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On 4-Regular Planar Hamiltonian Graphs

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ON 4-REGULAR PLANAR HAMILTONIAN GRAPHS

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Abstract
The task of generating large knots and links with uniform probability is very difficult. In order to research knots with large crossing numbers, one would like to be able to select a random knot from the set of all knots with $n$ crossings with as close to uniform probability as possible. The underlying graph of a knot diagram can be viewed as a 4-regular planar graph. The existence of a Hamiltonian cycle in such a graph is necessary in order to use the graph to compute an upper bound on rope length for a given knot. The algorithm to generate such graphs is discussed and an exact count of the number of graphs is obtained. In order to allow for the existence of such a count, a somewhat technical definition of graph equivalence is used. The main result of the thesis is the asymptotic results of how fast the number of graphs with $n$ vertices (crossings) grows with $n$. 
CHAPTER 1

Defining and Counting the Number of Graphs

1.1. Introduction

A knot is a simple closed curve in three space. A link is a collection of knots. In other words, a link is a group of simple closed curves. Each knot that is a member of a link is called a component of the link. Imagine a knot drawn on the plane. If the curve passes over itself, this intersection is called a crossing. Figure 1 shows an example of a knot with 9 crossings on the top. If one forgets the information of which strand goes over or under at a crossing, then the knot diagram turns into a 4-regular planar graph where at each crossings there is now a vertex of the graph. In fact, every 4-regular planar graph can arise in this way from a knot or link diagram.

Figure 1. A knot diagram representing a knot with nine crossings and its underlying 4-regular planar graph.
The task of generating large knots and links with uniform probability is very difficult. It is not known how many knots and links exist with $n$ crossings. It is also not known what a typical knot and link with $n$ crossings should look like [4].

In order to research knots with large crossing numbers, one would like to be able to select a random knot from the set of all knots with $n$ crossings with as close to uniform probability as possible. The motivation for this thesis arises in this context.

The rope length of a knot can be thought of as the shortest amount of rope needed to create a given knot. The goal is to eventually be able to compute an upper bound on rope lengths for knots with very large crossing numbers. To compute the upper bound on rope length, a Hamiltonian cycle must exist in the knot diagram [3]. A knot diagram can be viewed as a 4-regular planar graph $G$ and the Hamiltonian cycle in the knot diagram is now a Hamiltonian cycle in $G$. Therefore, instead of sampling the space of knots and links with very large crossing numbers, this thesis will concentrate on sampling the underlying planar graphs. In general, finding a Hamiltonian cycle in a given graph is computationally very difficult [6]. It is a well known NP-complete problem, thus the following methods are proposed.

(1) Instead of random knot diagrams, we shall generate random 4-regular planar graphs.

(2) Instead of generating such a graph and finding a Hamiltonian cycle, we shall begin with a given Hamiltonian cycle and construct the graph around the cycle.

A method to construct graphs around a Hamiltonian cycle has been proposed before, but a worst case run-time complexity of $O(n^3)$ for a single graph with $n$
vertices [4][5]. This thesis suggests a method that will run at a run-time complexity of \( O(n) \) to generate a single graph with \( n \) vertices. The issue of algorithmic complexity will not be addressed in this thesis (but details can be seen in [2]). In Chapter 1 the algorithm to generate the graphs is discussed and an exact count of the number of such graphs is obtained. In order to allow for the existence of such a count, a somewhat technical definition of graph equivalence is used (see Definition 1.3.2).

Chapter 2 contains the main result of this thesis, namely estimates on how fast the number of such graphs with \( n \) crossings grow with \( n \).

1.2. Basic Definitions

The following definitions are necessary to understand the content of this thesis, and can be found in any standard text in graph theory[6].

A graph \( G \) is a structure that consists of two sets \( V \) and \( E \). The elements of \( V \) are called vertices and the elements of \( E \) are called edges. Each edge has a set of one or two vertices associated to it, which are called its endpoints. If vertex \( v \) is an endpoint of edge \( e \), then \( v \) is incident on \( e \), and \( e \) is incident on \( v \).

A cycle of a graph \( G \) is a closed path of edges that contains no repeated vertices or edges.

A Hamiltonian cycle of a graph \( G \) is a cycle that contains every vertex of \( G \).

A graph isomorphism \( f: G \rightarrow H \) between two graphs \( G \) and \( H \) is a pair of bijections \( f_V: V_G \rightarrow V_H \) and \( f_E: E_G \rightarrow E_H \) such that for every edge \( e \in E_G \), the function \( f_V \) maps the endpoints of \( e \) to the endpoints of the edge \( f_E(e) \).
A 4-regular graph is a graph $G$ where every vertex is incident to four edges. If an edge has only one endpoint, then it is said to be a loop edge and counts as two edges incident to a vertex.

A cyclic graph $C_n$ is a graph with $n$ vertices such that all of its vertices and edges lie on one circle.

A drawing of a graph $G = (V, E)$ on a surface $S$ (or an embedding of $G$ on $S$) must satisfy the following conditions:

(i) The vertices of $G$ are disjoint points on $S$.

(ii) The drawing of an edge is a continuous path on $S$ such that

a) The drawing of an edge does not intersect itself except possibly at the endpoints of the edge.

b) The drawing of an edge does not intersect any vertices except at its endpoints.

c) The drawing of two edges do not intersect except possibly at their endpoints.

A diagram is a drawing of a graph $G$ on the surface $S$.

A planar graph is a graph that has an embedding in the plane or the sphere.

A spherical graph is a graph that has an embedding in the sphere.

The Riemann stereographic projection is the function $\rho$ that maps each point $w$ of the sphere (tangent at the south pole to the $xy$-plane in Euclidean 3-space) to the point $\rho(w)$ where the ray from the north pole through the point $w$ intersects the $xy$-plane; see Figure 2.
**Remark:** Note that every planar graph is spherical and every spherical graph is planar. This is a common theorem from any standard graph theory text [6]. These properties come from the idea of the Riemann stereographic projection. Given a graph drawn on the sphere, the projection allows a move to the plane.

Finally, we define some terms that can be found in a standard text in topology [7][1].

The *standard coordinate system* to be used in this paper is the three-dimensional system where the *x-axis* runs horizontal (left to right), the *z-axis* runs vertical, and the *y-axis* runs front to back (perpendicular to the *x-axis*).

A *homeomorphism* is a one-to-one, onto, continuous function with a continuous inverse.

### 1.3. What is a rooted Hamiltonian graph?

**Definition 1.3.1.** A rooted Hamiltonian graph $G$ is a quadruple $(S^2, G, H, i)$ that satisfies the following conditions:

(i) $G$ is a 4-regular planar graph embedded in $S^2$.

(ii) $H$ is an oriented Hamiltonian cycle in $G$ with labeled vertices (or equivalently labeled edges) that is $H = v_1e_1v_2e_2v_3 \ldots e_{n-1}v_nv_1$

(iii) $i$ identifies one of the disks bound by $H$ on $S^2$ as inside.

**Definition 1.3.2.** Two rooted Hamiltonian graphs $(S^2, G, H, i)$ and $(S^2, G', H', i')$ are equivalent if there exists a function $f : (S^2, G, H, i) \rightarrow (S^2, G', H', i')$ such that:
(i) \( f \) is a homeomorphism of \( S^2 \).

(ii) \( f(G) = G' \), and \( f|_G \) is an isomorphism of graphs.

(iii) \( f(H) = H' \), and \( f \) preserves the orientation of the Hamiltonian cycles such that \( f(v_i) = v_i' \) (or equivalently \( f(e_i) = e_i' \), for \( i = 1, 2, \ldots, n \)).

(iv) \( f(i) = i' \); that is, the inside disk of \( G \) maps to the inside disk of \( G' \).

The goal is to create rooted Hamiltonian graphs algorithmically and to count their number. The construction of an embedding of such a graph in \( S^2 \) begins with a cyclic graph on \( n \) vertices. Edges are then added between those vertices to create a 4-regular planar graph.

The following terminology will be used to describe the construction of rooted Hamiltonian graphs.

Let \( H \) be the Hamiltonian cycle.

**Crossing:** Any vertex \( v_i \) that lies on the cycle \( H \) (\( i = 1, 2, \ldots, n \)).

**Inside:** The side of the cycle \( H \) labelled as inside.

**Outside:** The side of the cycle \( H \) not labelled as inside.

**Inside edge:** Any edge \( e \in G \) that is completely contained in the inside of \( G \).

**Outside edge:** Any edge \( e \in G \) that is completely contained in the outside of \( G \).

**Double inside point (D-):** A crossing on \( H \) that is incident to only inside edges.

**Double outside point (D+):** A crossing on \( H \) that is incident to only outside edges.
Transition point \((T)\): A crossing on \(H\) that is incident to one inside edge and one outside edge.

Positive prefix vector: A string of 1s and 0s such that there is an equal number of 1s and 0s and the number of 0s is never greater than the number of 1s when considering an initial substring of 1s and 0s.

Using Definition 1.3.2, observe that each equivalence class of rooted Hamiltonian graphs admits a diagram \(D\) created by the following steps.

Let \(G\) be a rooted Hamiltonian graph.

1. On \(S^2\), deform \(G\) by an isotopy so that:
   
   - \(H\) is the equator.
   
   - The crossings \(v_1, v_2, \ldots, v_n\) are evenly spaced around \(H\).

2. If necessary, rotate \(S^2\) so that:
   
   - The crossings traverse in clockwise order when looking down at the sphere from the north direction.
   
   - \(v_1\) lies at the furthest negative \(y\) position of the sphere.

3. If the inside disk \(i\) is not the southern hemisphere of the sphere, modify \(G\) by the reflection \((x, y, z) \mapsto (x, y, -z)\) for every point \((x, y, z) \in G\).

4. If necessary, deform \(G\) by an isotopy so that no edge intersects the north pole.

5. Create a diagram of \(G\) by a Riemann stereographic projection (Figure 2).

Notice that the equator \(H\) will be mapped to a circle containing all the vertices, with the inside disk \(i\) now lying on the inside of this circle. Crossing \(v_1\) should lie at the
Figure 2. The Riemann stereographic projection. The point $w$ is mapped to the point $p(w)$ in the plane.

12:00 position on the circle, with the other crossings evenly spaced out in clockwise order.

**Definition 1.3.3.** A planar diagram of $G$ created by the steps 1, 2, 3, 4, and 5 will be called a **standard diagram** of $G$.

Figure 6 shows an example of a standard diagram. From now assume that all rooted Hamiltonian graphs are drawn using standard diagrams.

### 1.4. Generating rooted Hamiltonian graphs

The goal is to generate standard diagrams of rooted Hamiltonian graphs algorithmically. Each standard diagram represents one class of equivalent rooted Hamiltonian graphs. If one wishes to generate rooted Hamiltonian graphs with uniform probability, then it would be useful if one can count the number of different rooted Hamiltonian graphs with a fixed number of crossings $n$. 
The construction of such a diagram begins with a cyclic graph on \( n \) vertices \( C_n \). The vertices will be evenly spaced around the cycle with \( v_1 \) at the 12:00 position and traversing clockwise. This cycle of vertices and edges will serve as the Hamiltonian cycle. At \( v_1 \), a mark will be placed towards the disk on the right of the cycle (if traversing clockwise) to indicate the inside \( i \). Each vertex (or crossing) must become either a double inside point, double outside point, or transition point. The next step is to decide which crossings are to become which type of these three points.

First, choose \( 2t \) transition points from \( n \) crossings, where \( 2t \in \{0, 2, 4, \ldots, n\} \) if \( n \) is even, and \( 2t \in \{0, 2, 4, \ldots, n - 1\} \) if \( n \) is odd. Note that the number of transition points must be even. This can be seen as follows: Consider the inside edges of a graph \( G \). The \( s \) edges require \( 2s \) attachment points. The attachment points for the edges are either coming from double inside points or the transition points. The double inside points create an even number of attachment points on the inside and so the transition points must also create an even number of attachment points. The number of ways to choose \( 2t \) transition points from \( n \) crossings is \( \binom{n}{2t} \).

From the remaining \( n - 2t \) crossings, next choose \( p \) crossings to be double inside points. The remaining \( n - 2t - p \) crossings will all become double outside points. The total number of ways to choose these points is then:

\[
\binom{n}{2t} \binom{n - 2t}{p} \binom{n - 2t - p}{n - 2t - p} = \binom{n}{2t} \binom{n - 2t}{p}
\]

This value will be frequently referred to as the number of arrangements of points. Such an arrangement of points is shown in Figure 3.
Notice there is always an even number of inside edge-endpoints and an even number of outside edge-endpoints. An edge-endpoint is a fragment of a future edge. At this stage, for each crossing it is only known if it is going to be connected to only outside edges, only inside edges, or one of each. It is not yet known which crossings will form edges together. For an example of the edge-endpoints see Figure 4. From this point, the edges will be connected using two positive prefix vectors: one for the inside edge-endpoints and one for the outside edge-endpoints. These vectors will be known as the inside vector and the outside vector. Starting at $v_1$ and traversing clockwise, the first outside edge-endpoint is chosen and considered the starting outside edge-endpoint. The starting inside edge-endpoint is determined similarly (Figure 4).

**Connecting the edges:**

Suppose one wishes to connect the inside edges using the inside (positive prefix) vector. Because there are $2t$ transition points and $p$ double inside points, this results in $2t + 2p$ inside edge-endpoints. This means an inside vector of size $2t + 2p$ is needed. Each digit in the vector will represent a unique inside edge-endpoint. Beginning at the starting inside edge-endpoint and encountering the other inside edge-endpoints.
in clockwise order, if a 1 appears in the vector an edge is started and if a 0 appears an edge is closed with the nearest available started edge. For an example, see Figure 5.

The number of positive prefix vectors of size $2x$ is $\frac{1}{x+1} \binom{2x}{x}$, which is also commonly called a Catalan number [9]. Therefore, there are $\frac{1}{t+p+1} \binom{2t+2p}{t+p}$ ways to choose the inside vector. The outside edges are connected in the same way using an outside vector of size $2n - (2t + 2p)$, because there are $2n$ total edge-endpoints. There are then $\frac{1}{n-t-p+1} \binom{2n-2t-2p}{n-t-p}$ ways to choose the outside vector. It is then clear that there are

$$\frac{\binom{2t+2p}{t+p}}{(t + p + 1)} \frac{\binom{2n-2t-2p}{n-t-p}}{(n - t - p + 1)}$$

ways to connect all the edges. This value will be referred to as the number of edge constructions in the future. Figure 6 shows an example of a standard diagram after the edge connections.
Once all the edges are connected, these graphs become 4-regular, planar, standard diagrams. We now have our standard diagram, and we wish to count the total number of graphs we can construct in this manner. Recall that the orientation of the Hamiltonian cycle \( H \) is fixed as the clockwise direction the inside \( i \) points to the inside of the circle.

Given values for \( t \) and \( p \), we know there are \( \binom{n}{2t} \binom{n-2t}{p} \) ways to arrange the points, and \( \frac{(2t+2p)!}{t!p!(n-2t-2p)!} \frac{n-t-p+1}{(t+p+1)(n-t-p+1)} \) ways to connect all the edges.

This means that there are \( \binom{n}{2t} \binom{n-2t}{p} \binom{2t+2p}{t+p} \binom{2n-2t-2p}{n-t-p} \frac{n-t-p+1}{(t+p+1)(n-t-p+1)} \) total graphs for a fixed \( t \) and \( p \).
We now wish to exhaust all possibilities for $t$ and $p$. As mentioned before, $2t \in \{0, 2, 4, \ldots, n\}$ if $n$ is even, and $2t \in \{0, 2, 4, \ldots, n-1\}$ if $n$ is odd. So $t \in \{0, 1, 2, \ldots, \lfloor \frac{n}{2} \rfloor \}$ will ensure that $2t$ will be even and in the desired interval. Once $t$ is chosen, the number of double inside points $p$ must be chosen such that $p \in \{0, 1, 2, \ldots, n - 2t\}$. The number of double outside points will be dependent on both these values. So to exhaust all possibilities, we end up with the following double summation for our total number of graphs:

$$
\sum_{t=0}^{\frac{n}{2}} \sum_{p=0}^{n-2t} \binom{n}{2t} \binom{n-2t}{p} \frac{(2t+2p)}{(t+p+1)} \frac{(2n-2t-2p)}{(n-t-p+1)}
$$

(1.4.1)

1.5. Verifying the Count of Diagrams

The reason for the strict restrictions for equivalence in Definition 1.3.2 was to rule out the possibility of unnoticed symmetry in the graphs. For example, in Figure 7 parts of two standard diagrams $G$ and $H$ are shown. Assume the parts of $G$ and $H$ not
shown are identical. If this is the case, then the two graphs are isomorphic (Simply flip the "lunar shape" from the outside to the inside). If $G$ and $H$ were to be counted as one graph, the formula would have to account for all such flips, which would be difficult to do. Notice $G$ is not equivalent to $H$ by Definition 1.3.2. The situation is even more complicated if the Hamiltonian cycle need not be fixed between the two graphs. For example, the standard diagrams in Figure 8 are counted as distinct even though they are isomorphic as graphs. Algorithmically it is extremely difficult to find a single Hamiltonian cycle in a graph, let alone the set of all Hamiltonian cycles. Therefore, combinatorically it would be seemingly impossible to keep track of these graphs if one used a loose equivalence definition.

If one wants to generate these graphs with uniform probability, the first step is to create a count of these graphs. It will now be shown that every graph accounted for in our count is unequivalent by Definition 1.3.2.
Figure 8. $G$ and $H$ are two identical graphs. In $G$ and $H$, two different Hamiltonian cycles are chosen indicated by the thick lines. Only the parts where the Hamiltonian cycles differ are shown. Then $G$ and $H$ are not equivalent according to Definition 1.3.2.

Theorem 1.5.1. Suppose $G$ and $G'$ are rooted Hamiltonian graphs. Then $G$ is equivalent to $G'$ if and only if $G$ and $G'$ reflect the same element in the count

$$
\sum_{t=0}^{\frac{n}{2}} \sum_{p=0}^{n-2t} \binom{n}{2t} \binom{n-2t}{p} \frac{\binom{2t+2p}{t+p}}{(t+p+1)(n-t-p+1)} \left(\frac{2n-2t-2p}{n-t-p}\right)
$$

Proof. Suppose first that $G$ is equivalent to $G'$. Then they can be represented by standard diagrams $D$ and $D'$, respectively. We wish to show that $D$ and $D'$ are counted by the same element $\alpha$ in the count. Since $G \sim G'(\text{equivalent})$, there exists a homeomorphism $f$ of $S^2$ between the two graphs. This implies that the cyclic ordering of edges around each vertex must be preserved between the two graphs. Furthermore, since $f(H) = H'$, $f(\text{upper hemisphere of } G)$ must equal either the lower hemisphere of $G'$ or the upper hemisphere of $G'$. But since $f(i) = i'$, this forces $f(\text{upper hemisphere}) =$ upper hemisphere and $f(\text{lower hemisphere}) =$ lower hemisphere. In terms of $D$ and $D'$, the inside disk of $D$ will map to the inside disk of $D'$ and similarly the outside disk of $D$ will map to the outside disk of $D'$. This, along with the cyclic ordering preservation forces an identity around a thin strip of the equator between $D$ and $D'$. This implies that both equators will have the same edge-endpoint locations around the cycle. Furthermore, it follows that $D$ and $D'$ will have the same number
of double inside points, double outside points, and transition points. So it must be the case that they represent the same $t$ and $p$ values in 1.4.1.

The identity about a thin strip of the equator also implies that the arrangement of points will also be the same between $D$ and $D'$. Therefore they will represent the same entry in the arrangement of points quantity in our count value of $\left(\binom{n}{2t}\binom{n-2t}{p}\right)$.

*Claim 1:* The two prefix vectors must be the same in $D$ and $D'$. Claim 1 will be proven below. This implies that $D$ and $D'$ use the same entry in the edge construction quantity of our count value $\frac{(2t+2p)}{t+p+1} \frac{(2n-2t-2p)}{(n-t-p+1)}$. Therefore, it must be the case that $D$ and $D'$ represent the same element $\alpha$ in the count, and therefore $G$ and $G'$ must also both represent $\alpha$.

To prove the other direction, begin by assuming $G$ and $G'$ are embeddings that reflect the same element of the count. We want to show that $G \sim G'$. This will be done by showing that each element $\alpha$ represents a unique standard diagram $D$.

A random element $\alpha$ of the count reflects some $t$ and $p$ value. It will also reflect one unique way to arrange the points out of a possible $\left(\binom{n}{2t}\binom{n-2t}{p}\right)$ ways given $t$ and $p$. Also, $\alpha$ reflects one unique way to choose an outside vector and an inside vector out of a possible $\frac{(2t+2p)}{t+p+1} \frac{(2n-2t-2p)}{(n-t-p+1)}$ ways. We have only one method of connecting the edges, so $\alpha$ also reflects one unique way to connect the edges out of a possible $\frac{(2t+2p)}{t+p+1} \frac{(2n-2t-2p)}{(n-t-p+1)}$ ways. Therefore, $\alpha$ reflects a unique standard diagram that is one unique way to arrange the points and connect the edges out of the possible $\left(\binom{n}{2t}\binom{n-2t}{p}\right)$ ways to connect the edges given $t$ and $p$. 
Finally, $\alpha$ also reflects a unique value for $p$ out of the possible $n - 2t + 1$ ways to choose $p$ given $t$ and $n$, and reflects a unique value for $t$ out of the possible $\frac{n}{2} + 1$ ways to choose $t$ given $n$. Therefore given $n$, $\alpha$ reflects one unique way to choose a $t$ and a $p$, arrange the points, and connect the edges out of a possible ways. This implies that $\alpha$ reflects a unique standard diagram. Therefore, $G$ and $G'$ reflect the same standard diagram $D$, so it must be the case that $G \sim G'$. It remains to prove Claim 1.

Proof of Claim 1: It is known that the arrangement of points in the two graphs is identical. It needs to be shown that both graphs use the same outside vector and the same inside vector. Notice that because the arrangement of points is identical, both graphs will have the same starting outside edge-endpoint and the same starting inside edge-endpoint. First consider the outside vectors. Let $v$ be the outside vector for $G$ and $v'$ be the outside vector for $G'$. It needs to be shown that $v = v'$. Suppose instead that $v \neq v'$. We know both vectors will contain $m$ digits, where $m$ is the number of outside edge-endpoints. It is known that $v = a_1a_2\ldots a_m$ and $v' = b_1b_2\ldots b_m$ where $a_i$ and $b_i$ are either 1 or 0, for every $i \in \{1,\ldots, m\}$. Since $v \neq v'$, then $a_i \neq b_i$ for some $i \in \{1,\ldots, m\}$. Assume $i$ is the smallest such integer such that $a_i \neq b_i$.

In $v$, $(a_i, a_j)$ will form an edge $e$ between the $i^{th}$ and $j^{th}$ edge-endpoints in $G$. There are two cases to consider:

Case (1): Assume $j > i$. 
Then in $v$, $(a_i, a_j) = (1, 0)$. If $a_i \neq b_i$ then $b_i = 0$ and $b_i$ must be paired with some $b_k = 1$ such that $k < i$ in order to form an edge $e'$ in $G'$. $G$ is isomorphic to $G'$ and $f(H) = H'$, where $H$ and $H'$ are the Hamiltonian cycles of $G$ and $G'$ respectively. Therefore, since $e' \in G'$ connects vertices $i'$ and $k'$, there must be an outside edge $e''$ in $G$ that connects vertices $i$ and $k$. This implies $a_{i-1} = b_{i-1} = 0$ by the assumption that the index $i$ was the smallest index such that $a_i \neq b_i$. Now, in $G'$ vertex $i'$ is incident with two vertices whose indices are less than $i'$. while in $G$ this is impossible, see Figure 9a. Therefore, $G$ cannot be isomorphic to $G'$, which implies $G \not\cong G'$ and is a contradiction.

**Figure 9.** This figure is to aid in the understanding of Claim 1. In $a)$, vertex $i'$ in $G'$ will need to be paired with two vertices whose indices are less than $i'$. This is not possible for vertex $i$ in $G$ (according to the construction of edges). In $b)$, vertex $i$ in $G$ will need to be paired with two vertices whose indices are less than $i$. This is not possible for vertex $i'$ in $G'$.

**Case (2):** Assume $j < i$. 
Then in v, \((a_j, a_i) = (1, 0)\). So in \(G\), an edge \(e\) is formed between vertices \(j\) and \(i\). Since \(G\) is isomorphic to \(G'\) and \(f(H) = H'\), an outside edge \(e'\) must exist between vertices \(j'\) and \(i'\) in \(G'\). Furthermore, since \(a_i \neq b_i\) then \(b_i = 1\) and \(b_i\) must be paired with some \(b_k = 0\) such that \(k > i\) in order to form an edge \(e''\) in \(G'\). This implies \(b_{i-1} = a_{i-1} = 0\) by the assumption that the index \(i\) was the smallest index such that \(a_i \neq b_i\). Now, in \(G\) vertex \(i\) must be incident with two vertices whose indices are less than \(i\), while in \(G'\) this is impossible, see Figure 9b. Therefore, \(G\) cannot be isomorphic to \(G'\), which implies \(G \not\cong G'\) and is a contradiction.

Therefore, it must be the case that \(v = v'\). The argument is the same for the inside vectors of \(G\) and \(G'\). Hence, it must be true that \(G\) and \(G'\) use the same outside vector and the same inside vector. This completes the proof of Theorem 1.5.1. □
CHAPTER 2

Bounding the Formula

2.1. Introduction

If one looks at the formula from result 1.4.1, it is not clear how fast the number of rooted Hamiltonian graphs grows with the number of crossings. In this chapter upper and lower bounds for the number of rooted Hamiltonian graphs will be established. It will be shown that the bounds for the number of rooted Hamiltonian graphs \( X(n) \) satisfies

\[
\frac{(n!)^2}{(\frac{n}{2})^4} \leq X(n) \leq \frac{(n!)^3}{(\frac{n}{3})^3(\frac{n}{2})^4} \quad \text{for } (n \mod 6) = 0
\]

Because \( X(n) \) is clearly a strictly increasing function, investigating the asymptotic behavior for values of \( n \) that are divisible by 6 will suffice for an overall idea of how \( X(n) \) grows for very large \( n \). The reasons for this restriction on \( n \) will be explained in Section 2.3. The upper bound is much closer to the actual number of graphs \( X(n) \) than is the lower bound, and the reasoning will be explained in Section 2.4. In the same section, numerical evidence will be explored to discuss how close the bounds are for \( X(n) \), and a close numerical approximation of \( X(n) \) will be given without proof based only on numerical evidence.
2.2. Finding a Lower Bound

The goal of this section is to find a lower bound for the count of rooted Hamiltonian graphs,

\[
X(n) = \sum_{t=0}^{\frac{n}{2}} \sum_{p=0}^{n-2t} \binom{n}{2t} \binom{n-2t}{p} \frac{\binom{2t+2p}{t+p} \binom{2n-2t-2p}{n-t-p}}{(t+p+1)(n-t-p+1)}
\]

The goal is to express the lower bound for \(X(n)\) in terms of a simple function in \(n\), the number of crossings of a given graph \(G\). Let \(g(n, t, p) = \binom{n}{2t} \binom{n-2t}{p} \frac{\binom{2t+2p}{t+p} \binom{2n-2t-2p}{n-t-p}}{(t+p+1)(n-t-p+1)}\), which is one entry of the double summation in terms of \(n, t,\) and \(p\).

**Theorem 2.2.1.** For \(n\) even, \(g(n, t, p)\) is minimized when \(t = \frac{n}{2}, p = 0\).

**Proof.** Assume \(n\) is even. It needs to be shown that \(g(n, t, p)\) is minimized when \(t = \frac{n}{2}, p = 0\).

The arrangement of points \(\binom{n}{2t} \binom{n-2t}{p} = \binom{n}{0} \binom{n}{0} = 1\) when \(t = \frac{n}{2}, p = 0\). The arrangement of points is therefore clearly minimized for \(t = \frac{n}{2}, p = 0\).

Now if the edge construction \(\frac{\binom{2t+2p}{t+p} \binom{2n-(2t+2p)}{n-(t+p)}}{(t+p+1)(n-(t+p)+1)}\) is minimized when \(t = \frac{n}{2}, p = 0\), the proof is complete.

It needs to be shown that \(\frac{\binom{n}{2t} \binom{n-2t}{p}}{(\frac{n}{2}+1)(\frac{n}{2}+1)}\) is the minimum value for \(\frac{\binom{2t+2p}{t+p} \binom{2n-(2t+2p)}{n-(t+p)}}{(t+p+1)(n-(t+p)+1)}\). This expression is symmetric around the axis \((t+p) = \frac{n}{2}\), so the following general case is developed that will serve as the proof.

It is necessary to show for \(x = t + p = \frac{n}{2}\)

\[
\frac{\binom{2x}{x}}{(x+1)(x+1)} \leq \frac{\binom{2x+2k}{x+k}}{(x+k+1)(x-k+1)} \quad \text{for} \quad k = \{0, 1, 2, \ldots, x\}.
\]  

(2.2.1)
This is clearly equal for $k = 0$. It remains to be shown that the inequality is true for $k \in \{1, 2, \ldots, x\}$. That is, we must show
\[
\frac{(2x)!}{x!x!(x+1)} \leq \frac{(2x + 2k)!}{(x + k)!(x + k + 1)(x - k)!(x - k + 1)}
\]
and since every factor is positive, this inequality can be written as
\[
\frac{(x + k)!^2}{x!^2} \frac{(x - k)!^2}{(2x + 2k)!} \frac{(2x)!}{(x + k + 1)(x - k + 1)} \leq 1, \text{ or}
\]
\[
\frac{[(x + 1)(x + 2) \ldots (x + k)]^2}{[x(x - 1) \ldots (x - k + 1)]^2} \frac{[2x(2x - 1) \ldots (2x - 2k + 1)]}{[(2x + 1)(2x + 2) \ldots (2x + 2k)]} \frac{(x^2 + 2x + 1 - k^2)}{(x^2 + 2x + 1)} \leq 1
\]
It is clear that $0 \leq B \leq 1$ for $k \in \{1, 2, \ldots, x\}$. If it can be shown that $0 \leq A \leq 1$ for $k = \{1, 2, \ldots, x\}$, then clearly $AB \leq 1$ for $k = \{1, 2, \ldots, x\}$. We then have
\[
A = \frac{[(x + 1)(x + 2) \ldots (x + k)]^2}{[x(x - 1) \ldots (x - k + 1)]^2} \frac{[2x(2x - 1) \ldots (2x - 2k + 1)]}{[(2x + 1)(2x + 2) \ldots (2x + 2k)]}
\]
\[
= \frac{[(x + 1)(x + 2) \ldots (x + k)]^2}{[x(x - 1) \ldots (x - k + 1)]^2} \frac{22k[x(x - \frac{1}{2})(x - 1) \ldots (x - k + 1)(x - k + \frac{1}{2})]}{[(x + \frac{1}{2})(x + 1)(x + \frac{3}{2}) \ldots (x + k - \frac{1}{2})(x + k)]}
\]
\[
= \frac{[(x + 1)(x + 2) \ldots (x + k)]}{[x(x - 1) \ldots (x - k + 1)]} \frac{[(x - \frac{1}{2})(x - \frac{3}{2}) \ldots (x - k + \frac{1}{2})]}{[(x + \frac{1}{2})(x + \frac{3}{2}) \ldots (x + k - \frac{1}{2})]}
\]
\[
= \frac{1 + \frac{1}{x}}{x} \frac{x + 2}{x - 1} \ldots \frac{x + k}{x - k + 1} \frac{2x - 1}{2x + 1} \frac{2x - 3}{2x + 3} \ldots \frac{2x - 2k + 1}{2x + 2k - 1}
\]
\[
= \prod_{i=1}^{k} \frac{(x + i)}{(x - i + 1)} \frac{(2x - 2i + 1)}{(2x + 2i - 1)}
\]
Now consider a factor $F'$ of this product.
\[
F' = \frac{(x + i)}{(x - i + 1)} \frac{(2x - 2i + 1)}{(2x + 2i - 1)}
\]
\[
= \frac{2x^2 - 2xi + x + 2xi - 2i^2 + i}{2x^2 + 2xi - 2xi - 2i^2 + i + 2x + 2i - 1}
\]
\[
= \frac{2x^2 + x - 2i^2 + i}{2x^2 + x - 2i^2 + 3i - 1}
\]
It is clear that this quotient is greater than zero for any $x \geq 1$ because $i \leq k \leq x$.

It is also clear that the quotient is less than $1$ for all $i \geq 1$ because $3i - 1 \geq i$. This
means that for any factor $F$, it must be true that $0 \leq F \leq 1$. Therefore, $0 \leq A \leq 1$ for $k = \{1, 2, \ldots, x\}$ and hence $AB \leq 1$.

This completes the proof of inequality 2.2.1 and therefore $g(n, t, p)$ is minimized at $t = \frac{n}{2}, p = 0$ when $n$ is even. This concludes the proof of Theorem 2.2.1. □

The minimum values from Theorem 2.2.1 cause the arrangement of points value to be minimal, and cause the edge constructions value to be minimal also. Substituting these values into $g(n, t, p)$, one gets

$$
\binom{n}{n/2} \binom{0}{0} \binom{n/2}{n/2+1} = \frac{(n!)^2}{(n/2)!^4(n/2+1)^2}
$$

This value must be the minimal entry in the double summation of $X(n)$. To achieve a lower bound on $X(n)$, this minimal value can be used for each term of the double summation. Thus,

$$
X(n) \geq \sum_{t=0}^{n/2} \sum_{p=0}^{n-2t} \frac{(n!)^2}{(n/2)!^4(n/2+1)^2}
$$

The number of times the double summation runs in terms of $n$ can be found by evaluating the following:

$$
\sum_{t=0}^{n/2} \sum_{p=0}^{n-2t} 1 = \sum_{t=0}^{n/2} (n - 2t + 1) = \sum_{t=0}^{n/2} 1 + n \sum_{t=0}^{n/2} 1 - 2 \sum_{t=0}^{n/2} t
$$
\[
= \left(\frac{n}{2} + 1\right) + n\left(\frac{n}{2} + 1\right) - 2 \sum_{t=0}^{\frac{n}{2}} t \\
= \left(\frac{n}{2} + 1\right) + n\left(\frac{n}{2} + 1\right) - 2\left(\frac{n}{2}\left(\frac{n}{2} + 1\right)\right) \\
= \left(\frac{n}{2} + 1\right)(1 + n - \frac{n}{2}) \\
= \left(\frac{n}{2} + 1\right)^2
\]

Since the double summation is executed \((\frac{n}{2} + 1)^2\) times, the lower bound can be expressed as

\[
\frac{(n!)^2}{\left(\frac{n}{2}!\right)^4\left(\frac{n}{2} + 1\right)^2} = \frac{(n!)^2}{\left(\frac{n}{2}!\right)^4}
\]  \hspace{1cm} (2.2.2)

for rooted Hamiltonian graphs with an even number of \(n\) crossings. Stirling's Approximation Formula is a way to examine the growth of factorials [8]. This formula says that for large \(n\),

\[
n! \sim \sqrt{2\pi n}^{n+\frac{1}{2}} e^{-n}
\]

So in the lower bound,

\[
\frac{(n!)^2}{\left(\frac{n}{2}!\right)^4} \sim \frac{(\sqrt{2\pi})^2(n^{n+\frac{1}{2}})^2(e^{-n})^2}{\left(\sqrt{2\pi}\right)^4\left[\left(\frac{n}{2}\right)^{\frac{3}{2}} + \frac{1}{8}\right]^4[e^{-\frac{n}{2}}]^4} \\
= \frac{n^{2n+1}e^{-2n}}{2\pi\left(\frac{n}{2}\right)^{2n+2}e^{-2n}} \\
= \frac{n^{2n+1}2^{2n+2}}{2\pi n^{2n+2}} \\
= \frac{2^{n+1}}{\pi n} \\
= \left(\frac{2}{\pi}\right)\left(\frac{4^n}{n}\right)
\]
This gives a lower bound approximation, so for our number of rooted Hamiltonian graphs with even number \( n \) crossings \( X(n) \),

\[
X(n) \geq \left( \frac{2}{\pi} \right) \left( \frac{4^n}{n} \right)
\]

The reason \( n \) was restricted to being even in Theorem 2.2.1 is because that would involve factorials of non-integer values. Knowing \( X(n) \) is an increasing function means for \( n \) odd,

\[
X(n) > X(n - 1) \geq \left( \frac{2}{\pi} \right) \left( \frac{4^{n-1}}{n - 1} \right).
\]

2.3. Finding an Upper Bound

The goal of this section is to find an upper bound for the count of rooted Hamiltonian graphs,

\[
X(n) = \sum_{t=0}^{\frac{n}{2}} \sum_{p=0}^{n-2t} \binom{n}{2t} \binom{n-2t}{p} \frac{\binom{2t+2p}{t+p}}{(t+p+1)(n-t-p+1)}
\]

The following Lemma will be helpful.

**Lemma 2.3.1.** Let \( x \) be a nonnegative integer such that \( (x \mod 3) = 0 \). Then

\[
\left( \frac{x!}{(\frac{x}{3})!(\frac{x}{3})!(\frac{x}{3})!} \right) \geq \frac{x!}{a!b!c!}
\]

for any nonnegative integers \( a, b, c \) such that \( a + b + c = x \).

**Proof.** Let \((3x)!\) be a fixed sum and consider \( \frac{(3x)!}{a!b!c!} \) for nonnegative integers \( a, b, c \) such that \( a + b + c = 3x \).

To prove the lemma, it must be true that \( \frac{(3x)!}{x!x!x!} \) is maximal. In other words, it must be shown that \( x!x!x! \) is the smallest value by which \((3x)\)! can be divided. To show this, three cases must be considered:

1. \( x!x!x! \leq (x+k)!(x+l)!(x-k-l)! \) for \( k, l \) nonnegative integers such that \( k + l \leq x \)
(2) \(x!x!x! \leq (x-k)!(x-l)!(x+k+l)!\) for \(k, l\) nonnegative integers such that \(k+l \leq x\)

(3) \(x!x!x! \leq (x-k)!(x+l)!(x+k-l)!\) for \(k, l\) nonnegative integers such that \(k, l \leq x\)

Case (1):

\(x!x!x! \leq (x+k)!(x+l)!(x-k-l)!\) for \(k, l\) nonnegative integers such that \(k+l \leq x\)

All factors are always positive, so this inequality can be written as the following ratios while preserving the inequality:

\[
\frac{x!}{(x-k-l)!} \leq \frac{(x+k)!(x+l)!}{x!}, \text{ or }
\]

\[
\frac{[x(x-1)\ldots(x-k)(x-k-1)\ldots(x-k-l+1)]}{(k+l) \text{ factors}} \leq \frac{[(x+1)\ldots(x+k)(x+1)\ldots(x+l)]}{(k+l) \text{ factors}}
\]

One can clearly see that both sides contain \(k+l\) factors, where each factor on the right is greater than or equal to any factor on the left. So Case (1) is obvious.

Case (2):

\(x!x!x! \leq (x-k)!(x-l)!(x+k+l)!\) for \(k, l\) nonnegative integers such that \(k+l \leq x\)

Again, all factors are always positive so this inequality can be written as the following ratios while preserving the inequality:

\[
\frac{x!}{(x-k)!(x-l)!} \leq \frac{(x+k+l)!}{x!}, \text{ or }
\]

\[
\frac{[x(x-1)\ldots(x-k)][x(x-1)\ldots(x-l)]}{(k+l) \text{ factors}} \leq \frac{[(x+1)\ldots(x+k)(x+k+1)\ldots(x+k+l)]}{(k+l) \text{ factors}}
\]

Again, one can clearly see that both sides contain \(k+l\) factors, where each factor on the right is greater than or equal to any factor on the left. Thus, Case (2) also follows.

Case (3):

\(x!x!x! \leq (x-k)!(x+l)!(x+k-l)!\) for \(k, l\) nonnegative integers such that \(k, l \leq x\)

This case requires two subcases, one for \(k \geq l\) and one for \(l \geq k\).
Subcase a) Assume $k \geq l$. Now set $s = k - l$. This results in an example of Case (1) with $l = l$ and $k = s$ which has been established already.

Subcase b) Assume $l \geq k$. Now set $s = l - k$. This results in an example of Case (2) with $k = k$ and $l = s$ which has been established already.

This completes Case (3) and all three cases have been shown. Therefore, it must be true that if $a + b + c = 3x$, then $\frac{(3x)!}{a!b!c!}$ is maximal when $a = b = c = x$. \qed

Similar to finding the lower bound, the maximal entry in the double summation will be found, and then used as each term in the double summation. Recall that

$$g(n, t, p) = \binom{n}{2t} \binom{n - 2t}{p} \frac{(2t + 2p)}{(t + p + 1)(n - t - p + 1)}$$

**Theorem 2.3.2.** If $(n \mod 6) = 0$, $g(n, t, p)$ is maximized when $p = \frac{n - 2t}{2}$.

**Proof.** It needs to be shown that for $p = \frac{n - 2t}{2}$, then $g(n, t, p)$ is at a absolute maximum for $(n \mod 6) = 0$, $t = \{0, 1, \ldots, \frac{n}{2}\}$. To show this, it is necessary to consider the two cases below.

1. Suppose $p' = \frac{n}{2} - t + x$ for $x = \{1, 2, \ldots, \frac{n - 2t}{2}\}$. One needs to show $g(n, t, p') \leq g(n, t, \frac{n - 2t}{2})$.

2. Suppose $p' = \frac{n}{2} - t - x$ for $x = \{1, 2, \ldots, \frac{n - 2t}{2}\}$. One needs to show $g(n, t, p') \leq g(n, t, \frac{n - 2t}{2})$.

**Case (1):** Suppose $(n \mod 6) = 0$, $t = \{0, 1, \ldots, \frac{n}{2}\}$ and $p' = \frac{n}{2} - t + x$ for $x = \{1, 2, \ldots, \frac{n - 2t}{2}\}$. The following inequality needs to be established.

$$\binom{n}{2t} \binom{n - 2t}{\frac{n}{2} - t + x} \frac{(2t + n - 2t + 2x)}{(t + \frac{n}{2} - t + x + 1)(n - t - \frac{n}{2} + t - x + 1)} \leq$$
This inequality can be simplified to the following.

\[
\left( \frac{n}{2} - t + x \right) \left( \frac{n}{2} + x + 1 \right) \left( \frac{n}{2} - x + 1 \right) \leq \left( \frac{n}{2} - t \right) \left( \frac{n}{2} + 1 \right) \left( \frac{n}{2} + 1 \right)
\]

Writing the binomials as factorials we obtain:

\[
\frac{(n-2t)!}{(n-x)!} \leq \frac{(n-2x)!}{(n-2x)!} \frac{(n-2t-x)!}{(n-2t-x)!} \frac{(n-2t)!}{(n-2t)!} \frac{(n-2t-x)!}{(n-2t-x)!}
\]

which can be rewritten as the following inequality since all quantities are positive:

\[
\frac{(n/2)!}{(n/2+x)!} \frac{(n/2)!}{(n/2-x)!} \frac{(n/2)!}{(n/2-x)!} \frac{(n/2)!}{(n/2-x)!} \frac{(n/2)!}{(n/2-x)!} \frac{(n/2)!}{(n/2-x)!} \frac{(n/2)!}{(n/2-x)!} \frac{(n/2)!}{(n/2-x)!} \leq 1
\]

Inequality 2.3.1 will be proven using induction on x. For the base case of x = 1, the inequality simplifies to

\[
\frac{(n/2)!}{(n/2+1)!} \frac{(n/2)!}{(n/2-1)!} \frac{(n/2)!}{(n/2-t+1)!} \frac{(n/2)!}{(n/2-t-1)!} \frac{(n/2)!}{(n/2+1)!} \frac{(n/2)!}{(n/2+1)!} \frac{(n/2)!}{(n/2+1)!} \frac{(n/2)!}{(n/2+1)!} \leq 1
\]

It needs to be shown that this expression is less than or equal to 1. But we then have

\[
= \frac{(n/2)!}{(n/2+1)!} \frac{(n/2)!}{(n/2-1)!} \frac{(n/2)!}{(n/2-t+1)!} \frac{(n/2)!}{(n/2-t-1)!} \frac{(n/2)!}{(n/2+1)!} \frac{(n/2)!}{(n/2+1)!} \frac{(n/2)!}{(n/2+1)!} \frac{(n/2)!}{(n/2+1)!} \leq 1
\]
It can be assumed \( n \geq 6 \) since we are interested in the asymptotics as \( n \to \infty \). The denominator is always positive for \( n \geq 6 \) and \( t \in \{0, 1, \ldots, \frac{n}{2}\} \).

\[
\frac{n^3 + 3n^2 + 2n - 2n^2t - 6nt - 4t}{n^3 + 5n^2 + 2n - 2n^2t - 6nt + 8t - 8}
\]

So it needs to be shown that

\[
\frac{n^3 + 3n^2 + 2n - 2n^2t - 6nt - 4t}{n^3 + 5n^2 + 2n - 2n^2t - 6nt + 8t - 8} \leq 1 \tag{2.3.2}
\]

Since the denominator is positive, this inequality will be true whenever

\[
n^3 + 3n^2 + 2n - 2n^2t - 6nt - 4t \leq n^3 + 5n^2 + 2n - 2n^2t - 6nt + 8t - 8, \text{ or} \]

\[
0 \leq 2n^2 + 12t - 8
\]

which is true for \( n \geq 6, t = \{0, 1, \ldots, \frac{n}{2}\} \). So it must be true that Inequality (2.3.2) is true and the base case when \( x = 1 \) holds.

Now the inequality is assumed true for \( x = k \) and needs to be proven to hold true for \( x = k + 1 \) where \( k = \{1, 2, \ldots, \frac{n}{2} - t - 1\} \). In other words, it is needed to show:

\[
\frac{(\frac{n}{2})^2}{(\frac{n}{2} + k + 1)^2} \frac{(\frac{n}{2})^2}{(\frac{n}{2} - k - 1)^2} \frac{(\frac{n}{2} - t)^2}{(\frac{n}{2} - t + k + 1)(\frac{n}{2} - t - k - 1)!} \\
\times \frac{(n + 2k + 2)!}{n!n!} \frac{(n - 2k - 2)!}{(\frac{n}{2} + 1)(\frac{n}{2} + 1)} \frac{(\frac{n}{2} + 1)(\frac{n}{2} + 1)}{(\frac{n}{2} + k + 2)(\frac{n}{2} - k)} \leq 1
\]

But the above inequality can be rewritten as:

\[
\frac{(\frac{n}{2} - k)^2}{(\frac{n}{2} + k + 1)^2} \frac{(\frac{n}{2} - t - k)}{(\frac{n}{2} - t + k + 1)} \frac{(\frac{n}{2})^2}{(\frac{n}{2} + k)^2} \frac{(\frac{n}{2} - k)^2}{(\frac{n}{2} - k - 1)^2} \frac{(\frac{n}{2} - t)^2}{(\frac{n}{2} - t - k)!} \\
\times \frac{(n + 2k + 1)(n + 2k + 2)}{(n - 2k)(n - 2k - 1)} \frac{(\frac{n}{2} + k + 1)(\frac{n}{2} - k + 1)}{(\frac{n}{2} + k + 2)(\frac{n}{2} - k)}
\]
\[ \times \frac{(n+2k)!(n-2k)!}{n!n!} \frac{\left(\frac{n}{2}+1\right)\left(\frac{n}{2}+1\right)}{\left(\frac{n}{2}+k+1\right)\left(\frac{n}{2}-k+1\right)} \leq 1 \]

Now \( BD \leq 1 \) by the induction assumption, so if it can be shown that \( 0 \leq AC \leq 1 \) for \( n \geq 6, k = \{1, 2, \ldots, \frac{n}{2} - t - 1\}, t = \{0, 1, \ldots, \frac{n}{2}\} \) then it must be true that \( ABCD \leq 1 \) for the same values of \( n, k, \) and \( t \). We now have

\[
AC = \frac{\left(\frac{n}{2} - k\right)^2 \left(\frac{n}{2} - t - k\right) (n+2k+1)(n+2k+2) \left(\frac{n}{2}+k+1\right)\left(\frac{n}{2}-k+1\right)}{\left(\frac{n}{2}+k+1\right)^2 \left(\frac{n}{2} - t + k + 1\right) (n-2k)(n-2k-1) \left(\frac{n}{2}+k+2\right)\left(\frac{n}{2}-k\right)}
\]

\[
= \frac{\left(\frac{n}{2} - k\right) \left(\frac{n}{2} - t - k\right) (n+2k+1)(n+2k+2) \left(\frac{n}{2}+k+1\right)\left(\frac{n}{2}-k+1\right)}{\left(\frac{n}{2}+k+1\right) \left(\frac{n}{2} - t + k + 1\right) (n-2k)(n-2k-1) \left(\frac{n}{2}+k+2\right)\left(\frac{n}{2}-k\right)}
\]

\[
= \frac{(n-2t-2k) (n-2k+2)(n+2k+1)}{(n-2t+2k+2)(n-2k-1)(n+2k+4)}
\]

Consider \( \frac{n+2k+1}{n+2k+4} \) in \( AC \). It is true that \( 0 \leq \frac{n+2k+1}{n+2k+4} \leq 1 \) for \((n \mod 6), k = \{1, 2, \ldots, \frac{n}{2} - t - 1\}. Therefore if it can be shown that

\[
0 \leq \frac{(n-2t-2k) (n-2k+2)}{(n-2t+2k+2)(n-2k-1)} \leq 1
\]

for \( n \geq 6, t = \{0, 1, \ldots, \frac{n}{2}\}, k = \{1, 2, \ldots, \frac{n}{2} - t - 1\}, \) then it must be true that \( 0 \leq AC \leq 1 \) for those values of \( n, t, k \).

Consider the following expression

\[
\frac{(n-2t-2k) (n-2k+2)}{(n-2t+2k+2)(n-2k-1)}
\]

which is clearly non-negative for \( n \geq 6, t = \{0, 1, \ldots, \frac{n}{2}\}, k = \{1, 2, \ldots, \frac{n}{2} - t - 1\}. \)

Also,

\[
(n-2t+2k+2)(n-2k-1) > 0
\]

for those values of \( n, t, k \). It remains to be shown that \( \frac{(n-2t-2k) (n-2k+2)}{(n-2t+2k+2)(n-2k-1)} \leq 1 \). Since the denominator is always positive, this inequality will be true whenever any of the
following equivalent inequalities are satisfied.

\[(n - 2t - 2k)(n - 2k + 2) \leq (n - 2t + 2k + 2)(n - 2k - 1),\]
\[-4k + 4k^2 + 2n - 4nk + n^2 - 4t + 4kt - 2nt \leq -4k^2 + n^2 + n - 6k + 2t + 4kt - 2nt - 2, \text{ or}\]
\[n - 4nk + 8k^2 + 2k - 6t + 2 \leq 0 \quad (2.3.3)\]

But

\[n - 4nk + 8k^2 + 2k - 6t + 2 \leq n - 4nk + 8k^2 + 2k + 2,\]

so it will suffice to show

\[n - 4nk + 8k^2 + 2k + 2 \leq 0, \text{ or}\]
\[8k^2 + (2 - 4n)k + (n + 2) \leq 0 \quad (2.3.4)\]

If this inequality can be verified, then the induction is complete. Solving for \(k\), the two solutions are

\[k = \frac{-1 + 2n \pm \sqrt{4n^2 - 12n - 15}}{8}\]

Noticing 2.3.4 is a parabola in \(k\), it must be true that the sign of the function will be the same between the two zeros given by the quadratic formula above. The next goal is to show that these solutions bound the interval for \(k = \{1, 2, \ldots, \frac{n}{2} - t - 1\}\).

In other words, if \(z_1\) and \(z_2\) are the two zeros, then \(z_1 \leq \{1, 2, \ldots, \frac{n}{2} - t - 1\} \leq z_2\).

First, it will be shown that \(-1 + 2n - \sqrt{4n^2 - 12n - 15} < 1\) for all \(n \geq 6\). Recall that one can square both sides of an inequality while preserving the inequality if both sides are
nonnegative. Thus, we have the following equivalent inequalities:

\[
\frac{-1 + 2n - \sqrt{4n^2 - 12n - 15}}{8} < 1
\]

\[-1 + 2n - \sqrt{4n^2 - 12n - 15} < 8
\]

\[-\sqrt{4n^2 - 12n - 15} < 9 - 2n
\]

\[\sqrt{4n^2 - 12n - 15} > 2n - 9
\]

\[4n^2 - 12n - 15 > (2n - 9)^2
\]

\[4n^2 - 12n - 15 > 4n^2 - 36n + 81
\]

\[-12n - 15 > -36n + 81
\]

\[24n > 96
\]

\[n > 4
\]

So the values in question for \( k \) are bounded on the left by this zero. Next it will be shown that the zero \(-\frac{1 + 2n + \sqrt{4n^2 - 12n - 15}}{8}\) lies to the right of the value \( \frac{n}{2} - 1 \) for all \( n \geq 6 \). In other words,

\[
\frac{-1 + 2n + \sqrt{4n^2 - 12n - 15}}{8} > \frac{n}{2} - 1
\]

\[-1 + 2n + \sqrt{4n^2 - 12n - 15} > 4n - 8
\]

\[\sqrt{4n^2 - 12n - 15} > 2n - 7
\]

\[4n^2 - 12n - 15 > (2n - 7)^2
\]

\[4n^2 - 12n - 15 > 4n^2 - 28n + 49
\]

\[-12n - 15 > -28n + 49
\]

\[16n > 64
\]

\[n > 4
\]
Then it is clear that for \( n \geq 6 \), the zeros for \( k \) bound the interval for \( k = \{1, 2, \ldots, \frac{n}{2} - 1\} \), so they must bound the values of \( k = \{1, 2, \ldots, \frac{n}{2} - t - 1\} \). Recall the inequality from 2.3.4,

\[
n - 4nk + 8k^2 + 2k + 2 \leq 0
\]

The sign of the expression will be the same between the two zeroes found. From the previous two results, it is known that any value of \( k = \{1, 2, \ldots, \frac{n}{2} - t - 1\} \) lies between the zeroes. Substituting \( k = 1 \) into the expression results in \(-3n + 12 < 0\) which will be true for \( n \geq 6 \). This shows that Inequality (2.3.4) is true for the entire interval \( k = \{1, 2, \ldots, \frac{n}{2} - t - 1\} \), so Inequality (2.3.3) must be true for those values of \( k \). Therefore, it must be true that \( 0 \leq AC \leq 1 \) for \( n \geq 6 \), \( t = \{1, 2, \ldots, \frac{n}{2}\} \), and \( k = \{1, 2, \ldots, \frac{n}{2} - t - 1\} \), which completes the induction on \( k \). This concludes the proof of Case (1).

**Case (2):** Suppose \((n \mod 6) = 0\) and \(p' = \frac{n}{2} - t - x\) for \( x = \{1, 2, \ldots, \frac{n-2t}{2}\} \). One of the following equivalent inequalities needs to be shown.

\[
\binom{n}{2t} \left(\frac{n-2t}{2} - t - x\right) \leq \binom{n}{2t} \left(\frac{n-2t}{2} - t + x + 1\right)
\]

This last inequality can be written as Inequality (2.3.1) and the argument will be identical to that of Case (1). This completes both cases and therefore it must be the case that \( p = \frac{n-2t}{2} \) is the value of \( p \) in the absolute maximum of \( g(n, t, p) \). \( \square \)
Substituting \( p = \frac{n - 2t}{2} \) results in:

\[
\binom{n}{2t} \binom{n - 2t}{\frac{n - 2t}{2}} \frac{\binom{2t + n - 2t}{t + \frac{n - 2t}{2}}}{(t + \frac{n - 2t}{2} + 1)} \frac{\binom{2n - 2t - n + 2t}{n - t - \frac{n - 2t}{2}}}{(n - t - \frac{n - 2t}{2} + 1)}
\]

\[
= \binom{n}{2t} \binom{n - 2t}{\frac{n - 2t}{2}} \frac{\binom{n}{\frac{n}{2}} \binom{n}{\frac{n}{2}}}{(\frac{n}{2} + 1) (\frac{n}{2} + 1)}
\]

This term is maximized if \( A \) is maximized. Thus it suffices to consider \( A \) by itself.

\[
A = \binom{n}{2t} \binom{n - 2t}{\frac{n - 2t}{2}} \frac{n!(n - 2t)!}{(2t)!(n - 2t)!(\frac{n}{2} - t)!(\frac{n}{2} - t)!}
\]

\[
= \frac{n!}{(2t)!(\frac{n}{2} - t)!(\frac{n}{2} - t)!}
\]

From Lemma 2.3.1, \( A \) will be maximal when \( \frac{n}{3} \) is achieved. This result is accomplished with \( t = \frac{n}{6} \), so it must be the case that \( p = \frac{n - 2t}{2} = \frac{n}{3} \). Substituting these values results in the following expression:

\[
\binom{n}{2t} \binom{n - 2t}{\frac{n - 2t}{2}} \frac{\binom{2t + 2p}{t + \frac{n}{3}}}{(t + \frac{n}{3} + 1)} \frac{\binom{2n - 2t - 2p}{n - t - \frac{n}{3}}}{(n - t - \frac{n}{3} + 1)}
\]

\[
= \binom{n}{\frac{n}{3}} \binom{n - \frac{n}{3}}{\frac{n}{3}} \frac{\binom{\frac{n}{2}}{\frac{n}{2}} \binom{\frac{n}{2}}{\frac{n}{2}}}{(\frac{n}{2} + 1) (\frac{n}{2} + 1)}
\]

This is interesting because it has been seen in the proof of Theorem 2.2.1 that the edge constructions value is minimized when \( \frac{n}{3} \) occurs. This means that for \( (n \mod 6) = 0 \), \( g(n, t, p) \) is maximized when the edge constructions value is minimized and the arrangement of points value maximized. One would guess the upper bound will be much closer to the actual number of graphs \( X(n) \) than is the lower bound. Since the double summation is executed \( (\frac{n}{2} + 1)^2 \) times, the upper bound can be
expressed as

\[
\left(\frac{n}{2} + 1\right)^2 \frac{n!}{\left(\frac{n}{3}\right)!\left(\frac{n}{2}\right)!\left(\frac{n}{2}\right)!\left(\frac{n}{2}\right)!\left(\frac{n}{2} + 1\right)^2} \frac{n!n!}{(n!)^3} = \frac{(\frac{n}{3})^3}{(\frac{2!}{3})^3(\frac{2!}{2})^4}
\] 

(2.3.5)

for rooted Hamiltonian graphs with \(n\) crossings such that \((n \mod 6) = 0\). Stirling’s Approximation can be used again to approximate the growth of this value in terms of \(n\). So in the upper bound,

\[
\frac{(n!)^3}{(\frac{n}{3})^3(\frac{2!}{2})^4} \approx \frac{(\sqrt{2\pi})^3n^{3n+\frac{3}{3}}e^{-3n}}{n^{3n+\frac{3}{3}}(\frac{3}{2})^{2n+2}(\frac{3}{3})^{n+\frac{3}{2}}} = \frac{4^n3^{n+\frac{3}{3}}}{(2\pi)^2n^2(n!)^2} = \frac{12^n\sqrt{27}}{(\pi n)^2}
\]

This gives an upper bound approximation for our number of rooted Hamiltonian graphs with \(n\) crossings such that \((n \mod 6) = 0\):

\[
X(n) \leq \frac{12^n\sqrt{27}}{(\pi n)^2}
\]

Putting the two results together from 2.2.2 and 2.3.5, if \((n \mod 6) = 0\) the number of rooted Hamiltonian graphs \(X(n)\) satisfies

\[
\frac{(n!)^2}{(\frac{n}{3})^3(\frac{2!}{2})^4} \leq X(n) \leq \frac{(n!)^3}{(\frac{n}{3})^3(\frac{2!}{2})^4}
\] 

(2.3.6)
which can be approximated for large $n$ as

$$\frac{2}{\pi} \left(\frac{4^n}{n}\right) \leq X(n) \leq \frac{12^n \sqrt{27}}{(\pi n)^2}$$

(2.3.7)

The only restriction for the lower bound was for $n$ to be even. Since it must be true that $(n \mod 6) = 0$ in the upper bound, it will suffice to stay with the case when $(n \mod 6) = 0$ for both bounds. The reason $n$ must be divisible by 6 in the upper bound is because $p = \frac{n-2t}{2}$ requires $n$ to be even, and to apply Lemma 2.3.1 $n$ must also be divisible by three. If either of these cases fail one gets into non-integer factorials, which can be avoided if investigating asymptotics. For example, if one wishes to know how $X(602)$ behaves, it is true that $X(600) \leq X(602) \leq X(606)$, and then the growth of $X(602)$ can be estimated.

### 2.4. Quality of Bounds

Using Mathematica, one can see numerical evidence of how the upper bound and lower bound compare to the actual number of rooted Hamiltonian graphs, $X(n)$. Using the lower bound of $\left(\frac{n!}{(\frac{n}{2})^2}\right)$ and the upper bound of $\left(\frac{n!}{(\frac{n}{3})^3(\frac{n}{4})}\right)$, Table 2.4.1 was created.

Using Stirling’s Formula, the values in Table 2.4.2 were generated. As one can see, the upper bound is significantly better than the lower bound. When $t = \frac{n}{2}$, $p = 0$ were used to minimize $g(n, t, p)$, this minimized both the arrangement of points value and the edge constructions value. On the other hand, when $t = \frac{n}{6}$, $p = \frac{n}{3}$ were used to maximize $g(n, t, p)$, this maximized the arrangement of points value, but minimized the edge constructions value. This is the main reason for the significantly better quality of the upper bound.
Numerical evidence is the only basis for the following conjecture. It seems that the difference in the Stirling upper bound and \( X(n) \) for the same values of \( n \) is a factor of around \( \frac{1}{n} \). Numerical evidence is the only basis for the following conjecture.
CONJECTURE 1. $X(n)$ can be closely approximated by $\frac{12^n}{n^3}$.

This belief was developed by taking the Stirling upper bound $\frac{12^n\sqrt{2\pi n}}{(n^2)}$ and multiplying by a factor of $\frac{\pi}{\sqrt{2\pi n}}$. Table 2.4.3 shows numerical evidence to support Conjecture 1. The evidence supports all values of $n$, not just those $n$ divisible by 6. Thus

<table>
<thead>
<tr>
<th>n</th>
<th>$\frac{12^n}{n^3} / X(n)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>0.813132</td>
</tr>
<tr>
<td>200</td>
<td>0.799204</td>
</tr>
<tr>
<td>300</td>
<td>0.794588</td>
</tr>
<tr>
<td>400</td>
<td>0.792286</td>
</tr>
<tr>
<td>500</td>
<td>0.790906</td>
</tr>
<tr>
<td>600</td>
<td>0.789986</td>
</tr>
<tr>
<td>700</td>
<td>0.78933</td>
</tr>
<tr>
<td>800</td>
<td>0.788838</td>
</tr>
<tr>
<td>900</td>
<td>0.788456</td>
</tr>
<tr>
<td>1000</td>
<td>0.78815</td>
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<td>1100</td>
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<tr>
<td>1200</td>
<td>0.787691</td>
</tr>
<tr>
<td>1300</td>
<td>0.787514</td>
</tr>
<tr>
<td>1400</td>
<td>0.787363</td>
</tr>
<tr>
<td>1500</td>
<td>0.787232</td>
</tr>
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<td>0.787016</td>
</tr>
<tr>
<td>1800</td>
<td>0.786926</td>
</tr>
<tr>
<td>1900</td>
<td>0.786846</td>
</tr>
<tr>
<td>2000</td>
<td>0.786773</td>
</tr>
</tbody>
</table>

Table 2.4.3. A table displaying the ratio between $\frac{12^n}{n^3}$ and $X(n)$.

we have numerical evidence to claim:

$$X(n) \approx 1.27 \frac{12^n}{n^3}.$$
CHAPTER 3

Open Questions

There is plenty of further research that can be done surrounding this material. It has not been discussed in this thesis how to pick a random standard diagram with uniform probability. Although a count of total graphs has been provided, and algorithms have been developed to choose a standard diagram from this number [2], it is not trivial how to do this with uniform probability. Imagine two diagrams \( G \) and \( H \) with the same crossing number \( n=6 \). Next, imagine \( G \) has all transition points, and \( H \) has all double outside points. Then, there are \( \binom{6}{2} \binom{6}{2} = 25 \) ways to connect the edges in \( G \). There are \( \binom{12}{6} = 132 \) ways to connect the edges in \( H \). So it must be true that any standard diagram from \( G \) has a higher probability of occurring at random than a standard diagram from \( H \). This can be fixed if one picks \( t \) and \( p \) with a probability distribution that accounts for this. Such a distribution is not yet completely known, but it is being investigated [2].

A 4-edge-connected graph \( G \) is a graph that can not be disconnected by removing any three edges in \( G \). It would be interesting to know how many standard diagrams with a certain crossing number \( n \) have this property. One would guess that the majority of standard diagrams will not be 4-edge-connected. A loop edge is an edge that has the same vertex for both of its endpoints. If a loop edge occurs in any standard diagram, then it will not be 4-edge-connected. Indeed, suppose the loop
edge occurs at vertex $v$. Then the graph can be disconnected by removing the two Hamiltonian edges incident to $v$, hence it is not 4-edge-connected.

Furthermore, any loop edge corresponds to a knot or link diagram with a crossings that can be easily removed, see Figure 1. This gives rise to a question. Can one count and generate rooted Hamiltonian graphs with $n$ crossings and without loop edges?

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{loop_edge}
\caption{There is a loop edge at the vertex shown in the graph to the far left. The knot or link diagram corresponding to this has a crossing that can be removed by a simple twist.}
\end{figure}
Bibliography