thus, one walk is used. Due to the structure of the graph, we have four options to choose from to take another edge. We choose e_j. e_j leaves us at another vertex, v_m. We only have one more walk left. Because of the graphs structure we must take the same edge, e_j to return to the center vertex. We have used our three walks and

have not returned to our beginning vertex, v_n. Thus, we have reached our contradiction.

Case 2: Center vertex Asssume we start with the center vertex, v_p. v_p has four edges to choose from. v_p commits to an edge. Since there are no cycles within the graph, the walk must return to v_p. Thus, there are two walks already used and we already returned to our beginning vertex. Therefore, we have reached a contradiction.

□

The proof is characteristic of all vertices within the graph. We also know from the earlier chapters that there cannot be an odd total number of closed walks. This proposition furthers this claim.
In addition, we know that there are connections between the center and the rest of the vertices. Thus, we can propose the impact of the center vertex, as follows:

Proposition 4.0.2. *The total number of closed walks of length 4 from the outlying vertices will be equal to the number of closed walks of length 2 from the center vertex.*

Proof. We are given the methane graph and we wish to prove the total number of closed walks of length 4 is equal to the total number of closed walks of length 2. There are a total number of 4 closed walks for the length of 2.

Case 1: Outlying vertex Since, the first and last spot are already taken because we have to take the same edge back as we started with. Thus,

there are only two more spots left. Those steps are controlled by the center vertex. Once a step is commited to, the same step must be taken back. Thus, the inner walks of length 4 are the closed walks of length 2 from the center vertex. □

Theorem 4.1. *The hydrocarbons will not contain odd number of closed walks.*

Proof. Referring back to chapter 2 proposition 2.1.1 □

Lemma 4.2. *The hydrocarbons will only contain even number of closed walks that will be controlled by the center vertices.*

Let us explore our propositions. The total number of closed walks for even length can be found using the equation as a foundation.

$$W_G^1(2m) = W_G^5(2m-2) \tag{4.1}$$

Equation 4.1 demonstrates the total even closed walks from vertex 1. We can add these total even closed walks for every vertex to find the total number of even closed walks.

$$W_G^i(2m) = W_G^1(2m) + W_G^2(2m) + ...W_G^5(2m)W_G^i(2m) = 2^{2m+1}$$

Therefore, we can create an equation that establishes an overall definition for total even closed walks within a methane molecule.

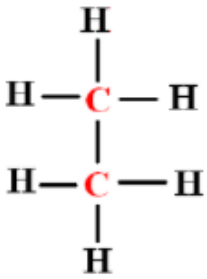


Figure 4.3: The molecular structure of the ethane.

$$W_G^i(2m) = 2^{2m+1} \tag{4.2}$$

Equation 4.2 can possibly used later to reveal a pattern within ethane - C_2H_6.

4.2 Ethane

There are three other hydrocarbons that can be explored for closed number of walks. Analyzing each may yield a pattern that facilitates the prediction of how a molecular structure forms, and how the structure looks.

This structure contains the same symmetry as methane, but with an added "methane" shape, that allows the same conditions to apply.

There are two cases that can be examined for the ethane molecule

1. Staying inside the structure formally known as methane – which we already have the formula for.

2. The closed walks must include new edges represented by the labelling (**a, b, d**) that are from the "methane" part of the molecule with a walk that begins at the "ethane" part of the molecule.

We can create a graphical illustration, like the methane graph made previously, to help follow the walks we wish to count from particular vertices using particular edges that are labeled. For simplicity, we will continue to add to the graph of the methane molecule, therefore having the same labelled edges and vertices to help seek out patterns from one part of the hydrocarbon to the other.

– add picture here –

When including new edges and the original case of remaining inside the "methane" shape, the equation below arises:

$$W^C_{G_{1,4}} = (W^l_{G_{1,4}}(4) - 1) \times 6 + W^C_{G_{1,4}}(6) + W^l_{G_{1,4}}(6) \tag{4.3}$$

4.3 Propane

We are going to explore propane to determine if there are any patterns that are similar to the previous 2 hydrocarbons.

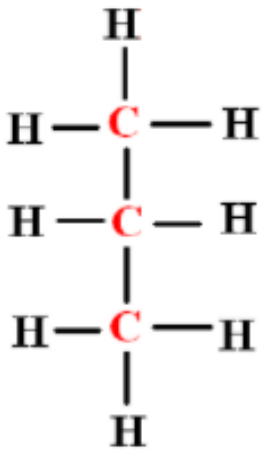


Figure 4.4: The molecular structure of the propane.

To continue our search further we want to find patterns from the methane and ethane molecules that are present in the propane molecule. First, we have two cases, which are:

1. The center vertex
2. The outlying vertices (which are the same due to symmetry therefore we can use one to represent all)

Let us examine. We already know due to our earlier proposition that there will not be any total number of odd closed walks within the molecule. Thus, we will examine the total number of even closed walks.

Analyzing a walk of length 2 we will discover that the pattern is the same as all of the other hydrocarbons thus far. We only have one edge that can

move away from the beginning vertex and the same edge to return to it. Therefore, we can move on to determine any patterns in a closed walk of length 4.

Looking at a closed walk of length 4 starting at vertex 1, we can see that we begin with only one option to move away from v_1 to get to v_4. Moreover, v_4 has 3 options to be chosen from. After the choice is made, there is only one choice that can be made to get back to v_4 and leave that particular vertex, and only one more walk left to return back to v_1. We can discern that the final 2 walks within the length 4 walk is actually a walk of length 2. We can generalize this discovery, but to be sure, we can confirm this pattern with one more even closed walk. Let us look at an even closed walk of length 6.

For the condition of a closed walk of length 6, we have two cases.

1. Staying within the partial graph that only contains v_4 as the center and 4 oulying vertices that are directly connected to it.

2. Moving to $G_{2,6}$ which is the ethane molecule.

For case 1, we already know that there will only be one option to leave v_1 and only option to return to v_1. Therefore, the first and last spots of our walk are already taken. Thus, we are left with a closed walk of length 4 from vertex 4. This is because v_1 – similar to other outlying vertices– are connected to v_4 and must return back to v_4 to ensure the walk will be closed (will return to the beginning vertex.)

For case 2, there still contains a closed walk of length 4, with the beginning and ending walks only containing one option.

Therefore, we can draw a conclusion from these patterns to generalize all hydrocarbon structures.

Proposition 4.2.1. *Let i be a leaf in $G_{C,H}$ and $a_{i,j} \in E(G_{C,H})$. Then,* $W^i_{G_{C,H}}(2m) = W^j_{G_{C,H}}(2m-2)$

Thus, we can use this equation to represent all outlying vertices for every hydrocarbon, because the shape never changes. Therefore, the properties of the hydrocarbon never change and the symmetry remains.

$$W^i_{G_{C,H}}(2m) = W^j_{G_{C,H}}(2m-2) \tag{4.4}$$

Chapter 5

Further Directions

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[2] Robin J. Wilson. *Introduction to graph theory*. Longman, Harlow, 1996. Fourth edition [of MR0357175].