Maximizing Spanning Trees in Almost Complete Graphs

by

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B Sc (Hon), University of Victoria, 1993

A Thesis Submitted in Partial Fulfillment of the
Requirements for the Degree of
MASTER OF SCIENCE
in the
Department of Computer Science

We accept this thesis as conforming
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Abstract

We denote the class of simple graphs with the same number of vertices, n, and same number of edges, e, by $\Omega(n,e)$. A graph in $\Omega(n,e)$ that has the most spanning trees is called Sp-optimal. Kel'mans and Chelnokov and independently Shier showed that the Sp-optimal graph in $\Omega\left(n, \binom{n}{2} - m\right)$, where $m \in (0, \left\lfloor \frac{n}{2} \right\rfloor]$, is the complement of a matching. This thesis characterizes the Sp-optimal almost-regular graphs in the class $\Omega\left(n, \binom{n}{2} - m\right)$, where $m \in (\left\lfloor \frac{n}{2} \right\rfloor, n]$. Petingi characterized the Sp-optimal graphs for m up to $n-2$ and for m up to n when m is divisible by three. Within the context of almost-regular graphs we extend his results. This is achieved with the following results.

We give a new proof of Kel'mans result: if G is composed of a collection of paths, then the number of trees in the complement of G is maximized when the path lengths are as equal as possible.

We give two new results for graphs whose complements are composed of cycles. A cycle on k vertices is denoted by C_k. Let $G = C_m$ and $H = C_k + C_{m-k}$ where $k \leq m-k$. Then the complement of G has more spanning trees than the complement of H if k is even and fewer if k is odd. Secondly, let $G = C_k + C_{m-k}$ and $H = C_{k+c} + C_{m-k-c}$, where $k \leq m-k$ and $c = 1$ or 2. Then the complement of G has more spanning trees than the complement of H if k is odd and fewer if k is even.

We also give results for graphs whose complements are composed of a mixture of cycles and paths. A path on k vertices is denoted by P_k. We give a new proof of Kel'mans claim that the complement of $C_3 + P_{k-3}$ has more spanning trees than the complement of P_k, where $k \geq 5$. We also show that the complement of $C_3 + P_k$ has more spanning trees than the complement of $C_{3+c} + P_{k-c}$, where $k > c > 0$.

We also review the formulas for counting the number of spanning trees in graphs whose complement is composed of path components or cycle components. One formula for cycle components is new and the algebraic formulas have been neglected in the literature. Before reviewing these formulas we collect and relate the major methods for counting the number of spanning trees in arbitrary graphs.

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Acknowledgements

I would like to thank Wendy Myrvold for starting me on this research topic long before I became a graduate student. Many of the results I present are due either to her work or our joint efforts. Essentially, the work I have accomplished could not have been done without her help.

I would also like to thank the University of Victoria for their support through the Fellowship program.

To Zosia

Chapter 1

Introduction

This thesis is concerned with the question "given n vertices and e edges how does one arrange the edges so that the resulting graph has as many spanning trees as possible?" In general, this question is difficult to answer and the primary objective of this thesis is to extend the subset of known results

To achieve this end, many different tools, from a variety of fields, are required For example, solutions have been obtained using results from linear algebra, combinatorics, and nonlinear optimization The secondary objective of this thesis is to extend the set of tools We do this by presenting new proofs for existing formulas plus new formulas for counting the number of spanning trees in special classes of graphs

For most classes of graphs the Sp-optimal graph can be described succinctly and its status can be verified with one main method In contrast, the results in Chapter 5 of this thesis and those by Petingi [64] require a number of methods and the solution statement is not succinct It is likely that the need for a diverse array of tools will persist in future work And so, future researchers in this field will need a broad background in all of the tools available This prompts the tertiary objective of this thesis to collect some background material that may aid future research

The rest of this introductory chapter provides basic definitions and describes the problem (Section 1 1), discusses the motivation for this research (Section 1 2), outlines known results (Section 1 3), previews the new results (Section 1 4), and provides an overview of the rest of the thesis (Section 1 5)

1.1 Problem statement

To define our problem and discuss the known results we need to define our terminology We start with basic graph theoretic definitions, discuss the problem and then close this section with some more definitions Essentially, these follow those of Bondy and Murty [13] We use common set notation and number theory notation (see, for example, [31]) and all notation, used in this thesis, is summarized in Appendix A

An undirected multigraph $G = (V(G), E(G))$ consists of a set $V(G)$ of $n = n(G)$ labeled vertices and a multiset $E(G)$ of $e = e(G)$ edges, where each edge is an unordered pair of vertices from V If G is understood, then we write V and E instead of $V(G)$ and $E(G)$ A multigraph with n vertices is called a multigraph of *order* n and a multigraph with e edges is said to have *size* e A *simple graph* G is a multigraph such that there is at most one edge between any pair of vertices Obviously, simple graphs are a subset of multigraphs

An edge x may be denoted by the unordered pair $x = \{u, v\}$ or as $x = uv$, where $u, v \in V$ We say the edge $e = uv$ is *incident* with u (or v) and two vertices connected by an edge are *adjacent* An edge whose endpoints are the same vertex, i e $x = vv$, is called a *loop* The *degree* of a vertex v, denoted d_v, is the number times an edge is incident to v (a loop is incident to a vertex twice). If there is no edge incident to a vertex v (i.e. $d_v = 0$), then v is called *isolated*. Edges are called *non-adjacent* if they have no vertices in common.

An xy-path, or simply a *path*, is a simple graph with vertex set $V = \{x = 1, 2, \ldots, k = y\}$ and edge set $E = \{\ \{i, i+1\} \mid 1 \leq i < k\}$. A *cycle* is a simple graph with vertex set $V = \{1, 2, \ldots, k\}$ and edge set $E = \{1, k\} \bigcup \{\ \{i, i+1\} \mid 1 \leq i < k\}$. A path of order k will be denoted by P_k and a cycle by C_k. The *length* of a path or cycle is equal to the number of edges. Note that, P_k has length $k-1$ whereas C_k has length k.

Let $G = (V, E)$ be a multigraph. A multigraph $G' = (V', E')$ is called a *subgraph* of G if $V' \subseteq V$ and $E' \subseteq E$. This relationship shall be denoted as $G' \subseteq G$. Two vertices $x, y \in V$ are *connected* if G has a subgraph which is an xy-path. A multigraph is *connected* if every pair of vertices is connected.

A *spanning subgraph* is any subgraph $G' = (V', E')$ of G satisfying $V' = V$. A *component* of a multigraph is a maximal connected subgraph.

A *tree* is a connected simple graph that contains no cycles. A spanning subgraph that is a tree is called a *spanning tree* of G. Two spanning trees, say T_1 and T_2, of G are considered distinct if $E(T_1)$ is not equal to $E(T_2)$. Let $\mathrm{Sp}(G)$ denote the number of spanning trees in the multigraph G.

Let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ be two multigraphs. These multigraphs are *isomorphic* if there exists a bijective function $f : V_1 \to V_2$ such that $\{x, y\} \in E_1$ if and only if $\{f(x), f(y)\} \in E_2$. We write $G_1 \cong G_2$ to show G_1 and G_2 are isomorphic.

Let $\Theta(n, e)$ denote the set of all multigraphs, up to isomorphism, with n vertices and e edges. Similarly let $\Omega(n, e)$ denote the set of simple graphs. Notation of this form is used by Cheng [18], Boesch and Suffel [11] and others. Any graph which maximizes the number of spanning trees in $\Theta(n, e)$ (or $\Omega(n, e)$) is called *Sp-optimal*.

Our problem is to find Sp-optimal graphs for a given number of vertices and edges. An obvious step to solving this problem is to discount graphs with loops since a loop can never be in a spanning tree. Thus, we assume that all our graphs are loop free.

As we review the known results we will denote the most general problem as *Problem M* (M for multigraph). Formally, let Problem M be:

> Given n and e, find G such that G is Sp-optimal with respect to all graphs in $\Theta(n, e)$.

But sometimes it has only been possible to find a solution for simple graphs. We denote this subproblem as *Problem S* (S for simple graphs). Formally, let Problem S be:

> Given n and e, find G such that G is Sp-optimal with respect to all graphs in $\Omega(n, e)$.

No total solution exists for either of these problems. Instead researchers have worked with smaller classes of graphs. For example, the class of graphs such that $e(G)$ is a particular function of $n(G)$ (e.g. $e = n + 2$). A review of these results is given in Section 1.3.

So far every solution has been a unique graph except for the case $e \leq n - 1$. This trend will probably not continue. Nevertheless, we informally say that one graph is *better* than another if it has more spanning trees. This makes the text easier to read. We will formally define a partial order over $\Theta(n, e)$ in Chapter 3 (page 51).

One way to solve Problem S for small n and each $e = n - 1, n, n + 1, \ldots, \binom{n}{2}$ is to generate every simple graph and then count the number of spanning trees using a counting formula (see Chapter 3). Our answer, for each n and e, is the graph that has the largest number. This approach has been done, for small graphs, by the author and others (Myrvold [59], Li [51]). Unfortunately, as n grows larger the number of graphs grows exponentially and so the computational task becomes impractical. Nevertheless, these early results are helpful for suggesting directions for research.

There remain a few terms, used throughout this thesis, that need definition. This thesis is concerned with graphs composed of some number of components. The operations described next facilitate this work. Let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$. The graphs G_1 and G_2 are *disjoint* if $V_1 \bigcap V_2 = \emptyset$ (this implies $E_1 \bigcap E_2 = \emptyset$). For the disjoint graphs G_1 and G_2, the binary operator $+$ is defined as $G = G_1 + G_2 = (V_1 \bigcup V_2, E_1 \bigcup E_2)$. The special case $G = G_1 + G_2 + \cdots + G_k$ where $G_1 \cong G_2 \cong \cdots \cong G_k$ is denoted by $G = k \cdot G_1$. Similarly, for the graphs G_1 and G_2, where $G_2 \subseteq G_1$, the binary operator $-$ is defined as $G = G_1 - G_2 = (V_1, E_1 - E_2)$.

A *complete graph* is a simple graph, of order n, with an edge between every pair of vertices. Such a graph is denoted by K_n. Since an edge is an unordered pair of two vertices, the number of edges in a complete graph is equal to the number of ways we can choose two vertices from the set of n vertices. Thus, there are $\binom{n}{2} = \frac{1}{2}n(n-1)$ edges in K_n. (Note that K_1 is an isolated vertex, $K_2 \cong P_2$, and $K_3 \cong C_3$.)

If $G \subseteq K_n$ then $\overline{G} = K_n - G$ is the *complement* of G with respect to K_n. (Often we just say $\overline{G}$ is the complement of G.) Note that G is in $\Omega(k, m)$ where $k \leq n$ and $m \leq \binom{n}{2}$. Furthermore, note that $\mathrm{Sp}(G)$ denotes a number but, $\mathrm{Sp}(K_n - G)$ denotes a function of n, since $K_n - G$ is an infinite family of graphs so long as $n \geq n(G)$.

A graph where every vertex has degree k is called *k-regular* (or just regular). A graph G is called *almost-regular* if $|d_u - d_v| \leq 1$ for all $u, v \in V(G)$. This thesis is concerned with a subproblem of Problem S, specifically almost-regular graphs in

$\Omega\left(n, \binom{n}{2} - m\right)$, where $\left\lfloor \frac{n}{2} \right\rfloor < m \leq n$ Formally, let Problem A (A for almost-regular) be:

> Given n and e, find G such that G is Sp-optimal with respect to all almost-regular graphs in $\Omega\left(n, \binom{n}{2} - m\right)$, where $\left\lfloor \frac{n}{2} \right\rfloor < m \leq n$

1.2 Motivation

The motivation for finding such extremal graphs arises from the notion that graphs with the most spanning trees are, in a sense, "more connected" than their peers. This is important in a number of fields, one of which is Network Reliability.

The *all-terminal network reliability model* is defined as follows. Vertices represent sites and edges represent links between the sites. The vertices are assumed to be perfectly reliable, but edges operate independently with the same probability p. The network is said to be operational if the underlying probabilistic graph is connected. The *reliability polynomial* of a graph G is a polynomial in p whose value for $0 \leq p \leq 1$ is the probability that G is operational. The reliability polynomial, for graph G, is defined as

$$Rel(p, G) = \sum_{i=1}^{e} N_i p^i (1-p)^{e-i}$$

where $e = e(G)$ and $N_i =$ the number of connected spanning i-edge subgraphs of G. Note that for $i < n - 1$ there are no connected spanning i-edge subgraphs so the sum can be considered to start at $n - 1$ instead of one.

In 1967, Kel'mans [36] first proposed this model of reliability, but there are other models Colbourn's' monograph [20] is an excellent and precise survey of reliability models For an accessible discussion on the validity of network reliability models see the discussion paper by Colbourn [21]

For completeness sake, we mention a set of papers by Kel'mans that Colbourn [20] and others have missed A number of Kel'mans' papers remain untranslated [39], [42], and [44] The following have been translated [38], [41], [40], and [46] Two other surveys that pertain specifically to the construction (synthesis) of reliable networks are by Boesch [8] and [9] The first paper discusses the probabilistic model outlined above while the second compares this model with a deterministic model

Since computing the all-terminal reliability of a network appears to be intractable (the problem is #P-complete [67]), various approximation schemes have been proposed (see Chapter 5 of [20]) Two of the more common of these is to let p approach either of its extreme values, zero or one

When edges are very unreliable, then the number of spanning trees is critical In particular we have the following theorem from Myrvold [59]

Theorem 1.2.1 *Let $G, H \in \Omega(n,e)$ If $N_i(G) = N_i(H)$ for $i = 1, 2, \ldots, k$ and $N_{k+1}(G) > N_{k+1}(H)$, then G is more reliable than H for p in the range $0 < p < \epsilon$ for some $\epsilon > 0$*

The key reason for this is because the dominant term of $Rel(p, G)$ is the low order term, namely the term with coefficient $N_{n-1}(G) = \mathrm{Sp}(G)$, for small p On the other hand for p very close to one we have the following theorem from the same source

Theorem 1 2 2 *Let $G, H \in \Omega(n,e)$ If $N_i(G) = N_i(H)$ for $i = e, e-1, \ldots, k+1$ and $N_k(G) > N_k(H)$, then G is more reliable than H for p in the range $1 > p > 1-\epsilon$ for some $\epsilon > 0$*

The proof of this theorem reasons as follows. For any graph G a *cutset* is a subset of the edge set whose removal disconnects the graph. Denote by $c(G)$ the size of the minimum cutset of G. For $i = e, e-1, \ldots, e-(c(G)+1)$ the number of connected spanning i edge subgraphs of G is just $\binom{e}{i}$. For example, when i equals $e-1$ (assuming $c(G) > 1$) there are e connected spanning subgraphs: one for each edge that can be deleted. Yet, when we delete $c(G)$ edges, then some subgraphs are disconnected so $N_{e-c(G)} < \binom{e}{e-c(G)}$.

For two graphs G and H let $c = \min\{c(G), c(H)\}$. From the above argument we have

$$N_i(G) = N_i(H) = \binom{e}{i}$$

for $i = e, e-1, \ldots, e-(c+1)$. Suppose, without loss of generality, that $c(G) > c(H) = c$. Then

$$\binom{e}{e-c} = N_{e-c(G)} > N_{e-c(H)},$$

and for p very close to one we have $Rel(p, G) > Rel(p, H)$. On the other hand suppose $c = c(G) = c(H)$. Then the graph that has the smallest number of minimum cutsets is more reliable.

It can happen that two non-isomorphic graphs can have the same minimum cutset size and have the same number of cutsets. In this case we need to examine the next term in the reliability polynomial to determine which graph is more reliable for p very close to one. Nadon did this for 3-regular graphs in her Master's thesis [63].

In summary, for p close to one we first need to maximize c. That is over all graphs we seek those with the largest minimum cut size. Then over the graphs that attain this maximum we seek those with the minimum number of minimum cutsets.

A graph $G \in \Theta(n, e)$ is said to be a *uniformly most reliable graph* if $Rel(p, G) \geq Rel(p, H)$, for all $H \in \Theta(n, e)$ and for all $p \in (0, 1)$. Clearly a uniformly most reliable graph will be a graph that attains the maximum number of spanning trees and has the minimum number of minimum size cutsets. Thus, the search for Sp-optimal graphs is a special case of the search for uniformly most reliable graphs.

Sometimes, however, a Sp-optimal graph is not uniformly most reliable because some other graph is better when p is sufficiently close to 0. It is known that uniformly most reliable graphs do not always exist. This was first discovered by Kel'mans and later independently discovered by Myrvold, Cheung, Page and Perry [59].

Further motivation comes from a field of study called optimum design theory. In 1981, Cheng [18] shows that finding Sp-optimal graphs is equivalent to finding a D-optimum incomplete block design. Cheng combined this observation with his 1978 work [17] to get his now famous result which we discuss below (p. 15).

1.3 Known Results

Table 1.1 presents all known results. The top portion of the table we call the sparse region because the graphs have relatively few edges. The lower portion of the table we call the dense region because the graphs have relatively many edges.

To solve problems in the sparse region, researchers treat e as a function of n. For example, $e = n$, $e = n + 1$, or $e = n + 2$. We will survey results of this type first. To solve problems in the dense region, e is determined by a range of functions of n. For example, $e = \binom{n}{2} - m$, where m is in the closed interval $(1, \lfloor n/2 \rfloor)$. This thesis uses the same approach but with m in the open interval $(\lfloor n/2 \rfloor + 1, n)$.

Class	Graphs with the most spanning trees	page
$\Theta(n,e)$ $e < n-1$	every graph since all are disconnected and hence have no trees	9
$\Theta(n,n-1)$	any tree	9
$\Theta(n,n)$	n-cycle	12
$\Theta(n,n+1)$	θ–graph with path lengths as even as possible [51, 60, 75]	12
$\Theta(n,n+2)$	a particular subdivision of K_4 [51, 70]	13
$\Theta\left(n,\frac{n^2}{4}\right)$	regular complete bipartite [18]	15
$\Omega\left(n,\frac{n^2}{2p}(p-1)\right)$	regular complete p–partite [18]	15
$\Omega\left(n,\binom{n}{2}-m\right)$ $\left\lfloor\frac{n}{2}\right\rfloor < m \leq n$	presented in this thesis for almost-regular graphs and [64] for $\left\lfloor\frac{n}{2}\right\rfloor < m \leq n-2$ and $m = n-1$ or $m = n$ provided $\binom{n}{2} - m$ is a multiple of three	
$\Omega\left(n,\binom{n}{2}-m\right)$ $0 < m \leq \left\lfloor\frac{n}{2}\right\rfloor$	K_n minus a matching [34, 68]	14
$\Theta\left(n,\binom{n}{2}\right)$	K_n [43, 47]	14

Table 1 1 Summary of known results

The most trivial solution to problem M is the case $e < n - 1$ Here every graph is Sp-optimal graph since all graphs are disconnected Another trivial case is for $e = n - 1$ In this case any connected graph is a tree and all other graphs are disconnected Hence the Sp-optimal graphs are trees and they have one spanning tree Currently these are the only known cases where the Sp-optimal graph is not unique This leads to the following conjecture

Conjecture 1 3 1 *The Sp-optimal graph for $\Theta(n, e)$, $e \geq n$, is unique*

Note that there are nontrivial cases where non-isomorphic graphs have the same number of spanning trees For example the complement of the graphs in Figure 1 1 have the same number of spanning trees for $n(G) \geq 7$ We discuss and prove this statement in Chapter 3, Section 3 5

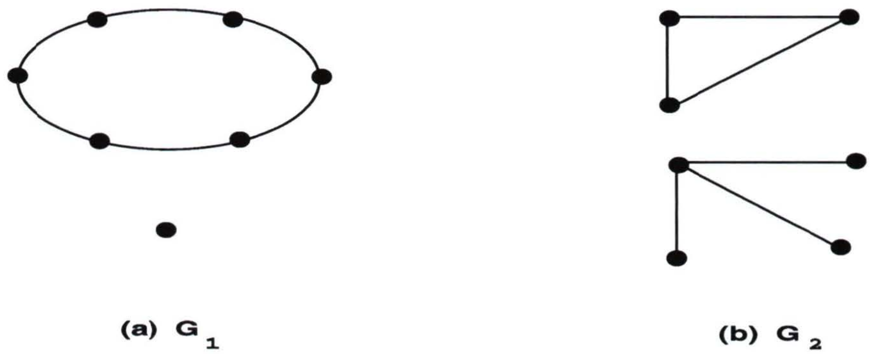


Figure 1 1 $K_n - G_1$ and $K_n - G_2$ have the same number of spanning trees, for $n \geq 7$

After the above simple cases problem M becomes more difficult Still it is not hard to see that for $e = n$ the best graph is a cycle with n edges Let us informally explore this simple case to exemplify the kind of task that we are attempting to solve in general (We will work with the class $\Omega(n, n)$ See Li [51] for a more formal proof for the class $\Theta(n, n)$) Figure 1 2 shows every graph in $\Omega(5, 5)$ with their respective number of spanning trees. Notice that each connected graph has exactly one cycle. Such graphs are called *unicyclic*.

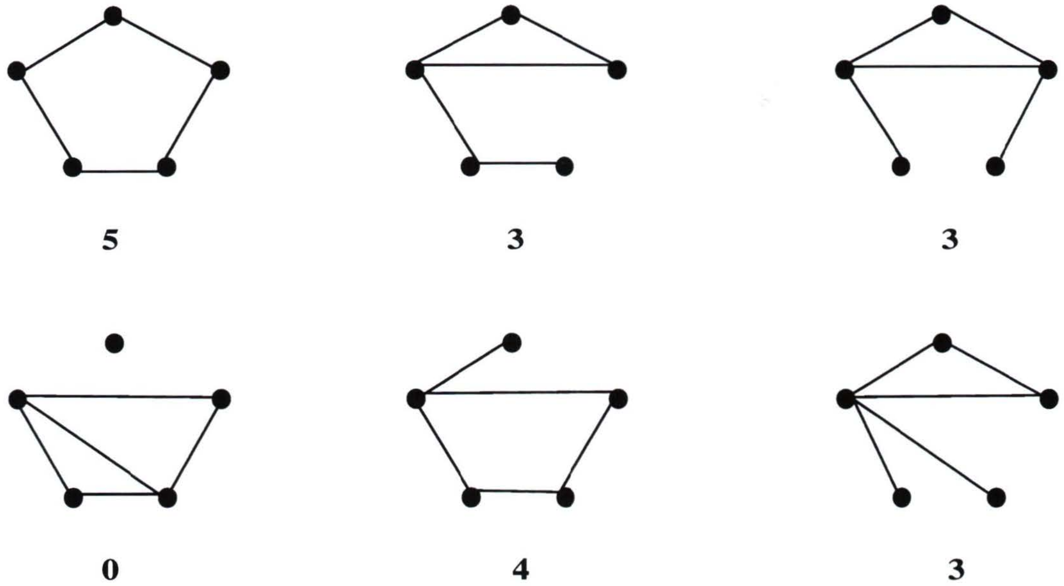
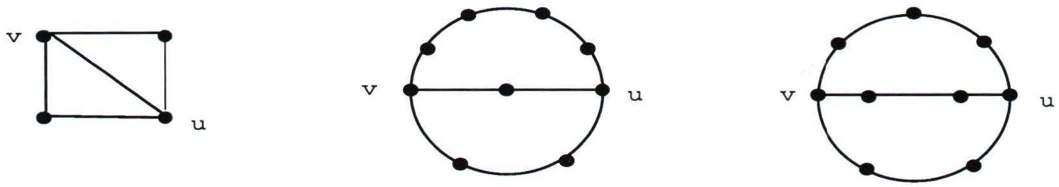


Figure 1.2: Graphs in $\Omega(5,5)$ and their number of spanning trees.

This arrangement is true for all graphs in $\Omega(n,n)$: if the graph is connected then it is unicyclic. First note that the non-cycle edges must be in every spanning tree. Then note that each edge in the cycle can be deleted in turn to produce a spanning tree. Since we can do this k ways, where k is the size of the cycle, the best graph in $\Omega(n,n)$ is the graph with the largest cycle: namely C_n.

The next entry of Table 1.1, $e = n+1$, is a relatively easy result which can be found in Li [51], Wang and Wu [75], and Myrvold [59]. It is interesting that three different approaches were used. Here is what they found.

A θ-graph $\in \Theta(n, n+1)$ has two distinct degree 3 vertices v and u plus three edge disjoint vu-paths. These graphs look like a cycle with a path across its middle. For example, Figure 1.3 shows three θ-graphs. It is possible to define such a graph G with



Θ(2,2,1) Θ(5,3,2) Θ(4,3,3)

(a) (b) (c)

Figure 1.3: Three θ-graphs

three integers, a, b and c, where $a+b+c=n+1$, the paths are P_a, P_b, and P_c, and for convenience, $a \geq b \geq c$. We shall denote such graphs as $\theta(a,b,c)$. When $e=n+1$ the Sp-optimal graph over all multigraphs is the $\theta(a,b,c)$-graph where $a-c \leq 1$. In other words, the path lengths are *nearly balanced*.

When $e = n+2$ we have a similar result due to Li [51] and independently by Tseng and Wang [70]. Li's result was subsequently published with Boesch and Suffel [10]. We present Li's formulation of the solution because Tseng and Wang's is more complicated. Furthermore, we present a simpler description than Li.

The *subdivision* of an edge $x = uv$ is accomplished by removing the edge uv, adding a new vertex w, and then adding two edges uw and wv. For example see Figure 1.4.

(a) edge uv (b) after subdivision

Figure 1.4: Subdivision of an edge

The Sp-optimal graph for $\Theta(n, n+2)$ is a *subdivision of a* K_4 which is constructed as follows. (Figure 1.5 shows the construction for $\Theta(7,9)$.) Form a K_4, label its six edges A, B, C, D, E, and F so that the three perfect matchings are $\{A, B\}, \{C, D\}$,

Figure 1 5 Construction of the Sp-optimal $\Theta(n, n+2)$ graph

and $\{E, F\}$ (See Figure 1 5(a)) Until the graph has n vertices subdivide the six original edges (making six paths) in lexicographic order Figure 1 5(b) shows the completed graph (the three edges A,B,C have been subdivided) Boesch, Suffel and Li [10] showed that the Sp-optimal graphs for $e = n, n+1$, and $n+2$ described above are also uniformly most reliable

For $e = n + 3$, Boesch, Li, and Suffel have shown that a subdivision of a $K_{3,3}$ (a 3-regular complete bipartite graph) is uniformly most reliable and hence Sp-optimal Our description of this graph follows Form a $K_{3,3}$, label its nine edges A, B, C, D, E, F, G, H, and I so that the three perfect matchings are

$$\{A, B, C\}, \{D, E, F\}, \text{ and } \{G, H, I\}$$

Until the graph has n vertices repeatedly subdivide the nine original edges (making nine paths) in lexicographic order

We have now reviewed all of the results in the sparse region and it is time to consider the dense region We start with $e = \binom{n}{2}$ Kiefer, in 1975 [47], and Kel'mans, in 1976 [43], showed that K_n is Sp-optimal over all graphs in $\Theta\left(n, \binom{n}{2}\right)$ Kiefer's work involved optimum design theory, a field of study which, in a restricted sense, is equivalent to problem M (see Cheng [17]) Kel'mans was the first to state this result in graph theoretic terms

We now restrict our attention to simple graphs. Since 1964, Kel'mans has investigated many topics related to problems M and S. One paper, written with Chelnokov in 1974 [34], contains the answer to problem S for graphs in $\Omega\left(n, \binom{n}{2} - m\right)$, $0 < m \leq \left\lfloor \frac{n}{2} \right\rfloor$. Independently, in 1974, Shier [68] derived the same answer. For graphs in this class, the best graph is $K_n - M$, where M is a matching (the graph $M = k \cdot K_2$, $k > 0$, is called a *matching*).

In his 1991 doctoral thesis, Petingi [64] states results for graphs in $\Omega\left(n, \binom{n}{2} - m\right)$, for $\left\lfloor \frac{n}{2} \right\rfloor < m \leq n - 2$ and $m = n - 1$ or $m = n$ provided $\binom{n}{2} - m$ is a multiple of three. This thesis strengthens his results and provides new methods for ranking almost-regular graphs in this class. In particular, this thesis finds the Sp-optimal almost-regular graphs in $\Omega\left(n, \binom{n}{2} - m\right)$, $\left\lfloor \frac{n}{2} \right\rfloor < m \leq n$. These results are previewed in the next section.

Finally, we briefly look at the work of Cheng [18]. First we need to describe two special types of graphs. A multigraph G is called *regular complete multi-partite* if $V(G)$ can be partitioned into p subsets of equal size such that there are k edges between any two vertices in the same subset and $k+1$ edges between any two vertices in different subsets, where $k \geq 0$ is an integer. (Note that if $k = 0$ the graph is simple.) If $p = 2$ then the graph is called *regular complete bipartite*. (Note that definitions for less specialized graphs exist but we don't need them for this thesis.)

Cheng [17] proved a result in optimum design theory that was later restated in graph theoretic terms [18]. If G is regular complete bipartite, $k \geq 0$, then G is Sp-optimal over all multigraphs in its class. Also in [18] he showed that if G is regular complete multi-partite, $k = 0$, then G is Sp-optimal over all simple graphs in its class.

This completes our look at known results.

1.4 New Results

As mentioned above, problem S is solved for the class $\Omega\left(n, \binom{n}{2} - m\right)$, $0 < m \leq \left\lfloor \frac{n}{2} \right\rfloor$ and this thesis will work with class $\Omega\left(n, \binom{n}{2} - m\right)$, $\left\lfloor \frac{n}{2} \right\rfloor < m \leq n$. This suggests the following (new) notation. Let

$$\begin{array}{rclcrcl}
\Omega^1 & = & \Omega\left(n, \binom{n}{2} - m\right), & & 0 & < m \leq & \left\lfloor \frac{n}{2} \right\rfloor \\
\Omega^2 & = & \Omega\left(n, \binom{n}{2} - m\right), & & \left\lfloor \frac{n}{2} \right\rfloor & < m \leq & n \\
\Omega^3 & = & \Omega\left(n, \binom{n}{2} - m\right), & & n & < m \leq & \left\lfloor \frac{3n}{2} \right\rfloor \\
\cdots & & \cdots & & & \cdots & \\
\Omega^k & = & \Omega\left(n, \binom{n}{2} - m\right), & & \left\lfloor \frac{(k-1)n}{2} \right\rfloor & < m \leq & \left\lfloor \frac{kn}{2} \right\rfloor
\end{array}$$

As discussed above for Ω^1, K_n minus a matching is Sp-optimal. This thesis and Petingi work with Ω^2. For each of these classes Cheng's result, regular complete multi-partite graphs are Sp-optimal for their respective class, may apply.

Observation 1.4.1 *For the class Ω^k a regular complete p-partite graph can be formed when kn is even and $(k+1)|n$. Thus, $e = \binom{n}{2} - (kn/2)$ (e.g. $m = kn/2$) and the number of partitions p is given by $p = n/(k+1)$.*

For example, let G be regular complete p-partite.

Ω^1. If $2|n$ then $m = n/2$, $p = n/2$ and G is the complement of p K_2's,

Ω^2. If $3|n$ then $m = n$, $p = n/3$ and G is the complement of p K_3's,

Ω^3 If $4|n$ then $m = 3n/2$, $p = n/4$, G is the complement of p K_4's

Before we discuss the main results of this thesis we make two observations about the known results In every case the Sp-optimal graph is regular or almost-regular (For example, for Ω^1 if n is not divisible by two, then $m = \left\lfloor \frac{n}{2} \right\rfloor$, $p = n$ and the Sp-optimal graph is the complement of p K_2's with a single isolated vertex Hence the graph is almost regular) Also, when a solution is known for all multigraphs in $\Theta(n, e)$, $e \leq \binom{n}{2}$, then the graph is simple Both of these observations make intuitive sense, yet there is no proof that they always hold Still, the next two conjectures are widely believed to be true

Conjecture 1 4 2 *If $e \leq \binom{n}{2}$ and G is Sp-optimal over all multigraphs, then G is simple*

Conjecture 1 4 3 *If $e \leq \binom{n}{2}$ and G is Sp-optimal, then G is regular or almost-regular*

For graphs with "sufficiently large" e the multigraph extension of Conjecture 1 4 3 has been proven true (e g e must be larger than $\binom{n}{2}$) Cheng et al [19] showed that for "sufficiently large" e the graphs with the most spanning trees are *nearly balanced* (almost regular and the number of multiple edges between any pair of vertices differs by at most one) From their work it is evident that there is no bound (even implicit) on what constitutes "sufficiently large e" Also, there is no clear way to restrict their work to the class of simple graphs

More important, in the context of this thesis, is Petingi's [64] doctoral thesis By complicated arguments he shows that in Ω^2 almost regularity is required when $m \leq n - 2$ or when $\left(\binom{n}{2} - n\right)$ is congruent to zero modulo three

Observation 1 4 4 *Let $G \in \Omega(n,m)$ so that $(K_n - G) \in \Omega^2$ Then $K_n - G$ is almost-regular if and only if G is almost regular*

Observation 1 4 5 *If the graph G in the previous observation is almost-regular then for all $v \in V(K_n - G)$, $d_v = n-2$ or $d_v = n-3$*

Thus almost-regular Ω^2 graphs have complements composed of paths and/or cycles We consider the following cases in turn

1. G is composed of path components
2. G is composed of cycle components
3. G is composed of a mixture of path and cycle components

For the path case, a result due to Kel'mans [43, Lemma 6 8,p 258] shows that given two paths it is best to make their lengths as equal as possible We give a new proof of this result and, at the same time, extend the result to show that given a path of length at least two and an isolated vertex that it is best to make two paths

For the cycle case, we present two new results Consider $C_k + C_{m-k}$, where $k \leq m-k$ If k is odd then $K_n - (C_k + C_{m-k})$ has more spanning trees than $K_n - C_m$ (the complement of one large cycle) However, if k is even then the converse holds $K_n - C_m$ is better Second, let $G = C_k + C_{m-k}$ and $H = C_{k+c} + C_{m-k-c}$, where $k \leq m-k$ and c is one or two Then the complement of G has more spanning trees than the complement of H if k is odd and fewer if k is even (This result is actually presented via two theorems) Although these results do not completely rank the graphs whose complements are a union of disjoint cycles, it does provide the means to find the Sp-optimal graph in this class, with one small provable exception We also give indication of a complete ranking for this class

For graphs whose complements are composed of a union of disjoint cycles and paths (mixed case), we show that breaking down large paths into a triangle and a smaller path increases the number of spanning trees (This result was stated by Kel'mans [43, 1976] We present the first proof) We also show that the complement of $C_3 + P_k$ has more spanning trees than the complement of $C_{3+c} + P_{k-c}$, where $k - c > 0$ and $c > 0$ We are then left with a set of three special cases which are proved algebraically Thus we are able to completely characterize the Sp-optimal almost-regular Ω^2 graphs

To obtain these results we review the major spanning tree counting methods and then summarize the known formulas for path components and cycle components We then derive some new formulas and give new proofs for some of the existing formulas

1.5 Thesis Overview

Chapter 2 contains basic linear algebra definitions, notation, and results needed for this thesis Chapter 3 presents the major spanning tree counting formulas We discuss a recursive formula, an inclusion exclusion formula and formulas derived from a special matrix associated with a graph We also discuss various properties of this matrix as they apply to counting spanning trees Chapter 3 concludes with a discussion of ranking graphs by their number of spanning trees

Since the thesis is concerned with finding the Sp-optimal almost-regular graphs in Ω^2, Chapter 4 presents spanning tree counting formulas for $K_n - P_k$ and $K_n - C_k$, $k \leq n$ We refer to these formulas as formulas for path and cycle components, respectively. We present trigonometric, combinatorial and analytic formulas for path and cycle components. The combinatorial formula for cycle components is new as is a relationship between the formulas for odd cycles and two paths. We give new proofs for the analytic formulas.

For other special classes of graphs formulas can be found in the literature. Berge [6] reviews combinatorial formulas. Moon [57] gives a comprehensive survey for counting trees. This work is extended in Moon [58]. Kel'mans and Chelnokov [34] present many analytic formulas – work that extends Kel'mans' [37]. A more recent survey of analytic formulas can be found in an unpublished report by Boesch and Suffel [11].

Chapter 5 presents the main results of this thesis which we have previewed in the previous subsection. Chapter 6 concludes with a discussion of possible directions for future research. The appendices include a summary of all notation used in this thesis and some formulas for path and cycle components for small k.

Chapter 2

Linear Algebra Definitions, Notation, and Basic Results

This chapter gives a brief review of the linear algebra necessary for this thesis. An excellent source of further information is Horn and Johnson's book "Matrix Analysis" [32]. This thesis only requires square real matrices and not the more general rectangular matrices over an arbitrary field. All vectors are assumed to be column vectors. The identity matrix of order n is denoted by I_n or just I if n is understood. The order n matrix composed entirely of ones is denoted J_n, or just J. The determinant of a matrix A is denoted by $|A|$. The transpose of matrix A is denoted A^{T}. Similarly for vectors. The sum of all elements on the main diagonal of matrix A is denoted by trace(A).

For matrix $A = [a_{ij}] \in \mathbf{R}^{n \times n}$ and for index sets $\alpha \subseteq \{1, \ldots, n\}$ and $\beta \subseteq \{1, \ldots, n\}$, we denote, by $A_{\alpha,\beta}$, the submatrix that remains after the rows of A indexed by α and the columns indexed by β are simultaneously deleted. The determinant of any such submatrix is called a *minor* of A.

If $\alpha = \beta$ then $A_{\alpha,\alpha}$ is called a *principal submatrix* of A and is abbreviated to A_α. For convenience we write A_i instead of $A_{\{i\}}$, and A_{ij} instead of $A_{\{i\}\{j\}}$. The determinant of any principal submatrix is called a *principal minor*. By convention, the empty principal minor is 1, that is, $\left|A_{\{1,2,\ldots,n\}}\right| = 1$.

The term $(-1)^{i+j}\,|A_{ij}|$ is called the $(i,j)^{\text{th}}$-*cofactor* of A. Using cofactors we can express the determinant of A as

$$\begin{aligned} |A| &= \sum_{j=1}^{n} a_{ij}\,(-1)^{i+j}\,|A_{ij}|, \quad 1 \le i \le n, \quad \text{(row expansion)} \\ &= \sum_{i=1}^{n} a_{ij}\,(-1)^{i+j}\,|A_{ij}|, \quad 1 \le j \le n, \quad \text{(column expansion)} \end{aligned}$$

Either of these expressions is called a *Laplace expansion* of the determinant of A.

Let $A \in \mathbf{R}^{n\times n}$. The transposed matrix of cofactors $B = [b_{ij}] \in \mathbf{R}^{n\times n}$, where

$$b_{ij} = (-1)^{i+j}\,|A_{ji}|,$$

is called the *adjugate* (sometimes called the *classical adjoint*) of A and is denoted by $\text{adj}(A)$. A calculation using the Laplacian expansion for the determinant shows that ([32, p. 20])

$$\text{adj}(A)\,A = A\,\text{adj}(A) = |A|\,\mathrm{I}. \tag{2.1}$$

Chapter 3

Spanning Tree Formulas

This chapter presents combinatorial and analytic formulas for counting the number of spanning trees in a graph. Whenever possible the methods are presented for multigraphs. However, when we count the number of spanning trees remaining after the deletion of a set of edges from the complete graph (complement graphs), then the method pertains to simple graphs.

The methods include a brief discussion of the well known recursive formula and a discussion of the inclusion exclusion formula. Then the rest of the chapter is devoted to a special matrix associated with a graph called the Laplacian (sometimes called the Kirchhoff matrix or the matrix of nodal admittance). From this matrix we derive analytic methods for counting the number of spanning trees in a graph. The chapter ends with a discussion of ranking simple graphs by their number of spanning trees.

3.1 Feussner's Recursive Formula

The following recursive formula is attributed to Feussner's 1904 paper [29]. The reader is referred to Moon's 1970 monograph for a discussion of the origin of this formula [57]. In this section, by graph we mean multigraph.

For a graph G an edge $x = uv \in E(G)$ is *contracted* when the vertices u and v are replaced by a new vertex, say w, all uv edges become loops incident with w, and each edge that was incident with u or v is replaced by an edge incident with w. Since we are counting spanning trees we can delete the loops.

Theorem 3.1.1 (Feussner) *Let x be any edge of graph G and let $G - x$ denote the graph obtained from G by deleting the edge x, and let G/x denote the graph obtained from G by contracting the edge x. Then*

$$Sp(G) = Sp(G - x) + Sp(G/x).$$

Proof For any spanning tree T of graph G, if $x \in E(T)$ then T is counted in $\mathrm{Sp}(G/x)$ otherwise T is counted in $\mathrm{Sp}(G - x)$. □

Li [51] made extensive use of Feussner's formula to derive Sp-optimal $\Theta(n, n+1)$ and $\Theta(n, n+2)$ graphs. He also gave a number of general results. One that he did not mention is the following simple result that is easily achieved with Feussner's formula.

Lemma 3.1.2 *If the graph $G \in \Theta(n, e)$, where $e \geq n$, is Sp-optimal, then G does not contain a vertex of degree one.*

Proof: Note that the condition $e \geq n$ insures there exists a connected graph in $\Theta(n, e)$. Let G be one of these graphs such that G has a degree one vertex u and let x be the edge incident to u. We show that, for any such G, there exists a graph $H \in \Theta(n,e)$ such that $\mathrm{Sp}(H) > \mathrm{Sp}(G)$. We do so by constructing H from G. Note that the condition $e \geq n$ insures that G contains a cycle. Choose an edge $y = vw$ on this cycle. Define H as

$$H = G - x - y + uv + uw.$$

Let $x' = uv$ and $y' = uw$.

Apply Feussner's formula twice to G:

$$\begin{aligned}\mathrm{Sp}(G) &= \mathrm{Sp}(G-y) + \mathrm{Sp}(G/y)\\ &= \big(\mathrm{Sp}(G-y-x) + \mathrm{Sp}(G-y/x)\big) + \big(\mathrm{Sp}(G/y-x) + \mathrm{Sp}(G/y/x)\big).\end{aligned}$$

Because the removal of x disconnects G this equals

$$\mathrm{Sp}(G-y/x) + \mathrm{Sp}(G/y/x).$$

Apply Feussner's formula twice to H as follows:

$$\begin{aligned}\mathrm{Sp}(H) &= \mathrm{Sp}(H-y') + \mathrm{Sp}(H/y')\\ &= \big(\mathrm{Sp}(H-y'-x') + \mathrm{Sp}(H-y'/x')\big) + \big(\mathrm{Sp}(H/y'-x') + \mathrm{Sp}(H/y'/x')\big)\end{aligned}$$

Note that $H - y' - x'$ is disconnected so $\mathrm{Sp}(H - y' - x') = 0$. Also note that, $(G - y/x) \cong (H - y'/x')$ and $(G/y/x) \cong (H/y'/x')$. So,

$$\mathrm{Sp}(H) - Sp(G) = \mathrm{Sp}(H/y' - x').$$

This result is at least one since $H/y' - x'$ is a connected graph. □

3.2 Temperley's Formula

This section presents Temperley's complement inclusion exclusion formula Since the formula is for complement graphs, it can only be used for simple graphs Hence in this section, by graph we mean simple graph The formula first appeared, implicitly, in Temperley's 1964 paper [69] (This paper's main focus was modeling the equation state of an imperfect gas) Since then it has been given and proved explicitly in two forms analytic and combinatorial The analytic version will be discussed later (Theorem 3 4 3) The combinatorial version (Theorem 3 2 3) and proof are due to Moon [55] Also see Berge [6] for a discussion of Moon's combinatorial approach

The next theorem is used to determine a single term in the complement inclusion exclusion formula It tells us exactly how many spanning trees of the complete graph K_n use all the edges of a given simple and acyclic graph (No spanning tree of K_n can use all of the edges of a cycle)

Theorem 3 2 1 *Let $V_1, V_2, \ldots, V_k$ be a partition of $V(K_n)$, $T_1 = (V_1, E_1)$, $T_2 = (V_2, E_2)$, $\ldots$, $T_k = (V_k, E_k)$ be trees, and let $n_i = |V(T_i)|, i = 1, 2, \ldots, k$ Then the number of spanning trees of K_n that have $T_1, T_2, \ldots$, and T_k as subgraphs is*

$$n_1 n_2 \cdots n_k n^{k-2}$$

Proof See Moon [55, Theorem 2, p 265] for a proof of this theorem (Also see Moon [57, Theorem 6 1, p 52] for a discussion of other uses of this result) □

For example, if $k = 1$ then T_1 is of order n and we have $nn^{1-2} = n/n = 1$ spanning tree of G that has T_1 as a subgraph Another example provides a simple proof for the most famous spanning tree formula Cayley's formula for the complete graph [16] The following is just one of the many ways to prove this important theorem See Moon's summary [56] for more

Theorem 3.2.2 (Cayley 1857) *For the complete graph K_n*

$$Sp(K_n) = n^{n-2}$$

Proof Using the notation of Theorem 3.2.1 we need the number of spanning trees of $G \cong K_n$ that have $T_1 \cong T_2 \cong \cdots \cong T_k \cong K_1$ as subgraphs. In this case $k = n$ and the order of each T_i, $1 \le i \le n$, is one. Thus, from Theorem 3.2.1

$$\mathrm{Sp}(K_n) = 1 \cdot 1 \cdots 1 \cdot n^{n-2} = n^{n-2}. \square$$

Define the function $\nu : \Omega(n, e) \to \mathbf{Z}^+$ such that if $G \in \Omega(n,e)$ has $k \ge 1$ components (not necessarily trees) of orders $n_1, n_2, \ldots, n_k$ then

$$\nu(G) = \begin{cases} 0 & \text{if } G \text{ contains a cycle} \\ n_1 n_2 \cdots n_k & \text{otherwise.} \end{cases} \tag{3.1}$$

Note that if the edge set of G is empty then there are n isolated vertices so $\nu(G) = 1^n = 1$.

We are now ready for the combinatorial version of Temperley's complement inclusion exclusion formula. This formula gives the number of spanning trees that do not use any edge in a given simple graph. In other words, the number of spanning trees contained in the complement of the graph.

Theorem 3.2.3 (Temperley's inclusion exclusion formula) *Let $G \subseteq K_n$. Then*

$$Sp(K_n - G) = n^{n-2} \sum_{\substack{F \subseteq G \\ V(F)=V(G)}} \nu(F)(-n)^{-e(F)} \tag{3.2}$$

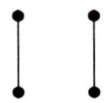


Figure 3.1: Graph $G = P_2 + P_2$

Since the sum is over all spanning subgraphs F of G, observe that the summation has an exponential nature. This is because the sum is taken, in effect, over the power set of $E(G)$.

For example, suppose $G = P_2 + P_2 \in \Omega(4,2)$ (see Figure 3.1). Then the four possible subgraphs of G are F_0, F_1, F_2, and F_3 shown in Figure 3.2.

Figure 3.2: The four subgraphs of $G = P_2 + P_2$.

Now using Theorem 3.2.3 we get:

$$\begin{aligned} \mathrm{Sp}(K_n - G) &= n^{n-2}\sum_{i=0}^{3}\nu(F_i)(-n)^{-e(F_i)} \\ &= n^{n-2}\Big(1 + 2(-n)^{-1} + 2(-n)^{-1} + 2\cdot 2(-n)^{-2}\Big) \\ &= n^{n-2}\Big(1 - \frac{4}{n} + \frac{4}{n^2}\Big) \end{aligned}$$

This is a formula for arbitrary n. For example, if $n = 4$ (Figure 3.3(a)) then $\mathrm{Sp}(K_n - G) = 4^2(\frac{4}{4^2}) = 4$ and if $n = 5$, which is larger than $n(G)$, then $\mathrm{Sp}(K_n - G) = 5^3(1 - \frac{4}{5} + \frac{4}{5^2}) = 5^3\frac{9}{5^2} = 45$ (see Figure 3.3(b)). So our formula for $\mathrm{Sp}(K_n - (P_2 + P_2))$ is really a formula for two paths of order two and any number of isolated vertices.

A complete proof of Theorem 3.2.3 can be found in Moon [55, Theorem 3, p. 267], but essentially it uses the inclusion exclusion principle discussed in many discrete

(a) $\overline{G}$ w.r.t. K_4 (b) $\overline{G}$ w.r.t. K_5

Figure 3.3: Complements of $G = P_2 + P_2$.

mathematics texts (e.g. Grimaldi [31] or Knuth [49]). The application of this principle starts with Sp(K_n) (Theorem 3.2.2) and uses Theorem 3.2.1 to get each term in the summation.

Following the notation of Moon [55, p. 266], let

$$f(n, G) = \sum_{\substack{F \subseteq G \\ V(F)=V(G)}} \nu(F)(-n)^{-e(F)} \tag{3.3}$$

for $G \in \Omega\,(k, e), k \leq n$. Bedrosian [3, p.314] calls the polynomial $f(n, G)$ the *generic form* of the graph G and in 1970 [4] he gives the generic form of certain classes of graphs. Later, in 1983, Bedrosian and Moon [58] give results for the generic form of multigraphs. In Chapter 4, we present Moon's formulas for the generic form of paths and cycles.

Notice that the definition of the generic form implies the following.

Corollary 3.2.4 *If $G \in \Omega\,(n, e)$ has $k \geq 1$ components $G_1, G_2, \ldots, G_k$, then*

$$Sp(K_n - G) = n^{n-2} \prod_{i=1}^{k} f(n, G_i)$$

Thus, it is advantageous to know the generic form of certain classes of uncomplicated graphs which can then be considered as components of more complicated graphs.

3.3 Laplacian Matrix

For this section by graph we mean multigraph. This allows us to develop the following results in their more general setting.

The matrix we are about to describe (called the Laplacian) is important if one wishes to develop formulas for the number of spanning trees in a graph, but it has also seen many other uses. Notably, Fiedler [26, 27] uses its second smallest eigenvalue and associated eigenvector to describe what he calls the algebraic connectivity of a graph. Fiedler's work has lead to several useful numerical algorithms [2, 54, 65, 66].

Other important uses of this matrix includes the determination of a necessary condition for a graph to have a Hamilton cycle. This result is due to Mohar [53]. And in the theory of flexible polymer molecules (a field of chemical physics) Forsman [28] states:

> the matrix incorporating entropy spring effects in the Rouse approach of describing chain dynamics is shown to be given by [the Laplacian].

The Laplacian matrix can be defined directly or in terms of other important matrices associated with a graph. The direct definition allows use to write the matrix by inspecting the graph. On the other hand, defining the matrix in terms of other matrices gives us additional information about the matrix itself. We begin with the direct definition and then we introduce the other important matrices.

For the graph $G \in \Theta(n, e)$, let $V(G) = \{1, 2, \ldots, n\}$ and let e_{ij} equal the number of edges $\{i, j\} \in E(G)$. Recall d_v denotes the degree of vertex $v \in V(G)$. The *Laplacian matrix*, $\mathcal{L}(G) = [\ell_{ij}] \in \mathbf{Z}^{n \times n}$, associated with the graph G is defined by

$$\ell_{ij} = \begin{cases} d_i & \text{if } i = j, \\ -e_{ij} & \text{if } i \neq j. \end{cases}$$

We write $\mathcal{L}$ instead of $\mathcal{L}(G)$ if G is understood. It follows that $\mathcal{L}$ is a real symmetric matrix. Note that the trace of $\mathcal{L}$ is the sum of the degrees of all vertices in G. By a well known result in graph theory (see Bondy and Murty [13, Theorem 1.1, p. 10]), trace$(\mathcal{L}) = 2\,e(G)$.

The *adjacency matrix*, $\mathcal{A}(G) = [\alpha_{ij}] \in \mathbf{Z}^{n \times n}$, is defined by

$$\alpha_{ij} = e_{ij}.$$

From the definition it follows that the trace of $\mathcal{A}$ is zero (all graphs are assumed to be loop free), and that $\mathcal{A}$ is a real symmetric matrix.

The matrix $\Delta(G) = [\delta_{ij}] \in \mathbf{Z}^{n \times n}$ is the diagonal matrix diag$(d_1, d_2, \ldots, d_n)$. Note that the Laplacian can be defined in terms of these two matrices since

$$\mathcal{L}(G) = \Delta(G) - \mathcal{A}(G) = [\delta_{ij} - \alpha_{ij}] \tag{3.4}$$

Before defining the last matrix, we introduce a useful device. For the graph $G \in \Theta(n, e)$, let $V(G) = \{v_1, v_2, \ldots, v_n\}$ and let $E(G) = \{x_1, x_2, \ldots, x_e\}$. For each edge $x = \{v_j, v_k\}$ of $E(G)$, we arbitrarily choose one of v_j, v_k to be the positive end of x and the other one to be the negative end. This procedure gives $E(G)$ an *orientation*. For example, Figure 3.4 shows a graph and a possible orientation.

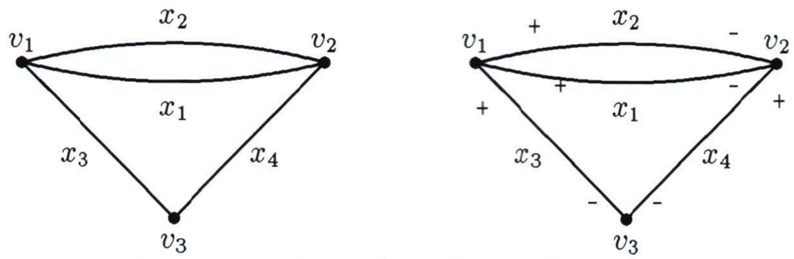


Figure 3.4. A graph with an arbitrary orientation.

The *incidence matrix*, $\Gamma(G) = [\eta_{ij}] \in \mathbf{Z}^{n \times e}$, for G and an arbitrary orientation of its edges, is defined by

$$\eta_{ij} = \begin{cases} +1 & \text{if } v_i \text{ is the positive end of edge } x_j \\ -1 & \text{if } v_i \text{ is the negative end of edge } x_j \\ 0 & \text{otherwise} \end{cases}$$

Note that the rows of this matrix correspond to the vertices of G, and the columns correspond to the edges of G. Also note that since all column sums are zero, $\Gamma(G)$ is singular. For example, the incidence matrix for the graph in Figure 3.4 is

$$\Gamma = \begin{pmatrix} 1 & 1 & 1 & 0 \\ -1 & -1 & 0 & 1 \\ 0 & 0 & -1 & -1 \end{pmatrix}$$

The following lemma with its proof is from Biggs [7, Prop. 4.8, p. 27].

Lemma 3.3.1 *For a graph $G \in \Theta(n, e)$ and some orientation of its edges, let $\Gamma = \Gamma(G)$, $\mathcal{A} = \mathcal{A}(G)$, and $\Delta = \Delta(G)$ be the matrices defined above. Then*

$$\Gamma\,\Gamma^{\mathrm{T}} = \Delta - \mathcal{A}$$

Proof. Note that $(\Gamma\,\Gamma^{\mathrm{T}})_{ij}$ (the (i,j) entry of $\Gamma\,\Gamma^{\mathrm{T}}$) is the inner product of row i and row j of Γ. If $i \neq j$ then these rows have a non-zero entry in the same column if and only if there is an edge joining v_i and v_j. In this case, the two non-zero entries are $+1$ and -1. Thus, $(\Gamma\,\Gamma^{\mathrm{T}})_{ij} = -e_{ij}$. Similarly, $(\Gamma\,\Gamma^{\mathrm{T}})_{ii}$ is the inner product of row i with itself, and since each term is $(-1)^2$ or $(+1)^2$ this entry is equal to the degree of v_i. □

For example consider the graph in Figure 3 4 Then

$$\Gamma\,\Gamma^{\mathrm{T}} = \begin{pmatrix} 1 & 1 & 1 & 0 \\ -1 & -1 & 0 & 1 \\ 0 & 0 & -1 & -1 \end{pmatrix} \begin{pmatrix} 1 & -1 & 0 \\ 1 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & -1 \end{pmatrix} = \begin{pmatrix} 3 & -2 & -1 \\ -2 & 3 & -1 \\ -1 & -1 & 2 \end{pmatrix}$$

This lemma and Equation 3 4 mean we also have

$$\mathcal{L}(G) = \Gamma\,\Gamma^{\mathrm{T}} \tag{3 5}$$

3.3.1 Characteristic polynomial of the Laplacian

For graph $G \in \Theta(n, e)$, the *characteristic polynomial*[1] of G is defined as

$$\mathcal{P}(t, G) = |t\mathrm{I} - \mathcal{L}(G)| \tag{3 6}$$

The characteristic polynomial of a graph is important in the counting of spanning trees and it will play a role in our attempt to rank graphs by their number of spanning trees

The n roots of $\mathcal{P}(t, G)$ are called the *eigenvalues* of $\mathcal{L}(G)$ and are denoted by $\lambda_i = \lambda_i(G)$, $i = 0, 1, \ldots, n-1$ With these eigenvalues we can write the characteristic polynomial as

$$\mathcal{P}(t, G) = \prod_{i=0}^{n-1} (t - \lambda_i) \tag{3 7}$$

[1]We adopt the convention of expressing the characteristic polynomial in terms of t for the same reasons discussed in Horn and Johnson's book [32, p 38]

We can also write the characteristic polynomial in general form as

$$\mathcal{P}(t,G) = \sum_{i=0}^{n-1} (-1)^i c_i(G)\, t^{n-i} \tag{3.8}$$

where $c_i(G)$ denotes the i^{th} coefficient. Later, in Lemma 3.3.12, we give Kel'mans' graph theoretic formula for these coefficients. Readers of Kel'mans note that his definition of the characteristic polynomial of a graph has an additional factor of $\frac{1}{t}$ and is $\mathcal{P}(t,G) = \frac{1}{t}\,|t\mathrm{I} - \mathcal{L}(G)|$.

Some authors (see Cvetković [23]) define the characteristic polynomial of a graph in terms of the adjacency matrix instead of the Laplacian. This polynomial is, in general, quite different. However, for regular graphs they are closely related. For example, let $G \in \Theta(n,e)$ be r-regular, $\mathcal{L} = \mathcal{L}(G)$, $\mathcal{A} = \mathcal{A}(G)$, and $\Delta = \Delta(G)$. Note that $\Delta = r\mathrm{I}$. So,

$$\begin{aligned} \mathcal{P}(t,G) &= |t\mathrm{I} - \mathcal{L}| \\ &= |t\mathrm{I} - (\Delta - \mathcal{A})| \\ &= |(t-r)\mathrm{I} + \mathcal{A}| \\ &= (-1)^n\ |(r-t)\mathrm{I} - \mathcal{A}| \end{aligned} \tag{3.9}$$

and this last equation, setting $\lambda = (r-t)$ and ignoring the sign term $(-1)^n$, contains the characteristic polynomial associated with $\mathcal{A}(G)$. Consequently, if $\mathcal{L}$ has eigenvalues $\lambda_0, \lambda_1, \ldots, \lambda_{n-1}$, then $\mathcal{A}$ has eigenvalues $r-\lambda_0, r-\lambda_1, \ldots, r-\lambda_{n-1}$. Thus, results derived from $|t\mathrm{I} - \mathcal{A}|$ for regular graphs apply to $\mathcal{P}(t,G)$. Cvetković has produced a continuing series of surveys on graph spectra [24, 22, 23].

The next result, due to Kel'mans [35] (1965), is related to Corollary 3.2.4 (p. 29) above since it too considers the individual components of a graph. The proof that follows differs from Kel'mans' since he worked with a variant of the Laplacian.

Lemma 3.3.2 (Kel'mans) *If $G \in \Theta(n,e)$ has $k \geq 1$ components $G_1, G_2, \ldots, G_k$, then*

$$\mathcal{P}(t,G) = \prod_{i=1}^{k} \mathcal{P}(t,G_i)$$

Proof Let $G' = G_1' + G_2' + \cdots + G_k'$ where the vertices of each component, G_i', are given consecutive labels, $G_i \cong G_i'$ and the vertices of G_i' are labelled before those of G_{i+1}'. This corresponds to the transformation $P\,\mathcal{L}(G)\,P^{\mathrm{T}} = \mathcal{L}(G')$, for some permutation matrix P. Since no vertex in component G_i' is adjacent to a vertex in component G_j', for all $i \neq j$, it follows that $\mathcal{L}(G')$ is block diagonal. Since $P^{\mathrm{T}} = P^{-1}$, $\mathcal{L}(G)$ is similar to a block diagonal matrix. By considering the Laplace expansion, it is clear that the determinant of a block diagonal matrix is the product of the determinants of the blocks. This gives the required result. □

3.3.2 Eigenvalues of the Laplacian

In the previous subsection, we introduced the n eigenvalues of $\mathcal{L}(G)$ as the roots of the characteristic polynomial. An alternative definition of an eigenvalue is any number, say λ, that satisfies the equation $\mathcal{L}(G)\,\mathbf{x} = \lambda\,\mathbf{x}$ for some nonzero vector $\mathbf{x}$.

This subsection summarizes some basic results concerning the eigenvalues of the Laplacian. As mentioned above the eigenvalues of a graph are important in a number of ways. As well, they play an important role in the context of counting spanning trees and ranking graphs by their number of spanning trees.

A matrix $C \in \mathbf{R}^{n \times n}$ is *positive semidefinite* if there exists a matrix M, not necessarily square, such that $C = M\,M^{\mathrm{T}}$ (see [77, Theorem 1.5.4] or [32, Theorem 7.2.7, p. 406]). Note that M can be singular implying that C can be singular as well. Let

$\mathcal{L} = \mathcal{L}(G)$ Equation 3.5 (p 33) says $\mathcal{L} = \Gamma\,\Gamma^{\mathrm{T}}$, therefore $\mathcal{L}$ is positive semidefinite Furthermore, since $\mathcal{L}$ is symmetric all of the eigenvalues of $\mathcal{L}$ are real by the Spectral Theorem (see Watkins [77, p 230] or Horn and Johnson [32, Theorem 2.5.6, p 104]) By a well known result in linear algebra, all of the eigenvalues of a real symmetric matrix are non-negative if and only if the matrix is positive semidefinite (see [32, Theorem 7.2.1, p 402]) Since all rows of $\mathcal{L}$ sum to zero, $\mathcal{L}$ is singular In particular, any constant multiple of the n-vector, u, composed of ones satisfies the equation $\mathcal{L}\,\mathrm{u} = 0\mathrm{u}$, and so zero is an eigenvalue of $\mathcal{L}$ These results allow us to order the eigenvalues of $\mathcal{L}$ in nondecreasing order For $G \in \Theta(n,e)$ let $\lambda_i = \lambda_i(G)$, $i = 0, 1, \ldots, n-1$ denote the eigenvalues of $\mathcal{L}$ such that

$$0 = \lambda_0 \leq \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_{n-1}$$

Furthermore, let

$$\sigma(G) = [0\ \lambda_1\ \lambda_2\ \ldots\ \lambda_{n-1}]^{\mathrm{T}} \in \mathbf{R}^n$$

In other words, $\sigma(G)$ is the n-vector containing all the eigenvalues of G arranged in non-decreasing order

The next result continues our look at the components of a graph

Lemma 3.3.3 (Kel'mans[35]) *If $G \in \Theta(n,e)$ has $k \geq 1$ components $G_1, G_2, \ldots G_k$, then*

$$\sigma(G) = \bigcup_{i=1}^{k} \sigma(G_i)$$

Proof By Lemma 3.3.2, $\mathcal{P}(t,G) = \prod_{i=1}^{k} \mathcal{P}(t,G_i)$ The result follows □

The next result states how the eigenvalues of a graph are affected by the deletion of an arbitrary edge

Lemma 3.3.4 (Kel'mans and Chelnokov) *For $G \in \Omega(n,e)$ and any edge $u \in E(G)$, let $G-u$ denote the graph obtained from G by deleting the edge u from $E(G)$. Then*

$$\lambda_k(G) \geq \lambda_k(G-u)$$

for $k = 0, 1, \ldots, n-1$.

Proof (From Kel'mans and Chelnokov [34, Lemma 2.2, p. 204].) Let $M = \mathcal{L}(G) - \mathcal{L}(G-u)$. For example, if $u = \{v_1, v_2\}$ then without loss of generality

$$M = \left(\begin{array}{cc|c} 1 & -1 & \\ -1 & 1 & 0 \\ \hline & & \\ \multicolumn{2}{c|}{0} & 0 \\ & & \end{array} \right)$$

Since $\mathcal{P}(t, M) = t^{n-1}(t-2)$, the eigenvalues (roots) of this polynomial are nonnegative, and so M is positive semi-definite. Apply Weyl's theorem, a specialization of the Courant-Fischer Theorem (see Horn and Johnson [32, Theorem 4.3.1, p. 181]), to get

$$\lambda_k(G) = \lambda_k(\mathcal{L}(G-u) + M) \geq \lambda_k(\mathcal{L}(G-u))$$

for $k = 0, 1, \ldots, n-1$. □

This next result was stated, in 1974, by Kel'mans [34] without proof but with reference to his 1965 paper [35]. Since the work in [35] deals with a variant of the Laplacian, the result is difficult to find. In a 1971 technical report Anderson and Morley present the same result in the proof of their Theorem 1. This technical report was subsequently published in 1983 [1]. Another proof appears in Boesch and Suffel's unpublished report [11, Theorem 1.2, p. 5].

Lemma 3.3.5 (Kel'mans) *For the graph $G \in \Omega(n,e)$ and for $\overline{G} = K_n - G$ the following relation holds*

$$\lambda_i(G) = n - \lambda_{n-i}(\overline{G}) \qquad \textit{for } i = 1, \ldots, n-1.$$

In linear algebra the spectral radius of a matrix A is equal to the maximum of the eigenvalues taken in absolute value. Thus for the graph $G \in \Theta(n, e)$ the *spectral radius* is the nonnegative real number $\rho(G) = \lambda_{n-1}(G)$. For simple graphs, Lemma 3.3.5 implies that $\rho(G) \leq n$. It is also important to note that,

$$\mathcal{P}(t, G) > 0 \qquad \text{for } t > \rho(G).$$

This is clear by Equation 3.7 (p. 33) and we shall use this fact later. In an untranslated 1967 Russian paper [37], Kel'mans shows that

$$\rho(G) \leq \max_{\substack{x,y \in V(G), \\ x \neq y}} (d_x + d_y).$$

Again this result appears in Anderson and Morley [1, Theorem 2, p. 143]. A less precise, but for our purposes equally useful result, is easily obtained from the Geršgorin Theorem. We present a version that pertains specifically to Laplacian matrices.

Theorem 3.3.6 (Geršgorin) *Let $G \in \Theta(n, e)$, and let*

$$d_{\max} = \max_{v \in V(G)} d_v.$$

Then for $\lambda \in \sigma(G)$

$$0 \leq \lambda \leq 2\, d_{\max}.$$

Proof. See Horn and Johnson [32, Theorem 6.1.1, p.344] for a proof of Geršgorin's Theorem and then note that for graphs $\mathcal{L} = \Delta - \mathcal{A}$. □

A lower bound on the spectral radius of a graph is given next.

Lemma 3.3.7 (Kel'mans and Chelnokov) *Let $G \in \Theta(n, e)$ where $e \geq 1$. Then*

$$\rho(G) \geq d_{\max} + 1$$

Proof See Kel'mans and Chelnokov [34, Lemma 2.3, p. 205]. □

Using these results we obtain the bounds for the complement of an almost-regular graph $\overline{G}$ in Ω^2 (G is composed of path and/or cycle components). For these graphs $d_{\max}$ equals two so,

$$3 \leq \rho(G) \leq 4 \tag{3.10}$$

Later, in Chapter 4 Section 4.1, we give a precise description of the spectrum of these graphs. We use this information for a proof of Theorem 5.3.3.

3.3.3 Matrix Tree Theorem

The following counting theorem is attributed to Kirchhoff [48] who did work in electric theory in the mid 1800's. The presentation adopted here and the next subsection is a composite of the work of Biggs [7, pp. 22-39], Cvetković [23, pp. 37-39], and Kel'mans [34, 43].

Theorem 3.3.8 (Kirchhoff Matrix–Tree Theorem) *For graph $G \in \Theta(n, e)$, the classical adjoint of $\mathcal{L}(G)$, $\mathrm{adj}(\mathcal{L}(G))$, equals $Sp(G)\mathrm{J}$.*

An algebraic proof of this theorem can be found in Biggs [7, Theorem 6.3, pp. 34-35] and a graph theoretic proof can be found in Gibbons [30]. This theorem is implicitly contained in Kirchhoff's 1847 paper [48], while the first proof can be found in the 1940 paper by Brooks, Smith, Stone and Tutte [14]. Many other equivalent results exist. For example, Maxwell's Rule [52], published in 1892, gives the weighted tree products of a graph and, in 1948, Tutte [71] gave the number of spanning trees in directed graphs. See Moon [57, pp. 41-42] for a discussion of these results.

The next two results follow directly.

Corollary 3.3.9 *For any* $i \in \{1, 2, \ldots, n(G)\}$, $|\mathcal{L}_i(G)| = Sp(G)$.

Proof: Obvious from Theorem 3.3.8. □

Corollary 3.3.10 *The number of spanning trees of a graph* G *is invariant under any permutation of the labels of* $V(G)$.

Proof: Let G' be the graph G with its vertices relabelled. Let $\mathcal{L}' = \mathcal{L}(G')$ and $\mathcal{L} = \mathcal{L}(G)$. This permutation of the labels of $V(G)$ corresponds to a permutation P (a permutation matrix) of $\mathcal{L}$. In other words, $\mathcal{L}' = P\,\mathcal{L}\,P^{\mathrm{T}}$. Then,

$$\mathrm{adj}(\mathcal{L}') = \mathrm{adj}(P\,\mathcal{L}\,P^{\mathrm{T}}).$$

Since the adjugate of a product equals the product of the adjugates (see Lemma 3.4.1 (p. 45) we can expand this equation to

$$\mathrm{adj}(P^{\mathrm{T}})\;\mathrm{adj}(\mathcal{L})\;\mathrm{adj}(P).$$

Since $|P| = \pm 1$ and $\mathrm{adj}(P) = |P|\,P^{-1} = P^{\mathrm{T}}$ this becomes

$$P\;\mathrm{adj}(\mathcal{L})\;P^{\mathrm{T}}.$$

But by Theorem 3.3.8 $\mathrm{adj}(\mathcal{L})$ is a constant matrix and remains so under any permutation. Thus, the above equals

$$\mathrm{adj}(\mathcal{L}) = \mathrm{Sp}(G)\,\mathrm{J}. \quad \square$$

From Theorem 3.3.8 it is possible to derive other spanning tree counting formulas. Two such methods follow, but first we generalize this theorem. This generalization is stated in 1976 (as self evident) by Kel'mans [43, Eqn. 2.2, p. 243]. The proof that follows is adapted from Cvetković et al. [24, p. 38].

Let $G \in \Theta(n, e)$ and let $\beta \subseteq V(G) = \{1, 2, \ldots, n\}$. Then the graph G_β is the multigraph obtained from G by identifying (amalgamating) the vertices in β into a single vertex while maintaining edges (yet, deleting loops). We write G_v instead of $G_{\{v\}}$, and note that $G_v = G$ for any $v \in V(G)$. (We use this fact in Corollary 3.3.13.)

Recall from page 22 that for a matrix A and index set β that A_β is a principal submatrix of matrix A (the rows and columns of A corresponding to the indices in β are simultaneously deleted).

Corollary 3.3.11 *Let $G \in \Theta(n, e)$, where $V(G) = \{1, 2, \ldots, n\}$, and let β be a nonempty subset of $V(G)$. Then*

$$Sp(G_\beta) = |\mathcal{L}_\beta(G)|$$

Proof Let $\imath$ be the label of the node resulting from identifying the vertices in β. But $\mathcal{L}_\imath(G_\beta) = \mathcal{L}_\beta(G)$ and, by Corollary 3.3.9,

$$\mathrm{Sp}(G_\beta) = |\mathcal{L}_\imath(G_\beta)| = |\mathcal{L}_\beta(G)|$$

as required. □

To allow for the case $\beta = \emptyset$, let $\mathrm{Sp}(G_\emptyset) = 0$ which is sensible because $|\mathcal{L}(G_\emptyset)| = |\mathcal{L}(G)| = 0$.

For a matrix $A \in \mathbf{R}^{n \times n}$, let $E_k(A)$ denote the sum of all principal minors of order k of A. (The notation is from Horn and Johnson [32, p. 42].) In particular, for a graph $G \in \Theta(n, e)$

$$E_k = E_k(\mathcal{L}(G)) = \sum_{\substack{\beta \subseteq V(G) \\ |\beta| = n-k}} |\mathcal{L}_\beta(G)| \tag{3.11}$$

Note that

$$E_1 = \text{trace}(\mathcal{L}(G)) = \sum_{v \in V(G)} d_v = 2e,$$

and

$$E_n = |\mathcal{L}(G)| = 0.$$

Lemma 3.3.12 (Kel'mans [37]) *For graph $G \in \Theta(n, e)$, the coefficients of $\mathcal{P}(t, G)$ are given by*

$$c_i = \sum_{\substack{\beta \subseteq V(G) \\ |\beta| = n-i}} Sp(G_\beta)$$

for $i = 0, 1, \ldots, n-1$.

Proof It is possible to show (inductively by Laplace expansion) [32, Eqn 1.2.11, p. 42] that

$$\mathcal{P}(t, G) = t^n - E_1 t^{n-1} + E_2 t^{n-2} - \cdots \pm E_n$$

Thus, $c_i = E_i$. By Equation 3.11 and by Corollary 3.3.11, $|\mathcal{L}_\beta(G)| = \text{Sp}(G_\beta)$ so the result follows. □

Corollary 3.3.13 *For graph $G \in \Theta(n, e)$,*

$$Sp(G) = \frac{1}{n} c_{n-1}$$

Proof Use Lemma 3.3.12 and let $i = n - 1$ Then

$$\begin{aligned} c_{n-1} &= \sum_{\substack{\beta \subseteq V(G) \\ |\beta|=1}} \mathrm{Sp}(G_\beta) \\ &= \sum_{v \in V(G)} \mathrm{Sp}(G_v) \\ &= n\,\mathrm{Sp}(G) \quad \square \end{aligned}$$

Kel'mans and Chelnokov [34, eqn 2.14, p 203] give another expression for the coefficients of $\mathcal{P}(t, G)$ Recall the function ν is defined on page 27

Lemma 3.3.14 *For graph $G \in \Theta(n, e)$, the coefficients of $\mathcal{P}(t, G)$ are given by*

$$c_i(G) = \sum_{\substack{F \subseteq G \\ e(F)=i}} \nu(F), \qquad \text{for } i = 0, 1, \ldots, n-1$$

We now develop a formula for $\mathrm{Sp}(G)$ based on the eigenvalues of the Laplacian First, for the n numbers $a_0, a_1, \ldots, a_{n-1}$, the k^{th} *elementary symmetric function*, $k \leq n-1$, is given by

$$S_k(a_0, a_1, \ldots, a_{n-1}) = \sum_{\substack{|P|=k \\ P \subseteq \{0,1,\ldots,n-1\}}} \prod_{i \in P} a_i$$

Theorem 3.3.15 *If $a_0, \ldots, a_{n-1}$ are the eigenvalues of matrix A, then*

$$S_k(a_0, \ldots, a_{n-1}) = E_k(A)$$

for $k \leq n$

Proof See, for example, Horn and Johnson [32, Theorem 1 2 12, p 42] □

The following is from Kel'mans and Chelnokov [34, Equation 2 18, p 203]

Theorem 3 3 16 *For graph $G \in \Theta(n, e)$*

$$Sp(G) = \frac{1}{n} \prod_{j=1}^{n-1} \lambda_j(G)$$

Proof By the definition of the k^{th} elementary symmetric function and the fact that $\lambda_0 = 0$, we have

$$S_{n-1}(\sigma(G)) = \prod_{j=1}^{n-1} \lambda_j$$

By Theorem 3 3 15 this equals E_{n-1} which equals $c_{n-1}(G)$ Apply Corollary 3 3 13 □

Notice how this counting method means the problem of finding the Sp-optimal graph is a problem of maximizing the product of $n-1$ numbers subject to the constraint that the numbers are eigenvalues of a graph It is this observation upon which Cheng [18] based his results As well, Theorem 3 3 16 gives a simple proof of a well known result

Corollary 3 3 17 *The multiplicity of 0 as an eigenvalue of the graph G is equal to the number of components in G*

Proof Since a component G_i is connected, it has at least one spanning tree, and so its $n(G_i) - 1$ largest eigenvalues are nonzero The smallest eigenvalue of each component is zero so each component contributes exactly one zero to the spectrum of G □

3.4 Complement Spanning Tree Formula

We now return to the consideration of simple graphs From here to the end of the thesis, by graph we mean simple graph In 1974, Biggs [7, Prop 6 4, p 35] gave a formula (Equation 3 12 below) that uses the determinant of a matrix instead of a cofactor of the Laplacian (e g Theorem 3 3 8) Biggs gives Temperley credit for this formula since it is implicit in his 1964 paper [69] First we need a result from linear algebra that says the adjugate of a product is the product of the adjugates

Lemma 3 4 1 *For the matrices $A, B \in \mathbf{R}^{n\times n}$ and for $C = AB$ the following holds*

$$\mathrm{adj}(B)\mathrm{adj}(A) = \mathrm{adj}(C)$$

Proof. The Cauchy-Binet formula [32, p 22] states that for $1 \leq r \leq n$, $\alpha, \beta \subseteq \{1, 2, \ldots, n\}$ and $|\alpha| = |\beta| = r$, that

$$\det C_{\alpha,\beta} = \sum_{\gamma} |A_{\alpha,\gamma}|\ |B_{\gamma,\beta}|$$

where the sum is taken over all index sets $\gamma \subseteq \{1, 2, \ldots, n\}$ of cardinality r Take this formula with $r = 1$ and consider the (i, j) entry of $\mathrm{adj}(C)$

$$(\mathrm{adj}(C))_{ij} = (-1)^{i+j} \det C_{ji}$$

$$= (-1)^{i+j} \sum_{k=1}^{n} \det A_{j\,k} \det B_{k\,i}$$
$$= \sum_{k=1}^{n} (-1)^{i+k} \det A_{j\,k} (-1)^{k+j} \det B_{k\,i}$$
$$= \sum_{k=1}^{n} (\mathrm{adj}(A))_{k\,j} (\mathrm{adj}(B))_{i\,k}$$

The result follows by the definition of matrix multiplication □

The proof for the next theorem is taken directly from Biggs [7, Prop 6 4, p 35], but each step is explained more fully

Theorem 3 4 2 (Temperley [69]) *For $G \in \Omega(n, e)$*

$$Sp(G) = n^{-2}\ |\mathrm{J} + \mathcal{L}(G)| \tag{3 12}$$

Proof For K_n we have $\Delta = (n-1)\mathrm{I}$ and $\mathcal{A} = \mathrm{J} - \mathrm{I}$ so

$$\mathcal{L}(K_n) = \Delta - \mathcal{A} = (n-1)\mathrm{I} - (\mathrm{J} - \mathrm{I}) = n\mathrm{I} - \mathrm{J} \tag{3 13}$$

By Theorem 3 3 8, $\mathrm{adj}(\mathcal{L}(K_n)) = \mathrm{Sp}(K_n)\mathrm{J}$ and by Theorem 3 2 2

$$\mathrm{adj}(\mathcal{L}(K_n)) = n^{n-2}\,\mathrm{J} \tag{3 14}$$

Let $\mathcal{L} = \mathcal{L}(G)$ Note that $n\mathrm{J} = \mathrm{J}^2$ and $\mathrm{J}\,\mathcal{L} = 0$ (all the column sums of $\mathcal{L}$ are 0) This allows us to write

$$(n\mathrm{I} - \mathrm{J})(\mathrm{J} + \mathcal{L}) = n\mathrm{J} + n\mathcal{L} - \mathrm{J}^2 - \mathrm{J}\,\mathcal{L} = n\mathcal{L},$$

and by Lemma 3 4 1

$$\mathrm{adj}(\mathrm{J} + \mathcal{L})\mathrm{adj}(n\mathrm{I} - \mathrm{J}) = \mathrm{adj}(n\mathcal{L})$$

Apply Equations 3.13 and 3.14 on the left and on the right and notice that each cofactor of $\mathrm{adj}(n\mathcal{L})$ is n^{n-1} times the corresponding cofactor of $\mathcal{L}$:

$$\mathrm{adj}(\mathrm{J}+\mathcal{L})n^{n-2}\mathrm{J} = n^{n-1}\mathrm{adj}(\mathcal{L}).$$

Simplify and then use Theorem 3.3.8.

$$\mathrm{adj}(\mathrm{J}+\mathcal{L})\mathrm{J} = n\,\mathrm{Sp}(G)\mathrm{J}$$

Next pre-multiply each side by $(\mathrm{J}+\mathcal{L})$ and use Equation 2.1 (page 22).

$$\begin{aligned}(\mathrm{J}+\mathcal{L})\mathrm{adj}(\mathrm{J}+\mathcal{L})\mathrm{J} &= n\,\mathrm{Sp}(G)\,(\mathrm{J}+\mathcal{L})\mathrm{J}\\ |\mathrm{J}+\mathcal{L}|\,\mathrm{J} &= n\,\mathrm{Sp}(G)\,(\mathrm{J}^2+\mathcal{L}\mathrm{J})\\ |\mathrm{J}+\mathcal{L}|\,\mathrm{J} &= n^2\mathrm{Sp}(G)\mathrm{J}.\end{aligned}$$

It follows that $n^{-2}\,|\mathrm{J}+\mathcal{L}| = \mathrm{Sp}(G)$, as required. □

This theorem alleviates the need to take a cofactor of the Laplacian, but a more flexible formula is obtainable using the next theorem. Note for any graph $G \in \Omega\,(n,e)$ that $G = K_n - \overline{G}$ so

$$\mathcal{L}(G) + \mathcal{L}(\overline{G}) = \mathcal{L}(K_n) = n\mathrm{I} - \mathrm{J}.$$

Thus

$$\mathrm{J} + \mathcal{L}(\overline{G}) = n\mathrm{I} - \mathcal{L}(G).$$

Since Theorem 3.4.2 says $\mathrm{Sp}(\overline{G}) = n^{-2}\left|\mathrm{J}+\mathcal{L}(\overline{G})\right|$, we have proven the following.

Theorem 3.4.3 *For the graph $G \in \Omega\,(n,e)$,*

$$Sp(\overline{G}) = n^{-2}\,|n\mathrm{I} - \mathcal{L}(G)|.$$

This is equivalent to the following (from Kel'mans and Chelnokov [34, Eqn 2 18, p 203])

Corollary 3 4 4 *For the graph* $G \in \Omega(n, e)$,

$$Sp(\overline{G}) = n^{-2}\mathcal{P}(n, G)$$

Proof By definition of the characteristic polynomial, $\mathcal{P}(n, G)$ equals $|n\,\mathrm{I} - \mathcal{L}(G)|$ □

Note that, unlike Temperley's complement inclusion exclusion formula (Theorem 3 2 3), the above is for fixed n That is, the formula $\mathrm{Sp}(\overline{G}) = n^{-2}\mathcal{P}(n, G)$ is for graphs G and $\overline{G}$, both of order n We can remedy this via a couple of corollaries First we have another result for the components for a graph

Corollary 3 4 5 *If* $G \in \Omega(n, e)$ *has* $k \geq 1$ *components* $G_1, G_2, \ldots, G_k$ *of orders* $n_1, n_2, \ldots, n_k$*, respectively, then*

$$Sp(\overline{G}) = n^{-2} \prod_{i=1}^{k} |n\mathrm{I}_{n_i} - \mathcal{L}(G_i)| = n^{-2} \prod_{i=1}^{k} \mathcal{P}(n, G_i)$$

Proof Combine Lemma 3 3 2 and Corollary 3 4 4 □

Corollary 3 4 6 (Temperley's complement spanning tree formula) *Let* $G \in \Omega(k, e)$*, and let* $k \leq n$ *Then*

$$Sp(K_n - G) = n^{n-2}\, n^{-k}\mathcal{P}(n, G)$$

Proof Graph G is of order k and $\overline{G} = K_n - G$ But $\overline{G}$ can be expressed as $\overline{G} = K_n - G'$, where G' is composed of the graph G plus $n-k$ isolated vertices Apply Corollary 3.4.5 and observe that $\mathcal{P}(n, K_1) = n$ to get

$$\begin{aligned}
\mathrm{Sp}(K_n - G) &= n^{-2}\Big(\prod_{i=1}^{n-k} \mathcal{P}(n, K_1)\Big)\mathcal{P}(n, G) \\
&= n^{-2}\, n^{n-k}\, \mathcal{P}(n, G) \\
&= n^{n-2}\, n^{-k}\, \mathcal{P}(n, G). \; \square
\end{aligned}$$

Now Theorem 3.2.3 gives the number of spanning trees of $K_n - G$ in terms of the generic form of the graph G (p. 29). On the other hand this corollary expresses $\mathrm{Sp}(K_n - G)$ in terms of the characteristic polynomial. So it is immediately evident that

$$f(n, G) = n^{-k}\, \mathcal{P}(n, G). \tag{3.15}$$

Therefore, the comments and results that pertain to the generic form of a graph also apply to the characteristic polynomial of a graph.

This observation motivates us to define the following matrix, sometimes called the *Complement Spanning Tree Matrix*. For the simple graph $G \in \Omega(k, e)$, and $k \leq n$ define the matrix $\mathcal{Q}(n, G) \in \mathbf{Z}^{k \times k}$ as

$$\mathcal{Q}(n, G) = n\mathrm{I}_k - \mathcal{L}(G) \tag{3.16}$$

It is also possible to define $\mathcal{Q}(n, G)$ directly from the graph G. The (i, j) entry is given by

$$(\mathcal{Q}(n, G))_{ij} = \begin{cases} n - d_{v_i} & \text{if } i = j \\ 1 & \text{if } i \neq j \text{ and } \{v_i, v_j\} \in E(G) \\ 0 & \text{otherwise} \end{cases}$$

Corollary 3.4.7 *Let $G \in \Omega(k, e)$. Then*

$$Sp(K_n - G) = n^{n-2} n^{-k}\, |\mathcal{Q}(n, G)|.$$

Proof This follows directly from Corollary 3.4.6 and the definition of $\mathcal{Q}(n, G)$. □

Therefore, as with generic forms, we are motivated to study families of graphs where $\mathcal{Q}$ is simple enough to permit an easy evaluation of $|\mathcal{Q}(n, G)|$. In the next chapter we present the formulas for $|\mathcal{Q}(n, P_k)|$ and $|\mathcal{Q}(n, C_k)|$. In the mean time, as an example of the usefulness of these results, we give an alternate simple proof for a result first given by Weinberg [78].

Theorem 3.4.8 *Let* $G \in \Omega\,(2k, k)$ *be a matching of size* k *and let* $0 \leq 2k \leq n$. *Then*

$$Sp(K_n - G) = n^{n-2}\, n^{-k}\, (n-2)^k$$

Proof The graph G is composed of k components with one edge each. By a suitable labeling of the vertices, the matrix $\mathcal{Q}$(n,G) can be made block diagonal composed of k two-by-two blocks of the form

$$n\mathrm{I}_2 - \mathcal{L}(K_2) = \begin{bmatrix} n-1 & 1 \\ 1 & n-1 \end{bmatrix}$$

These have determinant

$$|n\mathrm{I}_2 - \mathcal{L}(K_2)| = (n-1)^2 - 1 = n(n-2).$$

Thus,

$$\begin{aligned} \mathrm{Sp}(\overline{G}) &= n^{n-2}\, n^{-2k}\, (n(n-2))^k \\ &= n^{n-2}\, n^{-k}\, (n-2)^k \quad \Box \end{aligned}$$

For example consider $G = P_2 + P_2$ (like we did for Temperley's complement inclusion exclusion formula). By this theorem

$$\mathrm{Sp}(\overline{G}) = n^{n-2}\, n^{-2}\, (n-2)^k = n^{n-2}\left(1 - \frac{4}{n} + \frac{4}{n^2}\right)$$

This is the same expression we obtained earlier.

3.5 Ranking Graphs by Their Number of Spanning Trees

We close this chapter with a discussion of a partial order $\succ$ over $\Omega(n,e)$ (simple graphs) established by Kel'mans [43, p. 254]. We write $G \succ H$ if $G, H \in \Omega(n,e)$ and $\mathcal{P}(t,G) > \mathcal{P}(t,H)$ for all $t \geq n$. Note that $n \geq \max\{\rho(G), \rho(H)\}$ by Lemma 3.3.5 so $\mathcal{P}(t,G) > 0$ and $\mathcal{P}(t,H) > 0$ for $t \geq n$. Also note that $t = n$ gives $\text{Sp}(\overline{G}) > \text{Sp}(\overline{H})$ by Lemma 3.4.4. So, saying $G \succ H$ implies that $K_{n+k} - G$ has more spanning trees than $K_{n+k} - H$, for all $k \geq 0$. There are two equivalent ways to define $\succ$.

Theorem 3.5.1 *$G \succ H$ if and only if $|\mathcal{Q}(t,G)| > |\mathcal{Q}(t,H)|$ for $t > n(G) = n(H)$.*

Proof: This follows since $\mathcal{P}(n,G) = |\mathcal{Q}(n,G)|$. □

Theorem 3.5.2 *$G \succ H$ if and only if $f(t,G) > f(t,H)$, for $t > n(G) = n(H)$.*

Proof: Equation 3.15 says that $f(n,G) = n^{-k}\mathcal{P}(n,G)$ so the result follows. □

For later, we present the next rather obvious theorem.

Theorem 3.5.3 *Given two graphs $G, H \in \Omega(n,e)$ such that $G \succ H$, then for any other simple graph F we have $G + F \succ H + F$.*

Proof This is obvious since

$$\mathcal{P}(t, G+F) = \mathcal{P}(t, G)\mathcal{P}(t, F) \text{ and } \mathcal{P}(t, H+F) = \mathcal{P}(t, H)\mathcal{P}(t, F) \quad \square$$

We point out that $\succ$ is not a total order Kel'mans and Chelnokov give a complicated example of a pair of $\succ$-incomparable graphs in [34, p 211] Later, in a 1980 research announcement, Kel'mans [45] states, without details, a number of other examples of $\succ$-incomparable graphs Here we present a simple example of $\succ$-incomparable graphs

(a) $G = 2 \cdot C_3 + 2 \cdot K_1$ (b) $H = K_{1,3} + P_4$

Figure 3 5 A crossing example

Let $G, H \in \Omega(8,6)$, where $G = (2 \cdot C_3 + 2 \cdot K_1)$ and $H = (K_{1,3} + P_4)$ (Figure 3 5(a) and (b) respectively) Then using Theorem 3 2 3 and Corollary 3 2 4 it is possible to derive the following formulas

$$\mathrm{Sp}(K_n - G) = n^{n-2}\left[1 - \frac{12}{n^1} + \frac{54}{n^2} - \frac{108}{n^3} + \frac{81}{n^4}\right] \tag{3 17}$$

and

$$\mathrm{Sp}(K_n - H) = n^{n-2}\left[1 - \frac{12}{n^1} + \frac{55}{n^2} - \frac{122}{n^3} + \frac{138}{n^4} - \frac{76}{n^5} + \frac{16}{n^6}\right] \tag{3 18}$$

Evaluating these functions for $n = 8$ we see that $K_8 - G$ has more spanning trees than $K_8 - H$ yet $K_9 - H$ has more than $K_9 - G$ for $n = 9$ See Table 3 1 The author found two other $\Omega(8,6)$ graphs that have polynomials that cross with respect to G An open question is whether there exist graphs that have polynomials that cross twice

Another interesting fact is the existence of non-isomorphic graphs that have the same characteristic polynomial and hence the same spectrum Such graphs are called

	$n = 8$	$n = 9$
$Sp(K_n - G)$	40,000	944,784
$Sp(K_n - H)$	39,984	947,520

Table 3.1 A crossing example.

cospectral. Since these graphs have the same spectrum, they have the same number of spanning trees (by Theorem 3.3.16), and so these graphs are also incomparable.

For example, the graphs G_1 and G_2 in Figure 1.1 (p. 11) are cospectral graphs. Using Maple to evaluate the characteristic polynomials of these graphs we get

$$\begin{aligned} \mathcal{P}(t, G_1) &= \mathcal{P}(t, G_2) \\ &= t^6 - 12t^5 + 54t^4 - 112t^3 + 105t^2 - 36t \\ &= t(t-4)(t-1)^2(t-3)^2. \end{aligned}$$

Thus $K_n - G_1$ and $K_n - G_2$ have the same number of spanning trees for all $n \geq 7 = n(G_1) = n(G_2)$.

As well, Cvetković et al. [24, Chapter 6] discuss examples of regular graphs that are cospectral with respect to their adjacency matrices. By Equation 3.9 (p. 34) such graphs are also cospectral with respect to their Laplacians.

The existence of incomparable graphs shows that a strict ranking of all simple graphs, by the number of spanning trees in their complement, is not possible. It also suggests that a counterexample to Conjecture 1.3.1 may exist: Sp-optimal graphs may not be unique.

Chapter 4

Special Formulas

The counting formulas given in Chapter 3 are general and difficult to use for ranking families of graphs. So, for various classes, many special formulas have been developed. Two excellent summaries of results of this type are Moon's 1970 monograph [57] and Berge [6]. Since this thesis is concerned with graphs whose complements are composed of paths and/or cycles, we collect and develop formulas for such graphs in this chapter.

For these graphs, closed formulas exist in three formats: trigonometric, combinatorial and algebraic. These are all given in this chapter. In addition, we present a new combinatorial formula for cycles and we give a new proof for the algebraic formulas. Furthermore, the trigonometric formulas give us information about the eigenvalues of these graphs. We also look at the relationship between the generic forms of paths and cycles.

4.1 Trigonometric Formulas

In 1961, Bedrosian [3] posed the problem of finding the generic form for what he called the r, p, m, and s series of graphs. The r series represents graphs that are matchings on r edges, and the p series correspond to *star* graphs. (Star graphs are graphs that have p edges incident to the same vertex.) This thesis is concerned with his m and s series which correspond to the graphs C_m and P_{s+1}, respectively. In 1958 Wienberg obtained formulas for matchings (see Theorem 3.4.8 above) as well for star graphs. In 1969 Bercovici [5] obtained a formula for C_m and based on this Bedrosian, in 1970 [4], obtained a formula for P_{s+1}. For the cycle Bercovici's formula is as follows.

Theorem 4.1.1 (Bercovici) *For the cycle C_k the generic form is given by*

$$f(n, C_k) = n^{1-k} \prod_{i=1}^{k-1} \left(n - 4 \sin^2 \left(\frac{i \pi}{k}\right)\right) \tag{4.1}$$

For example, the generic form for the triangle, C_3, is as follows:

$$\begin{aligned} f(n, C_3) &= n^{-2} \prod_{i=1}^{2} \left(n - 4 \sin^2 \left(\frac{i \pi}{3}\right)\right) \\ &= n^{-2} \left(n - 4 \sin^2 \left(\frac{\pi}{3}\right)\right)^2 \\ &= n^{-2} \left(n^2 - 6n + 9\right) \end{aligned}$$

Formula 4.1 has been rediscovered a number of times, in various forms, during the course of finding a general formula for graphs whose Laplacian matrices are cycle matrices (c.f. [12, 76]). Bedrosian [4] pointed out that

$$(1 - \frac{4}{n}) f^2(n, P_k) = f(n, C_{2k}). \tag{4.2}$$

We give a new proof of this at the end of this chapter (Lemma 4.3.7). As well we present a new case for cycles of odd length (Lemma 4.3.8). (Moon [57, p. 54] misquotes Equation 4.2.) From Equation 4.2 Bedrosian obtained the following.

Theorem 4.1.2 (Bedrosian) *For the path P_k the generic form is given by*

$$f(n, P_k) = n^{1-k} \prod_{i=1}^{k-1} \left(n - 4 \sin^2\left(\frac{i\,\pi}{2\,k}\right)\right) \tag{4.3}$$

For example consider $G = P_2 + P_2$ (like we did for Temperley's complement inclusion exclusion formula). By this theorem

$$\begin{aligned} \mathrm{Sp}(K_n - G) &= n^{n-2} \left(n^{-1} \prod_{i=1}^{1} \left(n - 4 \sin^2\left(\frac{i\,\pi}{4}\right)\right)\right)^2 \\ &= n^{n-2} \left(1 - \frac{4}{n} \sin^2\left(\frac{\pi}{4}\right)\right)^2 \\ &= n^{n-2} \left(1 - \frac{4}{n} \left(\frac{\sqrt{2}}{2}\right)^2\right)^2 \\ &= n^{n-2} \left(1 - \frac{4}{n} + \frac{4}{n^2}\right) \end{aligned}$$

This is the same expression we got earlier.

Becovici and Bedrosian both expressed their results in terms of generic forms but it is clear from Equation 3.15 (p. 49) that they really gave results for $\mathcal{P}(n, P_k)$ and $\mathcal{P}(n, C_k)$. Furthermore the expressions they derived immediately give the eigenvalues of P_k and C_k, respectively.

Lemma 4.1.3 *The eigenvalues of $\mathcal{L}(P_k)$ are*

$$\lambda_i(P_k) = 4 \sin^2\left(\frac{i\,\pi}{2\,k}\right) \tag{4.4}$$

for $i = 0, 1, 2, \ldots, k-1$.

Observe that

$$0 < \frac{1}{2\,k} < \frac{1}{k} < \cdots < \frac{k-1}{2\,k} < \frac{1}{2} \tag{4.5}$$

so

$$0 < \sin\left(\frac{i\,\pi}{2\,k}\right) < 1 \tag{4.6}$$

for $i = 1, 2, \ldots, k-1$. Thus, the eigenvalues of P_k are arranged in increasing order. Furthermore, it is easy to derive bounds on the spectral radius of P_k. We need these bounds for a proof of Theorem 5.3.3.

Lemma 4.1.4 *The spectral radius, $\rho(P_k)$, of P_k has the following bounds, for $k \geq 4$.*

$$3 < \rho(P_k) < 4 \tag{4.7}$$

for $k \leq 3$, $\rho(P_3) = 3$, $\rho(P_2) = 2$, and $\rho(P_1) = 0$.

Proof. The spectral radius of P_k is given by $\rho(P_k) = 4\sin^2\left(\frac{(k-1)\pi}{2k}\right)$. The upper bound is immediate from Equation 4.6. The bounds for $k = 1, 2, 3$ are found by direct calculation. For example, when k equals three then

$$\sin\left(\frac{\pi}{3}\right) = \frac{\sqrt{3}}{2}.$$

Square this and multiply by four to get the result. For $k > 3$, observe that $(k-1)/k$ monotonicly increases. Therefore

$$\frac{\sqrt{3}}{2} < \sin\left(\frac{(k-1)\pi}{2k}\right).$$

Square both sides and multiply by four to get the result. □

Since taking the eigenvalues for C_k directly from Equation 4.1 does not give us a nondecreasing sequence, we express them as follows.

Lemma 4.1.5 *The eigenvalues of $\mathcal{L}(C_k)$ are*

$$\lambda_i = 4\sin^2\left(\left\lceil\frac{i}{2}\right\rceil\frac{\pi}{k}\right) \qquad \text{for } i = 1, 2, \ldots, k-1 \tag{4.8}$$

and $\lambda_0 = 0$.

Observe that $\lambda_1 = \lambda_2$, $\lambda_3 = \lambda_4$, etc , and if k is odd that $\lambda_{k-2} = \lambda_{k-1} < 4$ otherwise $\lambda_{k-3} = \lambda_{k-2}$ and $\lambda_{k-1} = 4$ It is interesting to note that when k is odd (e g $k = 2j+1$), then $\rho(C_k) = \rho(P_k)$

$$\rho(C_k) = 4\sin^2\left(\left\lceil\frac{(2j+1)-1}{2}\right\rceil\frac{\pi}{k}\right) = 4\sin^2\left(\frac{2j}{2}\frac{\pi}{k}\right) = 4\sin^2\left(\frac{(k-1)\pi}{2k}\right) = \rho(P_k)$$

With the above information we can give a refinement of Lemma 3 3 4 for P_k less an edge In particular, we can get strict inequality

Lemma 4 1 6 *For the path P_k and any edge $u \in E(P_k)$ then*

$$\lambda_i(P_k - u) < \lambda_i(P_k)$$

for $i = 1, \ldots, k-1$

Proof Consider that $P_k - u = P_{k-j} + P_j$ for some $j \in \{1, 2, \ldots, k-1\}$, and $\sigma(P_k - u) = \sigma(P_{k-j}) \cup \sigma(P_j)$ (see Lemma 3 3 3) Without loss of generality suppose $j \geq k - j$ To prove the lemma by induction requires a double induction on j and then i Instead let us look at the two extreme eigenvalues and leave the rest as an exercise For $i = 1$ we have $\lambda_1(P_k) > 0 = \lambda_1(P_k - u)$, and for $i = k-1$ we have

$$\rho(P_{k-j} + P_j) = 4\sin^2\left(\frac{(j-1)\pi}{2j}\right) < 4\sin^2\left(\frac{(k-1)\pi}{2k}\right) = \rho(P_k)$$

since $j \geq k - j$ and

$$0 < \left(\frac{(j-1)\pi}{2j}\right) < \left(\frac{(k-1)\pi}{2k}\right) < \left(\frac{\pi}{2}\right) \quad \square$$

On the other hand, for C_k less an edge we can not improve on Lemma 3 3 4 Note that $C_k - u = P_k$ So for any $i \in \{1, 2, \ldots, k-1\}$ we have

$$\lambda_i(P_k) = 4\sin^2\left(\frac{i}{2}\frac{\pi}{k}\right) \leq 4\sin^2\left(\left\lceil\frac{i}{2}\right\rceil\frac{\pi}{k}\right) = \lambda_i(C_k)$$

with equality only when i is even

4.2 Combinatorial Formulas

We now present the combinatorial formulas (i e the generic forms) of path and cycle components Both are due to Moon but we present a new simpler formula for the cycle

Theorem 4 2 1 (Moon) *For the path P_k, where $k \leq n$, the generic form is*

$$f(n, P_k) = \sum_{i=1}^{k} \binom{k+i-1}{k-i} \left(\frac{-1}{n}\right)^{k-i} \quad (4\ 9)$$

Proof See Moon [55, Theorem 6 5, p 56] □

For example consider $G = P_2 + P_2$ (like we did for Temperley's complement inclusion exclusion formula) By this theorem

$$\begin{aligned} \mathrm{Sp}(K_n - G) &= n^{n-2} f^2(n, P_k) \\ &= n^{n-2} \left(\sum_{i=1}^{2} \binom{2+i-1}{2-i} \left(\frac{-1}{n}\right)^{2-i} \right)^2 \\ &= n^{n-2} \left(1 - \frac{2}{n}\right)^2 \\ &= n^{n-2} \left(1 - \frac{4}{n} + \frac{4}{n^2}\right) \end{aligned}$$

Now, consider a simple example that ranks two graphs whose complements are composed of path components Let $G = P_3 + P_3$ and $H = P_2 + P_4$ (Figures 4 1(a)

(a) $G = P_3 + P_3$ (b) $H = P_2 + P_4$

Figure 4.1: Two graphs composed of path components.

and (b), respectively). For these graphs we use Theorem 4.2.1 and Lemma 3.4.5 to get

$$\begin{aligned} f^2(n, P_3) &= \left(\sum_{i=1}^{3} \binom{3+i-1}{3-i} \left(\frac{-1}{n} \right)^{3-i} \right)^2 \\ &= \left(1 - \frac{4}{n} + \frac{3}{n^2} \right)^2 \\ &= \left(1 - \frac{8}{n} + \frac{22}{n^2} - \frac{24}{n^3} + \frac{9}{n^4} \right) \end{aligned} \tag{4.10}$$

and

$$\begin{aligned} f(n, P_2)\, f(n, P_4) &= \left(\sum_{i=1}^{2} \binom{2+i-1}{2-i} \left(\frac{-1}{n} \right)^{2-i} \right) \left(\sum_{i=1}^{4} \binom{4+i-1}{4-i} \left(\frac{-1}{n} \right)^{4-i} \right) \\ &= \left(1 - \frac{2}{n} \right) \left(1 - \frac{6}{n} + \frac{10}{n^2} - \frac{4}{n^3} \right) \\ &= \left(1 - \frac{8}{n} + \frac{22}{n^2} - \frac{24}{n^3} + \frac{8}{n^4} \right) \end{aligned} \tag{4.11}$$

Clearly (4.10) is larger than (4.11) by $1/n^4$, for all $n > 0$. Thus $G \succ H$. Notice that the path lengths in G are more equal than those in H. In Chapter 5 we see this holds in general for graphs composed of path components.

The following formula for the generic form of a cycle appeared in Moon [57, Theorem 6.6, p. 56].

Theorem 4.2.2 (Moon) *For the cycle C_k, where $k \leq n$, the generic form is*

$$f(n, C_k) = \sum_{i=0}^{k-2} \sum_{j=1}^{i+1} j^2 \binom{2k-2-i-j}{i+1-j} \left(\frac{-1}{n} \right)^i + k^2 \left(\frac{-1}{n} \right)^{k-1} \tag{4.12}$$

For example, consider Equation 4 12 for C_3

$$\begin{aligned} f(n, C_3) &= \sum_{i=0}^{1} \sum_{j=1}^{i+1} j^2 \binom{4-i-j}{i+1-j} \left(\frac{-1}{n}\right)^i + \left(\frac{3}{n}\right)^2 \\ &= \sum_{j=1}^{1} j^2 \binom{4-j}{1-j} + \sum_{j=1}^{2} j^2 \binom{3-j}{2-j} \left(\frac{-1}{n}\right) + \left(\frac{3}{n}\right)^2 \\ &= 1 + \binom{2}{1}\left(\frac{-1}{n}\right) + 4\binom{1}{0}\left(\frac{-1}{n}\right) + \frac{9}{n^2} \\ &= 1 - \frac{6}{n} + \frac{9}{n^2} \end{aligned}$$

We now present a simpler formula suggested by Myrvold [61]

Theorem 4 2 3 *For the cycle C_k, where $k \le n$, the generic form is*

$$f(n, C_k) = \sum_{i=1}^{k} \binom{k+i-1}{k-i} \left(\frac{-1}{n}\right)^{k-i} \left(\frac{k}{i}\right) \tag{4 13}$$

Proof By Theorem 3 2 3

$$f(n, C_k) = \sum_{\substack{F \subseteq C_k \\ V(F)=V(C_k)}} \nu(F)(-n)^{-e(F)} \tag{4 14}$$

This formula sums over each spanning subgraph F of the cycle C_k Since $\nu(F)$ equals zero if F is a cycle, we consider instead $C_k - u = P_k$ for any $u \in E(C_k)$, and use

$$\sum_{\substack{F' \subseteq P_k \\ V(F')=V(P_k)}} \nu(F')(-n)^{-e(F')}$$

k times – once for each edge u But, this over-counts since each $k - i$ edge spanning subgraph F' is counted i times once for each edge missing from F' Thus Equation

4 14 equals

$$k \sum_{\substack{F \subseteq P_k \\ V(F)=V(P_k)}} \nu(F)(-n)^{-e(F)} \binom{1}{i}$$

Substitute Equation 4 9 to complete the proof □

To illustrate the over-counting argument consider C_3, and let $E(C_3) = \{1, 2, 3\}$ There are three ways to form P_3 and for each we use

$$\sum_{\substack{F \subseteq P_3 \\ V(F)=V(P_3)}} \nu(F)(-n)^{-e(F)}$$

For example, suppose u is chosen from $E(C_3)$ and the two remaining edges are x and y Then the four spanning subgraphs of P_3 are

$$\begin{aligned} F_1 &= 3 \cdot K_1 & E(F_1) &= \emptyset \\ F_2 &= K_1 + P_2 & E(F_2) &= \{x\} \\ F_3 &= K_1 + P_2 & E(F_3) &= \{y\} \\ F_4 &= P_3 & E(F_4) &= \{x, y\} \end{aligned}$$

For any $u \in E(C_3)$ the graph F_4 is unique and so it appears once – there is one edge missing At the other extreme, the graph F_1 appears once for each u and so $\nu(F_1)$ is counted three times – once for each of the three edges To see that the graph F_2 appears twice suppose $E(F_2) = \{1\}$ and consider $u = 1, 2, 3$ in turn

- When $u = 1$ then $E(P_3) = \{2, 3\}$, and F_2 can not be a subgraph
- When $u = 2$ then $E(P_3) = \{1, 3\}$, and F_2 can be a subgraph
- And finally, when $u = 3$ then $E(P_3) = \{1, 2\}$, and F_2 can be a subgraph

Similarly the graph F_3 appears two times – once for each edge missing.

Now to illustrate the theorem we calculate the generic form of C_3.

$$\begin{aligned} f(n, C_3) &= \sum_{i=1}^{3} \binom{3+i-1}{3-i} \left(\frac{-1}{n}\right)^{3-i} \binom{3}{i} \\ &= \binom{5}{0} \left(\frac{-1}{n}\right)^{0} \binom{3}{3} + \binom{4}{1} \left(\frac{-1}{n}\right)^{1} \binom{3}{2} + \binom{3}{2} \left(\frac{-1}{n}\right)^{2} \binom{3}{1} \\ &= 1 - \frac{6}{n} + \frac{9}{n^2} \end{aligned}$$

as expected.

Corollary 4.2.4 (to Theorem 4.2.1) *The number of spanning trees in $K_n - P_k$ is*

$$Sp(K_n - P_k) = n^{n-2} \sum_{i=1}^{k} \binom{k+i-1}{k-i} \left(\frac{-1}{n}\right)^{k-i}$$

Corollary 4.2.5 (to Theorem 4.2.3) *The number of spanning trees in $K_n - C_k$ is*

$$Sp(K_n - C_k) = n^{n-2} \sum_{i=1}^{k} \binom{k+i-1}{k-i} \left(\frac{-1}{n}\right)^{k-i} \binom{k}{i}$$

4.3 Algebraic Formulas

Each of the following algebraic formulas first appeared, implicitly, in Kel'mans' article [35]. Like many other results by Kel'mans, these formulas were overlooked in later works The reason is partly due to the delay in getting a translation of the Russian and partly to Kel'mans' presentation The formulas he presented are based on a matrix derived from the Laplacian matrix So, one needs to do some manipulations to get the formulas useful for counting spanning trees

Boesch and Suffel derive these formulas in an unpublished 1984 technical report [11] Later the formula for C_k appeared in a 1993 class assignment by Dimakopoulos [25] Based on this work, the author was able to obtain the path formula We present our derivation methods later and the results now because the derivations are lengthy

Theorem 4 3 1 *The number of spanning trees in $G = K_n - P_k$, for $k \leq n$, is given by*

$$
\begin{aligned}
&Sp(K_n - P_k) \\
&= \frac{n^{n-1-k}}{2^k\sqrt{n^2-4n}}\left((n-2+\sqrt{n^2-4n})^k - (n-2-\sqrt{n^2-4n})^k\right) \quad \text{if } n > 4 \\
&= 4^{3-k}k \quad \text{if } n = 4
\end{aligned}
$$

Proof. Apply Lemma 4 3 5 to Corollary 3 4 6 □

The restriction $n \geq 4$ is not a serious limitation because $\mathrm{Sp}(K_n - P_k)$ is trivial for $k \leq n \leq 4$

Theorem 4 3 2 *The number of spanning trees in $G = K_n - C_k$ is given by*

$$
\begin{aligned}
&Sp(K_n - C_k) \\
&= n^{n-2-k}\left(2^{-k}\left((n-2+\sqrt{n^2-4n})^k + (n-2-\sqrt{n^2-4n})^k\right) + 2(-1)^{k+1}\right)
\end{aligned}
$$

where $n \geq 4$ and $3 \leq k \leq n$

Proof Apply Lemma 4 3 6 to Corollary 3 4 6 □

Again the requirement $n \geq 4$ is not a problem since $C_3 \cong K_3$ is the smallest cycle and $K_3 - K_3$ is boring The first interesting case is $K_4 - K_3$

For notational convenience we define the following functions of n

$$\begin{aligned} r &\equiv r(n) = n - 2 \\ s &\equiv s(n) = \sqrt{n^2 - 4\,n} \\ p &\equiv p(n) = r + s \\ q &\equiv q(n) = r - s \end{aligned} \qquad (4\ 15)$$

With these abbreviations Theorem 4 3 1 can be written as

$$\mathrm{Sp}(K_n - P_k) = n^{n-2-k} \left(\frac{n}{2^k\, s}\right) \left(p^k - q^k\right)$$

and Theorem 4 3 2 can be written as

$$\mathrm{Sp}(K_n - C_k) = n^{n-2-k} \left(2^{-k} \left(p^k + q^k\right) + 2\,(-1)^{k+1}\right)$$

To derive these formulas we start by finding the determinant of a tri-diagonal matrix that is common to the Laplacians of both C_k and P_k

4.3.1 Determinants of Some Matrices

To derive the formulas in Theorems 4 3 1 and 4 3 2, we want to determine $|\mathcal{Q}(n, P_k)|$ and $|\mathcal{Q}(n, C_k)|$ Recall, $\mathcal{Q}(n, G) = n\,\mathrm{I}_k - \mathcal{L}(G)$, is the complement spanning tree matrix for $G \in \Omega\,(k, e)$ To find the determinants of these matrices, we initially use a Laplacian expansion and to make our work easier we judiciously choose the vertex labeling (Corollary 3 3 10)

Let $C_k = v_1, v_2, \ldots, v_k$. So,

$$\begin{aligned}
\mathcal{Q}(n, C_k) &= n\mathrm{I}_k - \mathcal{L}(C_k) \\
&= n\mathrm{I}_k - (\Delta(C_k) - \mathcal{A}(C_k)) \\
&= n\mathrm{I}_k - (2\mathrm{I}_k - \mathcal{A}(C_k)) \\
&= (n-2)\mathrm{I}_k + \mathcal{A}(C_k)) \\
&= \begin{pmatrix}
n-2 & 1 & & & & 1 \\
1 & n-2 & 1 & & & \\
 & 1 & n-2 & 1 & & \\
 & & \ddots & \ddots & \ddots & \\
 & & & 1 & n-2 & 1 \\
1 & & & & 1 & n-2
\end{pmatrix} \\
&= \begin{pmatrix}
r & 1 & & & & 1 \\
1 & r & 1 & & & \\
 & 1 & r & 1 & & \\
 & & \ddots & \ddots & \ddots & \\
 & & & 1 & r & 1 \\
1 & & & & 1 & r
\end{pmatrix}
\end{aligned}$$

where an empty space denotes a value of 0.

On the other hand, P_k has two degree one vertices and $(k-2)$ degree two vertices. Let $P_k = v_1, v_k, v_{k-1}, \ldots, v_3, v_2$ (see Figure 4.2).

Figure 4.2: Chosen labeling for a path.

$$
\begin{aligned}
\mathcal{Q}(n, P_k) &= \begin{pmatrix}
n-1 & & & & & & 1 \\
& n-1 & 1 & & & & \\
& 1 & n-2 & 1 & & & \\
& & \ddots & \ddots & \ddots & & \\
& & & 1 & n-2 & 1 & \\
& & & & 1 & n-2 & 1 \\
1 & & & & & 1 & n-2
\end{pmatrix} \\
&= \begin{pmatrix}
r+1 & & & & & & 1 \\
& r+1 & 1 & & & & \\
& 1 & r & 1 & & & \\
& & \ddots & \ddots & \ddots & & \\
& & & 1 & r & 1 & \\
& & & & 1 & r & 1 \\
1 & & & & & 1 & r
\end{pmatrix}
\end{aligned}
$$

We start by focusing on the common tri-diagonal submatrix. Let $\mathcal{T}_k = [t_{i,j}] \in \mathbf{Z}^{k \times k}$ where

$$
t_{ij} = \begin{cases} r & \text{if } i = j \\ 1 & \text{if } i+1 = j \text{ or } j+1 = i \\ 0 & \text{otherwise} \end{cases}
$$

Thus,

$$
\mathcal{Q}(n, P_k) = \left(\begin{array}{cc|ccc}
r+1 & & & & 1 \\
& r+1 & 1 & & \\
\hline
& 1 & & & \\
& & & \mathcal{T}_{k-2} & \\
1 & & & &
\end{array}\right) \tag{4.16}
$$

and

$$\mathcal{Q}(n, C_k) = \left(\begin{array}{c|ccc} r & 1 & & 1 \\ \hline 1 & & & \\ & & \mathcal{T}_{k-1} & \\ 1 & & & \end{array} \right) \tag{4 17}$$

Now we find the determinant of $\mathcal{T}_k$

Lemma 4 3 3 *Let $\tau_k = |\mathcal{T}_k|$, where $\mathcal{T}_k$ is the matrix defined above, and let $n \geq 4$ Then,*

$$\tau_k = r\,\tau_{k-1} - \tau_{k-2} \tag{4 18}$$

$$= \begin{cases} \left(\frac{1}{s2^{k+1}}\right)\left(p^{k+1} - q^{k+1}\right) & \text{if} \quad n > 4 \\ k+1 & \text{if} \quad n = 4 \end{cases} \tag{4 19}$$

with initial conditions $\tau_1 = r$ and $\tau_0 = 1$

(Equation 4 18 appears in the proof of Kel'mans [43, Lemma 6 9, p 258])

Proof By convention, the determinant of an empty matrix is one so $\tau_0 = 1$ And since $\mathcal{T}_1 = [r]$ we have $\tau_1 = r$ Now for $k > 1$, expand τ_k about the first first row to produce two $(k-1) \times (k-1)$ determinants, and expand the second of these about the first row For example

$$\tau_k = \begin{vmatrix} r & 1 & & & \\ 1 & r & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & r & 1 \\ & & & 1 & r \end{vmatrix}$$

$$= r\,\tau_{k-1} - \begin{vmatrix} 1 & & & & & \\ 1 & r & 1 & & & \\ & & \ddots & \ddots & \ddots & \\ & & & 1 & r & 1 \\ & & & & 1 & r \end{vmatrix}$$

$$= r\,\tau_{k-1} - \tau_{k-2}$$

This relation is called a second order linear homogeneous recurrence relation We solve this equation using standard techniques (see, for example, [15, 31] for a discussion on solving recurrence relations) The roots of the characteristic equation of $\tau_k = \tau_{k-1} - \tau_{k-2}$ are

$$\frac{r \pm \sqrt{r^2-4}}{2} = \frac{r \pm \sqrt{(n-2)^2-4}}{2} = \frac{r \pm \sqrt{n^2-4n}}{2} = \frac{r \pm s}{2} \qquad (4\ 20)$$

which we temporarily denote by b^+ and b^-, respectively So

$$\tau_k = c_1(b^+)^k + c_2(b^-)^k$$

where the constants c_1 and c_2 are to be determined Use the initial conditions to get the following system of equations

$$\begin{aligned} \tau_0 &= 1 = c_1 + c_2 \\ \tau_1 &= r = c_1(b^+) + c_2(b^-) \end{aligned}$$

Solving, we find that

$$c_1 = \frac{b^- - r}{b^- - b^+} \qquad \text{and} \qquad c_2 = \frac{r - b^+}{b^- - b^+} \qquad (4\ 21)$$

We can make the following simplifications For the denominator

$$b^- - b^+ = \frac{r-s}{2} - \frac{r+s}{2} = -s$$

And for the numerators

$$b^- - r = \frac{r-s}{2} - r = \frac{-(r+s)}{2} = -b^+,$$

and

$$r - b^+ = \frac{2r-(r+s)}{2} = \frac{r-s}{2} = b^-$$

Collecting these results we get

$$\begin{aligned}\tau_k &= \left(\frac{-b^+}{-s}\right)\left(b^+\right)^k + \left(\frac{b^-}{-s}\right)\left(b^-\right)^k \\ &= \frac{1}{s}\left((b^+)^{k+1} - (b^-)^{k+1}\right) \\ &= \frac{1}{s\,2^{k+1}}\left((r+s)^{k+1} - (r-s)^{k+1}\right) \qquad (4\,22)\end{aligned}$$

establishing the lemma if $n \neq 4$ But, if $n = 4$ then we have division by zero Instead, make use of the binomial theorem and cancellation, and write Equation 4 22 as

$$\begin{aligned}\tau_k &= \frac{1}{s\,2^{k+1}}\left(2\sum_{\substack{j=1\\ j\ \text{odd}}}^{k+1}\binom{k+1}{j} r^{k+1-j}\, s^j\right) \\ &= \frac{1}{2^k}\left(\sum_{\substack{j=1\\ j\ \text{odd}}}^{k+1}\binom{k+1}{j}(n-2)^{k+1-j}\left(\sqrt{n^2-4n}\right)^{j-1}\right) \qquad (4\,23)\end{aligned}$$

This form shows that the square root terms are always raised to an even power More importantly, if $n = 4$ (hence $s = 0$) then there is a formula for τ_k that does not have a zero divisor Put $n = 4$ into Equation 4 23 and note that the only nonzero term occurs when $j = 1$ We get

$$\begin{aligned}&\frac{1}{2^k}\binom{k+1}{1}(4-2)^k \\ =\ & k+1\end{aligned}$$

This completes the proof □

To get the formula for $|\mathcal{Q}(n, P_k)|$, we need the following intermediate result

Lemma 4.3.4 *Let $\mathcal{T}_k'$ denote the matrix derived from $\mathcal{T}_k = [t_{ij}]$, where $t_{11} = r+1$ instead of r. Then*

$$|\mathcal{T}_k'| = \tau_k + \tau_{k-1}$$

Proof Note that,

$$|\mathcal{T}_k'| = \begin{vmatrix} r+1 & 1 & & & \\ 1 & r & 1 & & \\ & & \ddots & \ddots & \\ & & 1 & r & 1 \\ & & & 1 & r \end{vmatrix}$$

Expand about the first row and expand the second determinant in this expansion about the first column. This gives

$$\begin{aligned} |\mathcal{T}_k'| &= (r+1)\,\tau_{k-1} - \tau_{k-2} \\ &= r\,\tau_{k-1} - \tau_{k-2} + \tau_{k-1} \\ &= \tau_k + \tau_{k-1} \end{aligned}$$

by Equation (4.18). □

4.3.2 Determinants of $\mathcal{Q}(n, P_k)$ and $\mathcal{Q}(n, C_k)$

It is now possible to prove Theorem 4.3.1, for P_k, using Lemmas 4.3.3 and 4.3.4 in the evaluation of the determinant of the matrix $\mathcal{Q}(n, P_k)$.

Lemma 4.3.5 *For a path P_k, where $k \leq n$ and $n \geq 4$,*

$$\begin{aligned} |\mathcal{Q}(n, P_k)| &= \frac{n}{s2^k}\left(p^k - q^k\right) & \text{if } n > 4 \\ &= 4\,k & \text{if } n = 4 \end{aligned}$$

Proof Note that

$$\mathcal{Q}(n, P_k) = \begin{pmatrix} r+1 & & & & & 1 \\ & r+1 & 1 & & & \\ & 1 & r & 1 & & \\ & & & \ddots & \ddots & \ddots \\ & & & 1 & r & 1 \\ 1 & & & & 1 & r \end{pmatrix}$$

contains $\mathcal{T}_{k-1}'$ as a submatrix. Expand $|\mathcal{Q}(n, P_k)|$ about the first row and then expand the second determinant of this expansion about its first column. Then use Lemma 4.3.4, collect terms and rearrange to take advantage of the recurrence relation $\tau_k = r\,\tau_{k-1} - \tau_{k-2}$.

$$\begin{aligned} |\mathcal{Q}(n, P_k)| &= (r+1)\,|\mathcal{T}_{k-1}'| + (-1)^{k+1}\,(-1)^{(k-1)+1}\,|\mathcal{T}_{k-2}'| \\ &= (r+1)\,(\tau_{k-1} + \tau_{k-2}) + (-1)^{2k+1}\,(\tau_{k-2} + \tau_{k-3}) \\ &= r\tau_{k-1} + r\tau_{k-2} + \tau_{k-1} - \tau_{k-3} \\ &= r\,\tau_{k-1} + \tau_{k-1} + (r\,\tau_{k-2} - \tau_{k-3}) \\ &= r\,\tau_{k-1} + \tau_{k-1} + \tau_{k-1} \\ &= (r+2)\tau_{k-1} \\ &= n\tau_{k-1} \qquad \text{since } r = n-2 \end{aligned}$$

The rest follows from Lemma 4.3.3. □

It is also possible to prove Theorem 4.3.2 for C_k using Lemma 4.3.3.

Lemma 4.3.6 *For cycle C_k, where $3 \le k \le n$ and $n \ge 4$,*

$$|\mathcal{Q}(n, C_k)| = \frac{1}{2^k}\left(p^k + q^k\right) + 2(-1)^{k+1}$$

Proof Recall,

$$\mathcal{Q}(n, C_k) = \begin{pmatrix} r & 1 & & & & 1 \\ 1 & r & 1 & & & \\ & 1 & r & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & 1 & r & 1 \\ 1 & & & & 1 & r \end{pmatrix}$$

Note that $\mathcal{Q}(n, C_k)$ contains $\mathcal{T}_{k-1}$ as a submatrix.

$$|\mathcal{Q}(n, C_k)| = \left| \begin{array}{c|ccc} r & 1 & & 1 \\ \hline 1 & & & \\ & & \mathcal{T}_{k-1} & \\ 1 & & & \end{array} \right|$$

Expand this about the first row

$$= r\,\tau_{k-1} - \left| \begin{array}{c|ccc} 1 & 1 & & \\ \hline & & \mathcal{T}_{k-2} & \\ 1 & & & \end{array} \right| + (-1)^{k+1} \left| \begin{array}{c|ccc} 1 & & & \\ & & \mathcal{T}_{k-2} & \\ \hline 1 & & & 1 \end{array} \right|$$

and expand the two unresolved determinants about their first columns

$$= r\,\tau_{k-1} - \left\{ \tau_{k-2} + (-1)^k \left| \begin{array}{ccccc} 1 & & & & \\ r & 1 & & & \\ 1 & r & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & r & 1 \end{array} \right| \right\} +$$

$$(-1)^{k+1}\left\{(-1)^k\tau_{k-2}+\begin{vmatrix}1 & r & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & r & 1\\ & & & 1 & r\\ & & & & 1\end{vmatrix}\right\}$$

and notice that the remaining determinants are lower and upper diagonal respectively, with ones along the diagonal. So we get

$$\begin{aligned}|\mathcal{Q}(n,C_k)| &= r\,\tau_{k-1}-(\tau_{k-2}+(-1)^k)+(-\tau_{k-2}+(-1)^{k+1})\\ &= r\,\tau_{k-1}-2\,\tau_{k-2}+2\,(-1)^{k+1}\end{aligned}$$

We can substitute into this expression the result for τ_k from Lemma 4.3.3 and simplify.

$$\begin{aligned}|\mathcal{Q}(n,C_k)| &= r\left(\frac{p^k-q^k}{s2^k}\right)-2\left(\frac{p^{k-1}-q^{k-1}}{s2^{k-1}}\right)+2(-1)^{k+1}\\ &= \frac{r}{s\,2^k}\left(p^k-q^k\right)-\frac{4}{s\,2^k}\left(p^{k-1}-q^{k-1}\right)+2(-1)^{k+1}\\ &= \frac{1}{s\,2^k}\left(r\left(p^k-q^k\right)-4\left(p^{k-1}-q^{k-1}\right)\right)+2(-1)^{k+1}\end{aligned}$$

Notice that $pq=(r+s)\,(r-s)=(n-2)^2-(n^2-4\,n)=4$ so we get

$$\begin{aligned}|\mathcal{Q}(n,C_k)| &= \frac{1}{s\,2^k}\left(r(p^k-q^k)-(p^kq-pq^k)\right)+2(-1)^{k+1}\\ &= \frac{1}{s\,2^k}\left(p^k\,(r-q)-q^k\,(r-p)\right)+2(-1)^{k+1}\end{aligned}$$

Now $r-q=r-(r-s)=s$ and $r-p=-s$ so we have

$$\begin{aligned}|\mathcal{Q}(n,C_k)| &= \frac{1}{s\,2^k}\left(sp^k+sq^k\right)+2(-1)^{k+1}\\ &= \frac{1}{2^k}\left(p^k+q^k\right)+2(-1)^{k+1}\end{aligned}$$

(Note that there is no division by s so we do not need a special formula for $n = 4$)

□

4.3.3 Generic Forms of Cycles and Paths

We now present a new proof of Bedrosian's result [4] relating the generic forms of an even length cycle and a path

Lemma 4.3.7 *For $k > 1$,*

$$f(n, C_{2k}) = \left(1 - \frac{4}{n}\right) f^2(n, P_k) \tag{4.24}$$

Proof: By Equation 3.15 (p 49) $f(n,G) = n^{-k} |\mathcal{Q}(n,G)|$ for any graph $G \in \Omega(k,e)$ Thus we can use Lemmas 4.3.5 and 4.3.6 to establish the above result The special case $n = 4$ is easily confirmed directly, so we assume $n > 4$ By Lemma 4.3.6,

$$\begin{aligned} f(n, C_{2k}) &= n^{-2k} |\mathcal{Q}(n, C_{2k})| \\ &= n^{-2k} 2^{-2k} (p^{2k} + q^{2k}) + 2(-1)^{2k+1-2k} \\ &= n^{-2k} 4^{-k} (p^{2k} + q^{2k} - 2 \cdot 4^k) \end{aligned} \tag{4.25}$$

By Lemma 4.3.5,

$$\begin{aligned} f^2(n, P_k) &= n^{-2k} |\mathcal{Q}(n, P_k)|^2 \\ &= n^{-2k} 2^{-2k} \frac{n^2}{s^2} \left(p^k - q^k\right)^2 \\ &= n^{-2k} 4^{-k} \left(\frac{n^2}{n^2 - 4n}\right) \left(p^{2k} + q^{2k} - 2p^k q^k\right) \\ &= n^{-2k} 4^{-k} \left(\frac{1}{1 - \frac{4}{n}}\right) \left(p^{2k} + q^{2k} - 2 \cdot 4^k\right) \end{aligned} \tag{4.26}$$

Clearly $\left(1-\frac{4}{n}\right)$ times Equation 4 26 equals Equation 4 25 □

We now present a new formula relating the generic forms of an odd length cycle and that of two paths

Lemma 4 3 8 *Let $m = 2k+1$, where $k > 0$ Then*

$$f(n, C_m) = \left(1-\frac{4}{n}\right) f(n, P_k) f(n, P_{k+1}) \; + \; n^{1-m} \tag{4 27}$$

Proof By Equation 3 15 and Lemma 4 3 6,

$$\begin{aligned} f(n, C_m) &= n^{-m}2^{-m}\left(p^m + q^m\right) + 2(-1)^{m+1} \\ &= n^{-m}2^{-m}\left(p^m + q^m + 2^{m+1}\right) \end{aligned} \tag{4 28}$$

By Equation 3 15 and Lemma 4 3 5,

$$\begin{aligned} &\left(1-\frac{4}{n}\right) f(n, P_k) f(n, P_{k+1}) \\ &= \left(1-\frac{4}{n}\right) n^{-m}2^{-m}\left(\frac{1}{1-\frac{4}{n}}\right)\left(p^k - q^k\right)\left(p^{k+1} - q^{k+1}\right) \\ &= n^{-m}2^{-m}\left(p^m + q^m - 2^{2k}(p+q)\right) \end{aligned} \tag{4 29}$$

Since $p = (n-2+\sqrt{n^2-4n})$ and $q = (n-2-\sqrt{n^2-4n})$ we have $p+q = 2(n-2)$ So Equation 4 29 becomes

$$n^{-m}2^{-m}\left(p^m + q^m + 2^{m+1} - 2^m n\right) \tag{4 30}$$

Rearranging we see this equation contains the generic form for the odd cycle plus a remainder In particular Equation 4 30 equals

$$\begin{aligned} &f(n, C_m) - n^{-m}2^{-m}2^m n \\ &= f(n, C_m) - n^{-m+1} \end{aligned} \tag{4 31}$$

as required □

Chapter 5

Main Results

In this chapter we find the Sp-optimal almost-regular graphs in $\Omega^2 (= \Omega\left(n, \binom{n}{2} - m\right)$, where $\left\lfloor \frac{n}{2} \right\rfloor < m \leq n)$ Also, when possible, we give a ranking of graphs in this class Both the algebraic and combinatorial formulas, from the previous chapter, will play a role in this work We also work with an elegant technique developed by Kel'mans and Chelnokov

Special mention is due to Myrvold [62] who suggested improvements to the proofs of Theorems 5 1 5, 5 2 1 and 5 3 3 These improvements allowed the author to derive Theorem 5 3 4 As well Myrvold provided Theorems 5 2 2, and 5 2 3

5.1 Ranking Path Components

The next two lemmas introduce new formulas which will be useful For the rest of this chapter let $x = p/2$, and let $s_k = (-1)^{k+1}$

Lemma 5.1.1 *For a path P_k, $k > 0$, and for $n > 4$,*

$$|\mathcal{Q}(n, P_k)| = x^{-k} \left(\frac{n}{s}\right) (x^{2k} - 1)$$

Proof From Lemma 4.3.5,

$$\begin{aligned} x^k \, |\mathcal{Q}(n, P_k)| &= \left(\frac{p}{2}\right)^k \left(\frac{n}{s}\right) \left(\left(\frac{p}{2}\right)^k - \left(\frac{q}{2}\right)^k\right) \\ &= \left(\frac{n}{s}\right) \left(\left(\frac{p}{2}\right)^{2k} - \left(\frac{p\,q}{2 \cdot 2}\right)^k\right) \\ &= \left(\frac{n}{s}\right) (x^{2k} - 1) \end{aligned}$$

since $p\,q = 4$. □

Lemma 5.1.2 *For a cycle C_k, $n \geq k \geq 3$, where $n \geq 4$,*

$$|\mathcal{Q}(n, C_k)| = x^{-k}(x^k + s_k)^2$$

Proof From Lemma 4.3.6,

$$\begin{aligned} x^k \, |\mathcal{Q}(n, C_k)| &= \left(\frac{p}{2}\right)^k \left(\left(\frac{p}{2}\right)^k + \left(\frac{q}{2}\right)^k + 2s_k\right) \\ &= \left(\frac{p}{2}\right)^{2k} + 1 + 2s_k \left(\frac{p}{2}\right)^k \\ &= (x^k + s_k)^2 \; \square \end{aligned}$$

For the rest of this chapter let $A(k) = (x^{2k} - 1)$ and let $B(k) = (x^k + s_k)^2$. Thus $|\mathcal{Q}(n, P_k)| = x^{-k} \left(\frac{n}{s}\right) A(k)$ and $|\mathcal{Q}(n, C_k)| = x^{-k} B(k)$.

Lemma 5 1 3 *Let $\mathcal{P}$ denote a graph composed of path components and $\mathcal{C}$ denote a graph composed of cycle components Let $G = \mathcal{P} + \mathcal{C}$, $k = n(G)$, and α equal the number of degree one vertices in G Then*

$$Sp(K_n - G) = n^{n-2-k} x^{-k} \left(\frac{n}{s}\right)^{\alpha} \left(\prod_{\substack{F \in \mathcal{P} \\ i = n(F)}} A(i) \right) \left(\prod_{\substack{F \in \mathcal{C} \\ i = n(F)}} B(i) \right) \qquad (5\ 1)$$

Proof This lemma follows directly from Corollary 3 4 5 and Lemmas 5 1 1 and 5 1 2 □

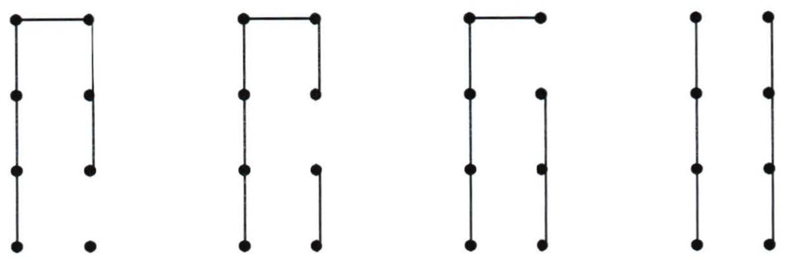
Observe that all graphs composed of path and cycle components, with n vertices and e edges, have the same number of degree one vertices (Consider that $2e = \sum_{i \in V(G)} d_i$ and that d_i equals one or two) So, when we rank the complement of two such graphs we can ignore all but the product terms in Equation 5 1 In particular we have the following

Lemma 5 1 4 *Let $G_1 = \mathcal{P}_1 + \mathcal{C}_1$ and $G_2 = \mathcal{P}_2 + \mathcal{C}_2$ Then $G_1 \succ G_2$ if and only if*

$$\left(\prod_{\substack{F \in \mathcal{P}_1 \\ i = n(F)}} A(i) \right) \left(\prod_{\substack{F \in \mathcal{C}_1 \\ i = n(F)}} B(i) \right) > \left(\prod_{\substack{F \in \mathcal{P}_2 \\ i = n(F)}} A(i) \right) \left(\prod_{\substack{F \in \mathcal{C}_2 \\ i = n(F)}} B(i) \right)$$

Our next theorem is due to Kel'mans [43] In 1976, he gave a proof of this theorem plus many other results A problem with this paper and his 1974 paper with Chelnokov [34] is the density of material and the new notation[1] This leads us to present our own (and quite different) proof of the theorem

[1] In a recent conversation, Kel'mans said foreign publication rights were restricted under the Soviet regime This lead to the necessity to put as much material as possible into his papers



$G(3) = P_7 + K_1$ (a) $G(2) = P_6 + P_2$ (b) $G(1) = P_5 + P_3$ (c) $G(0) = P_4 + P_4$ (d)

Figure 5.1. Comparison of paths on six edges.

Theorem 5.1.5 (Kel'mans) *Let $m \geq 4$, and let*

$$G(c) = P_{\lceil \frac{m}{2} \rceil + c} + P_{\lfloor \frac{m}{2} \rfloor - c}$$

where $0 \leq c < \left\lfloor \frac{m}{2} \right\rfloor$. Then

$$G(c) \succ G(c+1).$$

Actually Kel'mans theorem does not cover the case $c = 0$ although he does have another theorem that covers this case.

To demonstrate this theorem, suppose $m = 6$ and let $c = 0$. Then the theorem says that $P_3 + P_3 \succ P_2 + P_4$, as we already know from page 60. For another example, consider the graphs in Figure 5.1 where $m = 8$ and the graphs $G(c)$ are drawn for $c = 3, 2, 1, 0$ such that $G(3) \prec G(2) \prec G(1) \prec G(0)$.

Proof: For $m = 4$ the theorem is easily verified directly. Let $m \geq 5$. For a fixed c let $k = \left\lceil \frac{m}{2} \right\rceil + c$. From Lemma 5.1.4 it suffices to show that $A(k)A(m-k) > A(k+1)A(m-k-1)$. We have

$$\begin{aligned} A(k)A(m-k) &= (x^{2k}-1)(x^{2(m-k)}-1) \\ &= x^{2m} - x^{2(m-k)} - x^{2k} + 1 \qquad (5.2) \end{aligned}$$

And

$$\begin{aligned} A(k+1)A(m-k-1) &= (x^{2(k+1)}-1)(x^{2(m-k-1)}-1) \\ &= x^{2m} - x^{2(m-k-1)} - x^{2(k+1)} + 1 \end{aligned} \tag{5.3}$$

Subtract Equation 5.3 from Equation 5.2 to get

$$x^{2(m-k-1)} - x^{2(m-k)} + x^{2(k+1)} - x^{2k} \tag{5.4}$$

$$= x^{2k}\left(x^{2m-4k-2} - x^{2m-4k} + x^2 - 1\right)$$

$$= x^{2k}\left((1-x^2)(x^{2m-4k-2}-1)\right) \tag{5.5}$$

Now $x = p/2 > 2$ since $p > 5$ so $1 - x^2$ is negative. Also,

$$2m - 4k - 2 = 2m - 4\left\lceil \frac{m}{2} \right\rceil - 4c - 2$$

is negative for any $c \geq 0$ and so, $(x^{2m-4k-2} - 1)$ is negative. The product of two negatives is positive so Equation 5.5 is positive. Hence the theorem is proven. □

Thus, if we are given a graph whose complement contains path components then we can increase the number of spanning trees by dividing the paths into as many paths as possible (using any isolated vertices) and then evening out their lengths. As an aside, note that we have a result that extends beyond the class of graphs that are almost-regular.

5.2 Ranking Cycle Components

We now proceed to consider the graphs in Ω^2 whose complements are composed entirely of cycles. The next theorem is new and allows us to extend the work done by

Kel'mans [43], Kel'mans and Chelnokov [34], and Petingi [64] Petingi has a version of the following where k is fixed at three

Theorem 5 2 1 *Let* $m \geq 6$ *and* $3 \leq k \leq m-k$ *then*

$$C_k + C_{m-k} \succ C_m \qquad \text{if } k \text{ is odd}$$

and

$$C_k + C_{m-k} \prec C_m \qquad \text{if } k \text{ is even}$$

Proof Note that $n(C_m) = n(C_k + C_{m-k}) \geq 6$ so we can safely use the formula derived in Lemma 5 1 2 (p 78) From Lemma 5 1 4 it suffices to compare $B(k)B(m-k)$ and $B(m)$ For k odd we will show that $\sqrt{B(k)B(m-k)} - \sqrt{B(m)}$ is positive, and for k even we will show that $\sqrt{B(k)B(m-k)} - \sqrt{B(m)}$ is negative First,

$$B(k)B(m-k) = (x^k + s_k)^2(x^{m-k} + s_{m-k})^2 \tag{5 6}$$

so,

$$\sqrt{B(k)B(m-k)} - \sqrt{B(m)} \tag{5 7}$$
$$= (x^k + s_k)(x^{m-k} + s_{m-k}) - (x^m + s_m)$$
$$= s_k x^{m-k} + s_{m-k} x^k + s_k s_{m-k} - s_m \tag{5 8}$$

Now, $s_k s_{m-k} = (-1)^{k+1}(-1)^{m-k+1} = (-1)(-1)^{m+1} = -s_m$ so Equation 5 6 can be written as

$$s_k x^{m-k} + s_{m-k} x^k - 2s_m$$
$$= x^k(s_k x^{m-2k} + s_{m-k}) - 2s_m \tag{5 9}$$

The sign of Equation 5.9 equals the sign of s_k since $2k \leq m$ and $x > 2$. For example if $2k = m$ then $s_{m-k} = (-1)^{2k-k+1} = s_k$ and Equation 5.9 becomes

$$x^k(s_k x^0 + s_k) + 2 = 2(s_k x^k + 1)$$

So if k is odd, then s_k is positive and Equation 5.9 is positive. Therefore, Equation 5.7 is positive and $C_k + C_{m-k} \succ C_m$. On the other hand, when k is even Equations 5.6 and 5.7 are negative so $C_k + C_{m-k} \prec C_m$. □

The above theorem compares one large cycle with two smaller ones. The next two theorems compare pairs of cycles. The first theorem compares two pairs of cycles in which the lengths have the same parity. The second theorem handles the case in which the parities differ.

Theorem 5.2.2 *Let $m \geq 6$ and $3 \leq k \leq m - k$. Then*

$$C_k + C_{m-k} \succ C_{k+2} + C_{m-k-2} \qquad \text{if } k \text{ is odd}$$

and

$$C_k + C_{m-k} \prec C_{k+2} + C_{m-k-2} \qquad \text{if } k \text{ is even.}$$

Theorem 5.2.3 *Let $m \geq 6$ and $3 \leq k \leq m - k$. Then*

$$C_k + C_{m-k} \succ C_{k+1} + C_{m-k-1} \qquad \text{if } k \text{ is odd}$$

and

$$C_k + C_{m-k} \prec C_{k+1} + C_{m-k-1} \qquad \text{if } k \text{ is even.}$$

To prove these theorems we first prove the following theorem.

Theorem 5.2.4 *Let $m \geq 6$ and $3 \leq a, b \leq m-k$ and let*

$$D(k) = s_k x^{m-k} + s_{m-k} x^k, \tag{5.10}$$

where $x = p/2$ and $s_i = (-1)^{i+1}$ as above. Then

$$C_a + C_{m-a} \succ C_b + C_{m-b}$$

if and only if

$$D(a) > D(b).$$

Proof. By Lemma 5.1.4 $C_a + C_{m-a} \succ C_b + C_{m-b}$ holds if

$$B(a)B(m-a) > B(b)B(m-b) \tag{5.11}$$

or if

$$\sqrt{B(a)B(m-a)} > \sqrt{B(b)B(m-b)}. \tag{5.12}$$

For an arbritrary c

$$\begin{aligned} \sqrt{B(c)B(m-c)} &= (x^c + s_c)(x^{m-c} + s_{m-c}) \\ &= x^m + s_c x^{m-c} + s_{m-c} x^c - s_m \end{aligned} \tag{5.13}$$

So, Equation 5.12 can be written as

$$s_a x^{m-a} + s_{m-a} x^a > s_b x^{m-b} + s_{m-b} x^b \tag{5.14}$$

which is the same as saying $D(a) > D(b)$. □

Proof. (Theorem 5.2.2) We must show that $D(k) - D(k+2)$ is positive when k is odd and negative when k is even. Algebraic manipulation gives the following

$$\begin{aligned} D(k) - D(k+2) &= s_k x^{m-k} + s_{m-k} x^k - s_{k+2} x^{m-k-2} - s_{m-k-2} x^{k+2} \\ &= s_k x^{m-k} + s_{m-k} x^k - s_k x^{m-k-2} - s_{m-k} x^{k+2} \\ &= x^k (s_k x^{m-2k} + s_{m-k} - s_k x^{m-2k-2} - s_{m-k} x^2) \\ &= x^k (s_{m-k} - s_k x^{m-2k-2})(1 - x^2). \end{aligned} \tag{5.15}$$

Note that $x > 2$, so $1 - x^2$ is negative Therefore Equation 5 15 is positive when k is odd and negative when k is even □

We use a similar proof technique for Theorem 5 2 3

Proof (Theorem 5 2 3) We must show that $D(k) - D(k+1)$ is positive when k is odd and negative when k is even Algebraic manipulation gives the following

$$\begin{aligned} D(k) - D(k+1) &= s_k x^{m-k} + s_{m-k} x^k - s_{k+1} x^{m-k-1} - s_{m-k-1} x^{k+1} \\ &= s_k x^{m-k} + s_{m-k} x^k + s_k x^{m-k-1} + s_{m-k} x^{k+1} \\ &= x^k (s_k x^{m-2k} + s_{m-k} + s_k x^{m-2k-1} + s_{m-k} x) \\ &= x^k (s_{m-k} + s_k x^{m-2k-1})(1+x) \qquad (5\ 16) \end{aligned}$$

Clearly, this equation is positive when k is odd and negative when k is even □

Let Ω^2_{2reg} denote the sub-class of Ω^2 that have 2-regular complements (i e composed of cycle components only) With Theorems 5 2 1, 5 2 2, and 5 2 3 we can rank most, but not all, of the Ω^2_{2reg} graphs To illustrate what these theorems can and cannot do, we present some ranking results for all graphs in Ω^2_{2reg} for up to 13 deleted edges

Table 5 1 shows the ranking of graphs in Ω^2_{2reg} for $m = 6, 7, \ldots, 13$, where m is the number of edges deleted Each graph is listed by the cycle components in its respective complement For example, the entry 3, 3, 3, for $m = 9$, represents the graph $\overline{C_3 + C_3 + C_3}$ The graphs whose complement, for a given m, has the most spanning trees is at the top of the column, while the graph with the least spanning trees is at the bottom This data was compiled using Maple and Theorem 4 2 3 (see Appendix B)

Theorems 5 2 1, 5 2 2, and 5 2 3 can be used to rank all but two cases in Table 5 1 We will point out the two exceptions below but first we consider the graphs for $m = 10$

number of edges	6	7	8	9	10	11	12	13
component lists	3,3	3,4	3,5	3,3,3	3,3,4	3,3,5	3,3,3,3	3,3,3,4
	6	7	8	3,6	3,7	3,8	3,3,6	3,3,7
			4,4	9	5,5	3,4,4	3,9	3,5,5
				4,5	10	5,6	3,4,5	3,10
					4,6	11	5,7	3,4,6
						4,7	12	5,8
							6,6	13
							4,8	6,7
							4,4,4	4,9
								4,4,5

Table 5 1 Ranking of some graphs whose complement is 2-regular

Theorem 5 2 1 gives us

$$C_3 + C_3 + C_4 \succ C_3 + C_7,$$

$$C_5 + C_5 \succ C_{10},$$

and

$$C_{10} \succ C_4 + C_6$$

Theorem 5 2 2 gives us

$$C_3 + C_7 \succ C_5 + C_5$$

This covers all of the graphs in this category On the other hand the theorem does not deal with $C_3 + C_4 + C_4$ versus $C_5 + C_6$, for $m = 11$, and $C_3 + C_4 + C_6$ versus $C_5 + C_8$, for $m = 13$ These were found directly (See Appendix B) Generally, as m increases, more of these cases appear Nevertheless, the data in Table 5 1 and other experiments with Theorem 4 2 3 suggests the following conjecture for ranking all graphs in Ω^2_{2reg}

Conjecture 5 2 5 *Let $G, H \in \Omega(n, m)$, where $\left\lfloor \frac{n}{2} \right\rfloor < m \leq n$ and let $G = C_{a_1} + C_{a_2} + \cdots + C_{a_k}$, $H = C_{b_1} + C_{b_2} + \cdots + C_{b_j}$, such that $G \ncong H$ Let $A = (a_1, a_2, \ldots, a_k)$ and*

$B = (b_1, b_2, \ldots, b_j)$ *denote the lists of components for* G *and* H *respectively, where the elements are arranged in lexical order. Suppose* $a_1 = b_1, a_2 = b_2, \ldots, a_{i-1} = b_{i-1}$ *for* $0 \leq i < \min(j, k)$. *Suppose, without loss of generality, that* $a_i < b_i$ *then*

$$G \succ H = \begin{cases} \text{if} & \begin{array}{l} a_i \text{ is odd and } b_i \text{ is even, or} \\ a_i \text{ and } b_i \text{ are both odd} \end{array} \end{cases} \tag{5.17}$$

$$H \succ G = \begin{cases} \text{if} & \begin{array}{l} b_i \text{ is odd and } a_i \text{ is even, or} \\ a_i \text{ and } b_i \text{ are both even} \end{array} \end{cases} \tag{5.18}$$

Even without a proof of this conjecture it is possible to find the Sp-optimal graph in Ω^2_{2reg}.

Lemma 5.2.6 *Let* $G \in \Omega^2_{2reg}$. *To increase the number of spanning trees in* G, *apply the following spanning-tree-increasing operations on* $\overline{G}$.

Step 1. Repeatedly break any cycle, C_k, with $k \geq 6$ into a C_3 and a C_{k-3}. (When done this leaves a number of C_3's, C_4's, and C_5's.)

Step 2. Repeat the next two steps until there is at most one C_4 and at most one C_5.

Step 2.a. Transform each pair of C_4's into a C_3 and a C_5. (This leaves one C_5 for every pair of C_4's, at most one C_4, and more C_3's.)

Step 2.b. Transform each pair of C_5's into two C_3's and a C_4. (This leaves one C_4 for every pair of C_5's, at most one C_5, and more C_3's.)

Step 3. If there is a C_4 C_5 pair then replace it by three C_3's.

Proof Step 1 follows directly from Theorem 5.2.1

For the two C_4's in Step 2.a apply Theorem 5.2.1 with $k = 4$ and $m = 8$ to get a C_8. Then transform the C_8 into $C_3 + C_5$. Alternatively we can use Theorem 5.2.3 to directly transform $C_4 + C_4$ to $C_3 + C_5$.

Theorem 5.2.2 transforms the two C_5's in Step 2.b to $C_3 + C_7$. Then use Theorem 5.2.1 to get $C_3 + C_3 + C_4$.

For the C_4, C_5 pair in Step 3 apply Theorem 5.2.1 with $k = 4$ and $m = 9$ to get a C_9. Repeat twice to get the three C_3's as required. □

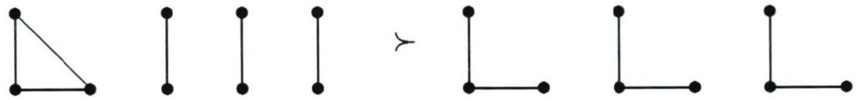
Notice that these spanning tree increasing operations produce as many C_3's as possible and at most one C_4 or one C_5. More importantly we have found the graph with the most spanning trees in Ω^2_{2reg}.

5.3 Ranking Mixed Path and Cycle Components

To find the Sp-optimal almost-regular graph in the class Ω^2 we have observed that only graphs whose complements are composed of cycles and paths need to be considered. In this section we finish off the work of the two previous sections by considering a mixture of cycle and path components.

Given an almost regular graph in Ω^2, one can perform the operations described above to break all paths into as many paths with lengths as even as possible and to break all cycles into as many triangles as possible. In this section we will work with a mixture of cycle and path components. In particular we show the following:

(a) $C_3 + P_3 + P_2 \succ P_4 + P_4$



(b) $C_3 + 3 \cdot P_2 \succ 3 \cdot P_3$

(c) $C_3 + P_2 + P_2 \succ P_3 + P_4$

Figure 5.2. Special cases.

(a) $C_3 + P_{k-3} \succ P_k$, for $k \geq 5$.

(b) $C_3 + P_k \succ C_{3+c} + P_{k-3}$, for $k - c > 0$ and $c > 0$.

(c) $C_3 + P_3 + P_2 \succ P_4 + P_4$ (Figure 5.2 (a)).

(d) $C_3 + 3 \cdot P_2 \succ 3 \cdot P_3$ (Figure 5.2 (b)).

(e) $C_3 + P_2 + P_2 \succ P_3 + P_4$ (Figure 5.2 (c)).

We present two proofs for Item (a) in the Subsection 5.3.2 and we prove Item (b) in Subsection 5.3.3. Then we deal with Items (c), (d), and (e) in Subsection 5.3.4. Finally, in Subsection 5.3.5, we show how these results give the Sp-optimal almost-regular graphs in Ω^2.

Our first objective is to show $C_3 + P_{k-3} \succ P_k$, for $k \geq 5$. Kel'mans states, without proof [43, p. 260], that this is a spanning tree increasing operation. He probably had a proof but didn't publish it due to restrictions imposed by the Soviet regime We present two proofs The first proof is the one Kel'mans most likely derived since it uses a technique he developed with Chelnokov [34] The second proof uses the techniques developed above

5.3.1 Technique of Kel'mans and Chelnokov

The purpose in presenting the Kel'mans and Chelnokov technique is twofold First the papers [34] and [43] present this technique in a very brief manner and we hope to provide a more detailed derivation that may help future researchers Secondly we wish to show how this technique is useful in the current context Besides these reasons the technique is interesting because it uses integration

The following polynomial was introduced in Kel'mans and Chelnokov [34] For $G \in \Theta(n, e)$, let

$$\Phi(t, G) = t^{e-n}\mathcal{P}(t, G) \tag{5.19}$$

Thus,

$$\begin{aligned} \Phi(t, G) &= t^{e-n}\sum_{i=0}^{n-1}(-1)^i c_i(G)t^{n-i} \\ &= \sum_{i=0}^{n-1}(-1)^i c_i(G)t^{e-i} \end{aligned} \tag{5.20}$$

Note that this polynomial can be used to rank graphs in the same manner as the characteristic polynomial

Lemma 5.3.1 *$G \succ H$ $(G, H \in \Omega(n, e))$ if and only if $\Phi(t, G) > \Phi(t, H)$ for $t \geq n$*

Proof This is clear from the definition of Φ and $\succ$ □

We need this polynomial because it changes the exponent of t in the characteristic polynomial and this is necessary to get the next lemma The following lemma, due to Kel'mans and Chelnokov, is an elegant tool for ranking some classes of graphs They used this tool to prove that K_n minus a matching is Sp-optimal in Ω^1 We are going to use this tool to show $C_3 + P_{k-3} \succ P_k$

Lemma 5.3.2 (Kel'mans and Chelnokov) *Let $G \in \Omega(n,e)$, and let $G-u$ denote the graph obtained from G by deleting the edge $u \in E(G)$ Then*

$$\Phi(t,G) = \Phi(a,G) + \sum_{u \in E(G)} \int_a^t \Phi(x, G-u)dx \tag{5.21}$$

Proof (This is the same proof as in [34, Lemma 2 4, p 205]) with more explanation provided) By Lemma 3 3 14 (p 43)

$$c_i(G) = \sum_{\substack{F \subseteq G \\ e(F)=i}} \nu(F), \qquad \text{for } i = 0, 1, \ldots, n-1 \tag{5.22}$$

So,

$$c_i(G-u) = \sum_{\substack{F \subseteq G-u \\ e(F)=i}} \nu(F), \qquad \text{for } i = 0, 1, \ldots, n-1 \tag{5.23}$$

Equation 5 23 sums over every i edge subgraph F of G that does not contain the edge u We first show that

$$\sum_{u \in E(G)} c_i(G-u) = (e-i)c_i(G) \qquad \text{for } i = 0, 1, \ldots, n-1 \tag{5.24}$$

Suppose $E(G) = \{1, 2, \ldots, e\}$ We argue by example but we skip the trivial cases of $i = 0$ or $i = 1$ Suppose $i = 2$ and look at $c_2(G)$ By Equation 5 22 this sums over every two edge subgraph of G Pick one of these, say F', where w.o.l.g. $E(F') = \{1,2\}$. Notice that $\nu(F')$ does not appear in the left hand side of Equation 5.24 when $u = 1$ or $u = 2$ but it does when $u = 3, 4, \ldots, e$. Thus, $\nu(F')$ is counted $e - 2$ times. Similarly for all other two edge subgraphs of G. A similar argument holds for any $i = 0, 1, \ldots, n-1$. That is for any i edge subgraph F', $\nu(F')$ is counted $e - i$ times in the left hand side of Equation 5.24. End of proof of claim.

We next prove that

$$\sum_{u \in E(G)} \Phi(t, G - u) = \Phi'(t, G). \tag{5.25}$$

By definition

$$\sum_{u \in E(G)} \Phi(t, G - u) \quad = \quad \sum_{u \in E(G)} t^{e-1-n} \, \mathcal{P}(t, G - u).$$

Rearrange to get

$$\begin{aligned}
& \sum_{u \in E(G)} t^{e-1-n} \sum_{i=0}^{n-1} (-1)^i \, c_i(G-u) \, t^{n-i} \\
= \; & \sum_{u \in E(G)} \sum_{i=0}^{n-1} (-1)^i \, c_i(G-u) \, t^{e-1-i} \\
= \; & \sum_{i=0}^{n-1} \sum_{u \in E(G)} (-1)^i \, c_i(G-u) \, t^{e-1-i} \\
= \; & \sum_{i=0}^{n-1} (-1)^i \, t^{e-1-i} \sum_{u \in E(G)} c_i(G-u).
\end{aligned}$$

By Equation 5.24 this equals

$$\sum_{i=0}^{n-1} (-1)^i \, t^{e-1-i} \, (e - i) c_i(G).$$

But this is the derivative with respect to t of Equation 5.20, so we have

$$\begin{aligned}
& \frac{\mathrm{d}}{\mathrm{dt}} \left(\sum_{i=0}^{n-1} (-1)^i \, t^{e-i} \, c_i(G) \right) \\
= \; & \Phi'(t, G).
\end{aligned}$$

Finally, the function $\Phi(t, G)$ satisfies the conditions required for the Fundamental Theorem of Calculus (e.g. Larson and Hostetler [50, Theorem 5.14, p.290]) since it is continuous over the closed interval $[a, t]$, where $0 < a < t$. So,

$$\int_a^t \Phi'(x, G)dx = \Phi(t, G) - \Phi(a, G).$$

Incorporate Equation 5.25 and rearrange to get

$$\begin{aligned}\Phi(t, G) &= \Phi(a, G) + \int_a^t \sum_{u \in E(G)} \Phi(x, G-u)dx \\ &= \Phi(a, G) + \sum_{u \in E(G)} \int_a^t \Phi(x, G-u)dx\end{aligned}$$

as required. □

5.3.2 $C_3 + P_{k-3}$ verses P_k

We now show that $C_3 + P_{k-3} \succ P_k$, for $k \geq 5$. As mentioned, Kel'mans stated this result without proof in [43, p. 260]. We will give two proofs, the first will be the proof he most likely derived and the second will use the techniques we have developed.

Theorem 5.3.3 (Paths to C_3's) *Let $k \geq 5$. Then*

$$C_3 + P_{k-3} \succ P_k.$$

Proof. (1) Induction on k. For $k = 5$ we claim $\mathcal{P}(t, C_3)\mathcal{P}(t, P_2) > \mathcal{P}(t, P_5)$ $(t \geq 5)$. The following are easily computed.

$$\begin{aligned}\mathcal{P}(t, C_3) &= t\,(t^2 - 6\,t + 9) \\ \mathcal{P}(t, P_2) &= t\,(t - 2) \\ \mathcal{P}(t, P_5) &= t\,(t^4 - 8\,t^3 + 21\,t^2 - 20\,t + 5)\end{aligned}$$

Compute

$$\begin{aligned}\mathcal{P}(t,C_3)\mathcal{P}(t,P_2) &= t^2\,(t-2)\,(t^2-6\,t+9)\\ &= t^2\,(t^3-6\,t^2+9\,t-2\,t^2+12\,t-18)\\ &= t^2\,(t^3-8\,t^2+21\,t-18)\\ &= t^5-8\,t^4+21t^3-18t^2\end{aligned}$$

Subtract

$$\begin{aligned}&\mathcal{P}(t,C_3)\mathcal{P}(t,P_2)-\mathcal{P}(t,P_5)\\ &= (t^5-8\,t^4+21t^3-18t^2)-t\,(t^4-8\,t^3+21\,t^2-20\,t+5)\\ &= 2\,t^2-5\,t\\ &> 0\end{aligned}$$

for $t > \frac{5}{2}$ End of proof of claim

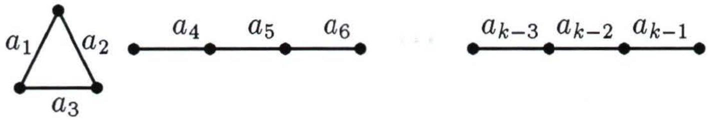


Figure 5 3 $G = C_3 + P_{k-3}$

Figure 5 4 $H = P_k$

IN the induction step, we assume $k \geq 6$ Let $G = C_3 + P_{k-3}$ and let $E(G) = \{a_1, a_2, \ldots, a_{k-1}\}$ where the edges are labelled as in Figure 5 3 (e g $E(C_3) = \{a_1, a_2, a_3\}$) Let $H = P_k$ and let $E(H) = \{b_1, b_2, \ldots, b_{k-1}\}$ where the edges are labeled as in Figure 5 4 For a mapping of the edges of G to those of H, let $\gamma(a_i) = b_i$ for $1 \leq i \leq k-1$

So, using Lemma 5.3.2 we can write

$$\Phi(t,G)-\Phi(t,H)=$$
$$\Phi(\mu,G)-\Phi(\mu,H)+\sum_{u\in E(G)}\int_{\mu}^{t}\Big[\Phi(x,G-u)-\Phi(x,H-\gamma(u))\Big]\mathrm{d}x \quad (5.26)$$

for $\mu < t$. We claim this equation is positive and demonstrate this in two steps.

Claim

$$\Phi(x,G-u)-\Phi(x,H-\gamma(u))\geq 0 \quad (5.27)$$

for any $u\in E(G)$. And for at least one edge this expression is positive.

For $u\in\{a_1,a_2,a_3\}$ we have $G-u\cong P_3+P_{k-3}$. Compare this to $H-\gamma(u)$. When $u=a_3$ then $G-a_3\cong H-\gamma(a_3)$ so that $\Phi(x,G-u)-\Phi(x,H-\gamma(u))=0$. For $u=a_1,a_2$ then Theorem 5.1.5 applies to give $G-u\succ H-\gamma(u)$ since the path lengths are more equal in $G-u$ than in $H-\gamma(u)$. Thus $\Phi(x,G-u)-\Phi(x,H-\gamma(u))>0$.

For $i=1,2,\ldots,k-4$ we have $G-a_{3+i}\cong C_3+P_i+P_{k-3-i}$ and $H-\gamma(a_{3+i})\cong P_{i+3}+P_{k-3-i}$. Disregarding the common subgraph P_{k-3-i} we note that the inductive hypothesis gives $\Phi(t,C_3+P_i)>\Phi(t,P_{i+3})$. This means Equation 5.27 is positive for each of these edges.

Next consider that for μ equal to the spectral radius, $\rho(P_k)$, of P_k that $\Phi(\mu,P_k)=0$. From $\mathcal{P}(t,C_3)=t(t-3)^2$ we know that $\rho(C_3)=3$ so $\rho(G)=\max\{3,\rho(P_{k-3})\}$. And from Lemma 4.1.6 we know that

$$\mu=\rho(P_k)>\rho(P_{k-3}).$$

Thus,

$$\mu=\rho(P_k)>\rho(G)$$

since $k\geq 5$. Therefore,

$$\Phi(\mu,G)-\Phi(\mu,P_k)=\Phi(\mu,G)>0$$

and Equation 5.26 is positive. □

Proof (2) We must show $B(3)A(k-3) - A(k)$ is positive. We have

$$\begin{aligned} B(3)A(k-3) - A(k) &= (x^6+1)^2(x^{2(k-3)}-1) - (x^{2k}-1) \\ &= 2x^{2k-3} + x^{2k-6} - x^6 - 2x^3. \end{aligned}$$

This is clearly positive since $x > 2$ and $k \geq 5$. □

5.3.3 $C_3 + P_k$ verses $C_{3+c} + P_{k-c}$

After we apply the spanning-tree-increasing operations for cycle components (Lemma 5.2.6), we may have one C_4 or one C_5. After we break down long paths into shorter ones with a triangle (Theorem 5.3.3) we may have some short paths as well. This subsection presents one theorem that handles the case of a C_4 or a C_5 with short paths. In particular we will show that a triangle and path is better than a larger cycle and shorter path.

Theorem 5.3.4 *Let $k - c > 0$, and let $c > 0$. Then*

$$C_3 + P_k \succ C_{3+c} + P_{k-c}.$$

Proof As before we use the functions $A(k)$ and $B(k)$ introduced in Section 5.1 (p. 78). In particular we show that

$$B(3)A(k) - B(3+c)A(k-c) \tag{5.28}$$

is positive. First we develop a formula for $B(a)A(b)$. Let $m = a + b$ then

$$\begin{aligned} B(a)A(b) &= (x^a + s_a)^2(x^{2b}-1) \\ &= (x^{2a} + 2s_a x^a + 1)(x^{2b}-1) \\ &= x^{2m} - 1 - x^{2a} + x^{2b} + 2s_a x^a(x^{2b}-1) \end{aligned} \tag{5.29}$$

We now develop Equation 5.28 as follows

$$B(3)A(k) - B(3+c)A(k-c)$$
$$= -x^6 + x^{2k} + 2s_3x^3(x^{2k}-1) - \left[-x^{2(3+c)} + x^{2(k-c)} + 2s_{3+c}x^{3+c}(x^{2(k-c)}-1)\right]$$

Now since $s_3 = 1$ and $s_{3+c} = -s_c$ this equals

$$-x^2 - 2x^3 + x^{6+2c} - 2s_cx^{3+c} + x^{2j} + 2x^{2j+3} - x^{2(j-c)} + 2s_cx^{3+c+2j-2c}$$

Collect the terms without k's and factor out an x^3 and collect the terms with k's and factor out an x^{2k} to get

$$x^3\left(-x^3 - 2 + x^{3+2c} - 2s_cx^c\right) + x^{2k}\left((1 - x^{-2c}) + 2x^3(1 + s_cx^{-c})\right)$$

Factor the two inner terms

$$x^3\left(x^3(x^{2c}-1) - 2(1 + s_cx^c)\right) + x^{2k}\left((1 - x^{-2c}) + 2x^3(1 + s_cx^{-c})\right)$$

Since $x > 2$ and $c > 0$ this expression is positive. Hence Equation 5.28 is positive and the result follows. □

Corollary 5.3.5 *The following special cases hold*

(a) $C_3 + P_3 \succ C_4 + P_2$

(b) $C_3 + P_4 \succ C_4 + P_3$

(c) $C_3 + P_5 \succ C_4 + P_4$

(d) $C_3 + P_4 \succ C_5 + P_2$

(e) $C_3 + P_5 \succ C_5 + P_3$

(f) $C_3 + P_6 \succ C_5 + P_4$

Proof. These follow directly from Theorem 5.3.4. □

5.3.4 Special Cases

We have found that if there is a C_4 or a C_5 and any paths that we can increase the number of spanning trees by replacing the cycle with a triangle and making the path a bit longer (Theorem 5.3.4). Of course if the longer path has length greater than five, then we shorten it and make another triangle (Theorem 5.3.3). So what if there are no cycles larger than C_3 yet there are some paths? Observe that they will have length two, three, or four because otherwise we apply Theorem 5.3.3 to shorten them. The next lemma says that if the collection of paths have enough degree two vertices, then we can make a triangle. Note that if there are not enough degree two vertices, then there are no further spanning tree increasing operations. The graphs described in this lemma are drawn in Figure 5.2.

Lemma 5.3.6 *(a)* $C_3 + P_3 + P_2 \succ P_4 + P_4$

(b) $C_3 + 3 \cdot P_2 \succ 3 \cdot P_3$

(c) $C_3 + 2 \cdot P_2 \succ P_4 + P_3$

Proof. The following algebra was done with Maple. See Appendix D. For Item (a)

$$\begin{aligned} & B(3)A(3)A(2) - A(4)A(4) \\ =\ & (x^3+1)^2(x^6-1)(x^4-1) - (x^8-1)^2 \\ =\ & x^3\left(x^2+1\right)\left(2x^4 - x^3 + 2x^2 - x + 2\right)(x-1)^2(x+1)^2 \end{aligned}$$

For Item (b)

$$\begin{aligned} & B(3)A(2)^3 - A(3)^3 \\ =\ & (x^3+1)^2(x^4-1)^3 - (x^6-1)^3 \\ =\ & x^3\left(2x^2 + x + 2\right)\left(x^2 - x + 1\right)^2(x-1)^3(x+1)^3 \end{aligned}$$

And for Item (c)

$$
\begin{aligned}
& B(3)A(2)^2 - A(4)A(3) \\
&= (x^3+1)(x^4-1)^2 - (x^8-1)(x^6-1) \\
&= 2x^3\left(x^2+1\right)\left(x^2-x+1\right)(x-1)^2(x+1)^2
\end{aligned}
$$

Clearly each of these expressions are positive for $x > 1$ □

Petingi's Lemma 5.10 parts (a), (d) and (e) [64, p. 38] are equivalent to our Lemma 5.3.6 parts (a), (b) and (c) respectively.

5.3.5 Solution for Almost-Regular Graphs in Ω^2

We now describe the Sp-optimal almost-regular graph in Ω^2.

Lemma 5.3.7 *Given an almost-regular graph G' in Ω^2, perform the spanning-tree-increasing operations prescribed in Theorem 5.1.5 (p. 80, balance paths lengths) and Lemmas 5.2.6 (p. 88, decompose cycles) and 5.3.3 (p. 93, long path to triangle and shorter path) to produce the graph G. Then the complement of G has the following components.*

- *zero P_k's, where $k \geq 5$,*
- *zero C_j's, where $j \geq 6$,*
- *$a \cdot P_4$, where $a \geq 0$,*
- *$b \cdot P_3$, where $b \geq 0$,*
- *$c \cdot P_2$, where $c \geq 0$,*

- *d C_3, where $d \geq 0$,*
- *and at most one of a C_4 or a C_5*

Proof. Suppose the complement of G' has path components. To these apply Theorem 5.1.5 and balance the path lengths. Then while there is any path with length greater than five decompose (Lemma 5.3.3) it into a triangle and a path shorter by three edges. This proves there are no paths with length greater than five and the remaining paths have lengths of two, three, or four.

Next suppose the complement of G' has cycle components. To these apply Lemma 5.2.6 resulting in some number of C_3's and at most one C_4 or one C_5. □

Lemma 5.3.8 *Given an almost-regular graph G' in Ω^2, perform the spanning-tree-increasing operations prescribed in Lemma 5.3.7 followed by the operations prescribed in Corollary 5.3.5 and Lemma 5.3.6 to produce the graph G. Let a, b, c, d have the values resulting from the application of Lemma 5.3.7. Then the complement of G has the following components:*

- *zero P_k's, where $k \geq 5$,*
- *zero C_j's, where $j \geq 6$,*
- *c' P_2, where $c' \geq c$,*
- *d' C_3, where $d' \geq d$,*
- *and at most one of these graphs $\{P_4, P_3, P_3 + P_3, C_4, C_5\}$.*

Proof. After performing the operations in Lemma 5.3.7 we perform the following.

- If there is a C_5 and a path, say P_k for $k = 2, 3, 4$, then apply the appropriate Step (d,e, or f) of Corollary 5.3.5 ($C_5 + P_k \to C_4 + P_{k+1}$). If $k = 4$ then take the resulting P_5 and make a C_3 and P_2 ($P_5 \to C_3 + P_2$).

- If there is a C_4 and a path, say P_k for $k = 2, 3, 4$, then apply the appropriate Step (a,b, or c) of Corollary 5.3.5 ($C_4 + P_k \to C_3 + P_{k+1}$). If $k = 4$ then take the resulting P_5 and make a C_3 and P_2 ($P_5 \to C_3 + P_2$).

- For each P_4, P_4 pair repeatedly apply Step (a) of Lemma 5.3.6 ($2 \cdot P_4 \to C_3 + P_3 + P_2$).

- For each P_3, P_3, P_3 triple repeatedly apply Step (b) of Lemma 5.3.6 ($3 \cdot P_3 \to C_3 + 3 \cdot P_2$).

- If there is a P_3, P_4 pair then apply Step (c) of Lemma 5.3.6 ($P_3 + P_4 \to C_3 + P_2 + P_2$).

We are left with some P_2's, some C_3's and at most one of these graphs: $\{P_4, P_3, P_3 + P_3, C_4, C_5\}$. □

The result of this lemma is clearly the Sp-optimal almost-regular graph in its respective class because no further decompositions can be performed. Essentially the complement of the Sp-optimal graph uses as many of the degree two vertices as possible in triangles with the remaining degree two vertices going to a C_4 or a C_5 provided there are no paths or the degree two vertices go to a P_3, a P_3, P_3 pair, or a P_4 only if there is no C_4 or C_5. The rest of the components, if they exist, are P_2's or triangles. We summarize these observations in our final theorem. This theorem also includes the Kel'mans, Chelnokov and Shier result (Case E) as well as two special cases of Cheng's result (Cases A.1 and D.1).

Theorem 5.3.9 *Let $G \in \{\Omega^1 \bigcup \Omega^2\}$ be almost-regular and be Sp-optimal. Then G has the following form.*

(A) Case $m = n$

(A.1) $n = 3k$ $\quad G = k \cdot C_3$

(A.2) $n = 3k + 1$ $\quad G = (k-1) \cdot C_3 + C_4$

(A.3) $n = 3k + 2$ $\quad G = (k-1) \cdot C_3 + C_5$

(B) Case $m = n - 1$

(B.1) $n = 3k$ $\quad G = (k-1) \cdot C_3 + P_4$

(B.2) $n = 3k + 1$ $\quad G = k \cdot C_3 + P_2$

(B.3) $n = 3k + 2$ $\quad G = k \cdot C_3 + P_3$

(C) Case $\left\lfloor \frac{n+2}{2} \right\rfloor < m < n - 1$

(C.1) $n - 2m \equiv 0 \bmod 3$

Let k and j be positive integers that satisfy the following system of equations

$$n = 3k + 2j \geq 5, \text{ and } m = 3k + j$$

Then

$$G = k \cdot C_3 + j \cdot P_2$$

(C.2) $n - 2m \equiv 1 \bmod 3$

Let k and j be positive integers that satisfy the following system of equations

$$n = 3k + 3 + 2j \geq 8, \text{ and } m = 3k + 2 + j$$

Then

$$G = k \cdot C_3 + j \cdot P_2 + P_3$$

(C.3) $n - 2m \equiv 2 \bmod 3$

Let k and j be positive integers that satisfy the following system of equations

$$n = 3k + 6 + 2j \geq 11, \text{ and } m = 3k + 4 + j$$

Then

$$G = k \cdot C_3 + j \cdot P_2 + 2 \cdot P_3$$

(D) *Case* $\left\lfloor \frac{n}{2} \right\rfloor \leq m \leq \left\lfloor \frac{n+2}{2} \right\rfloor$

(D.1) $m = \frac{n}{2}$ $\quad G = m \cdot P_2$

(D.2) $m = \frac{n+1}{2}$ $\quad G = (m-2) \cdot P_2 + P_3$

(D.3) $m = \frac{n+2}{2}$ $\quad G = (m-4) \cdot P_2 + 2 \cdot P_3$

(E) *Case* $0 < m < \left\lfloor \frac{n}{2} \right\rfloor$

$$G = m \cdot P_2 + (n-m)K_1$$

Items E and D.1 are due to Kel'mans and Chelnokov [34] and independently Shier [68]. Items D.1 and A.1 are two cases covered by Cheng's result [18] that complete multipartite graphs are Sp-optimal for their respective classes. Items A.2, A.3, B.2 and B.3 are presented for the first time here while the remaining items are due to Petingi [64].

Chapter 6

Future Research

This thesis has characterized the Sp-optimal almost-regular graphs in $\Omega\left(n, \binom{n}{2} - m\right)$, $\left\lfloor \frac{n}{2} \right\rfloor < m \leq n$, which we have denoted as Ω^2. Petingi obtained similar results by different methods and he showed that the Sp-optimal graph in Ω^2 is almost-regular if

- m is in the open interval $(\lfloor n/2 \rfloor + 1, n - 2)$, or if,
- $m \in \{n-1, n\}$ and e is a multiple of three.

As well, we have collected and developed formulas for the number of spanning trees in graphs whose complements are composed of disjoint unions of cycles or paths.

Our motivation for finding Sp-optimal graphs comes from the all-terminal reliability question from the theory of network reliability. And it is from this point of view that we ask where do we go from here. Nevertheless, there are many interesting problems yet to be solved that are graph theoretic, combinatorial, or related to optimization theory. The following is a list of possible directions for future research.

- Are the Sp-optimal graphs that we have found uniformly most reliable? (See page 8 for the definition of this term.) To be uniformly optimal a graph must be optimal at both ends of the reliability polynomial.

- What about the next term in the reliability polynomial? Which graphs on n vertices and e edges have the most connected spanning n edge subgraphs. Notice that a subproblem of this is how to count Hamilton cycles in a graph. Recall that determining if a graph has a Hamilton cycle is NP-complete.

  This topic is important in the case two graphs have the same number of spanning trees. Then the reliability of one over the other will be determined by the number of n edge subgraphs. The same will hold if the two graphs have close to the same number of spanning trees and the probability of edge failure is not very close to zero.

- What happens when we take the complement of a simple graph with respect to complete bipartite graphs instead of complete graphs? Can we characterize the Sp-optimal graph(s) in this subclass?

- Can we prove the almost-regularity conjecture (Conjecture 1.4.3)? We discuss some of the possibilities below in Section 6.1.

- Can we find the Sp-optimal almost-regular graphs in Ω^3? (See page 16.)

- Sp-optimal graphs are known for $e \leq n+3$. Can we extend this to $e = n+4$ or larger?

- Is it possible to prove the conjecture that Sp-optimal graphs are simple for $e \leq \binom{n}{2}$?

- There is a need for a thorough survey of all known results. This would include a survey of the counting methods, specialized counting formula, ranking methods, and ranking results. To effectively conduct a survey one needs to be fluent in

English, German, Russian, Chinese, and probably other languages Even within results published in English we have seen poor accreditation (e g Kel'mans work)

Beyond the above, the survey should explore the inter-relations of the various methods We did this in part throughout this thesis For example, we exploited the relationship between generic forms and characteristic polynomials, and later this facilitated the development of results for cycle and path components

Furthermore, there are related theories that need to be better understood, developed and utilized These include the relationship between the eigenvalues of the Laplacian and adjacency matrices of regular graphs (and for line graphs), the theory of optimal block design, and the inverse eigenvalue problem

6.1 The Importance of Being Almost-Regular

This section is concerned with the almost-regularity conjecture (Conjecture 1 4 3) We ask is it possible to prove the conjecture that Sp-optimal graphs are almost-regular? We outline some possible approaches

- One starting point for further research may use the Lagrange multiplier technique from non-linear optimization Cheng [18] used this technique to show that regular complete p-partite graphs are Sp-optimal in their respective classes of simple graphs

  The author attempted to extend this work but to no avail The approach involved expressing Cheng's non-linear optimization problem as

$$\max_{\mathbf{x} \in \mathbf{R}^{n-1}} \prod_{i=1}^{n-1} x_i,$$

where x_i is the i^{th} component of the vector $\mathbf{x}$, subject to

$$\begin{aligned}\sum_{i=1}^{n-1} x_i - 2e &= 0,\\ \sum_{i=1}^{n-1} x_i^2 - g(n,e) &\geq 0,\\ x_i &\geq 0, \text{ for } i = 1, 2, \ldots, n-1\end{aligned}$$

In this problem, e is the number of edges, n is the number of vertices, and the function $g(n, e)$ is

$$g(n,e) = na^2 + k(2a+1) + 2e,$$

where $a = \left\lfloor \frac{2e}{n} \right\rfloor$, $k = 2e - a\,n$. This function is the solution to the minimization problem.

$$\min_{\mathbf{d} \in \mathbf{Z}^n} \sum_{i=1}^{n} d_i^2 + 2e$$

subject to

$$\begin{aligned}\sum_{i=1}^{n} d_i &= 2e\\ d_i &\geq 0 \text{ for } i = 1, 2, \ldots n,\\ d_i &\leq n-1 \text{ for } i = 1, 2, \ldots n\end{aligned}$$

This function and its corresponding constraint arise from the fact that the sum of the squares of the eigenvalues of the Laplacian equals the sum of the squares of the degrees of the vertices plus $2e$.

The author believes that we need another constraint on the x_i that insures they are eigenvalues. This is an *inverse eigenvalue problem*. In our context, the problem is: given a set of $n-1$ numbers, do they constitute the eigenvalues of some graph?

- Can we extract any more information from Cheng's nearly balanced result? It is only the last portion of his proof that requires the graphs have multiple edges

Perhaps some further work would dispose of this requirement, at least in some special circumstances. The general problem is as follows.

Question. Given a simple graph G that is not almost-regular, is there an operation that produces G' such that the spectrum of G' majorizes the spectrum of G?

- Can we add loops to a graph to make it regular and then use any results for the spectrum of the adjacency matrix?

  This question is prompted by a result due to Hutschenreuther [33] (see Cvetkovic [24, Proposition 1.4, p. 39]).

Theorem 6.1.1 *For any regular multigraph G of degree r,*

$$Sp(G) = \frac{1}{n}\prod_{i=1}^{n-1}(r-\lambda_i) = \frac{1}{n}\frac{\mathrm{d}}{\mathrm{dn}}\left|n\mathrm{I} - \mathcal{A}(G)\right|, \qquad (6.1)$$

where $\lambda_i \in \sigma(G)$ and $\mathcal{A}(G)$ is the adjacency matrix of G.

This result corresponds to Lemma 3.3.16 (page 44), for regular graphs. Notice that the process of adding loops has no influence on the number of spanning trees. So we can take any non-regular graph and make it regular. The important thing is to use the eigenvalues of the regular graph created and not the original graph. Cvetkovic says this observation is due to D.A. Waller ([72, 74, 73]).

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Appendix A

Notation

A.1 Set Theory Notation

The set notation used in this thesis follows [31]). For sets A and B.

$A \subseteq B$	A is a subset of B	
$A \subset B$	A is a proper subset of B	
$\emptyset$	the empty set	
$A \cup B$	A union B	$\{x \mid x \in A \bigvee x \in B\}$
$A \cap B$	A intersect B	$\{x \mid x \in A \bigwedge x \in B\}$
$A - B$	relative complement of B in A	$\{x \mid x \in A,\ x \notin B\}$

A.2 Number Theory Notation

The number theory notation used in this thesis follows [31]).

$\mathbf{R}$	the set of real numbers
$\mathbf{Z}$	the set of integers
$\mathbf{Z}^+$	the set of nonnegative integers
$\mathbf{C}$	the set of complex numbers
$a \mid b$	a divides b, for $a, b \in \mathbf{Z}, a \neq 0$
$a \nmid b$	a does not divides b, for $a, b \in \mathbf{Z}, a \neq 0$
$a \equiv b \pmod{c}$	a is congruent to b modulo c
$\lfloor x \rfloor$	equals i where $i \in \mathbf{Z}$ is the maximum integer such that $i \leq x$
$\lceil x \rceil$	equals j where $j \in \mathbf{Z}$ is the minimum integer such that $j \geq x$
$\binom{n}{2}$	$\frac{n!}{(n-2)!2!} = n(n-1)/2$

A.3 Linear Algebra

The page number indicates the page where the symbol is defined

Symbol	Description	Page
$\mathbf{x}$	a vector	
u	n-vector of ones	
I_n	identity matrix of order n	21
J_n	matrix of all ones of order n	21
N	equals the set $\{1, 2, \ldots, n\}$	
A^{T}	transpose of matrix A	21
$\|A\|$	determinant of matrix A	21
$A_{\alpha,\beta}$	a submatrix of A, for $\alpha, \beta \subseteq N$ delete the rows indexed by α and columns indexed by β	22
A_α	a principal submatrix of A, for $\alpha \subseteq N$ delete the rows and columns indexed by α	22
A_i	a principal submatrix of A, delete row and column i	22
$A_{i,j}$	a submatrix of A, delete row i and column j	22
$\|A_\alpha\|$	a principal minor of A	22
$E_k(A)$	sum of all principal minors of A of order k	41
$\mathrm{trace}(A)$	sum of diagonal elements of A	21
$\mathrm{adj}(A)$	adjugate of A	22
$S_k(\lambda_0, \lambda_1, \ldots, \lambda_{n-1})$	k^{th} elementary symmetric function	43

A.4 Graph Theoretic

The page number indicates the page where the symbol is defined

Symbol	Description	Page
G	a graph	2
$V(G)$	vertex set of G	2
$E(G)$	edge multiset of G	2
$n = n(G)$	number of vertices in G	2
$e = e(G)$	number of edges in G	2
$\Theta(n, e)$	set of multigraphs on n vertices and e edges	3
$\Omega(n, e)$	set of simple graphs on n vertices and e edges	3
Ω^k	$\Omega\left(n, \binom{n}{2} - m\right)$, $\left\lfloor \frac{(k-1)n}{2} \right\rfloor < m \leq \left\lfloor \frac{kn}{2} \right\rfloor$	16
K_n	complete graph on n vertices	5
$\overline{G}$	denotes the complement of G w r t K_n	5
d_v	degree of vertex v	2
$G \cong H$	graphs G and H are isomorphic	3
$G \subseteq H$	graph G is a subgraph of H	3
$G + H$	disjoint union of graphs G and H	5
G/x	graph G where edge x is contracted	24
G_β	$\beta \subset V(G), \beta \neq \emptyset$ vertices in β are amalgamated	41
$\mathrm{Sp}(G)$	number of spanning trees of graph G	3
P_k	path of order k	3
C_k	cycle of order k	3
$\nu(F)$		27
$f(n, G)$	generic form	29
$\succ$	e g $G \succ H$	51

A.5 Special Matrices and Functions

The page number indicates the page where the symbol is defined.

Symbol	Description	Page
$\mathcal{L}(G) = [\ell_{ij}]$	Laplacian matrix of graph G	30
$\mathcal{A}(G) = [\alpha_{ij}]$	adjacency matrix of G	31
$\Gamma(G) = [\eta_{ij}]$	incidence matrix of G	31
$\Delta(G) = [\delta_{ij}]$	$\mathrm{diag}(d_{v_1}, d_{v_2}, \ldots, d_{v_n})$	31
$\mathcal{P}(t, G)$	characteristic polynomial of matrix $\mathcal{L}(G)$	33
$\sigma(G)$	spectrum of $\mathcal{L}(G)$	36
$\mathcal{Q}(n, G)$	complement spanning tree matrix	49
$\mathcal{T}_n = [t_{ij}]$	a special tri-diagonal matrix of order n	67
$\tau_n = \|\mathcal{T}_n\|$	determinant of $\mathcal{T}_n$	68
r	$r(n) = n - 2$	65
s	$s(n) = \sqrt{n^2 - 4n}$	65
p	$p(n) = r + s$	65
q	$q(n) = r - s$	65

Appendix B

Polynomials for Cycle Components

The data in Figure 5 1 (page 86) is calculated by using the formula in Theorem 4 2 3. The process starts by computing a polynomial for each graph. These polynomials are then evaluated and the results are compared. The table below shows the coefficients for the polynomials for these graphs. The top row gives the i^{th} exponent for n and the complete formula is obtained by multiplying the given polynomial by n^{n-2}. For example, the graph $C_3 + C_4$ has polynomial

$$n^{n-2}\left(1 - \frac{14}{n} + \frac{77}{n^2} - \frac{208}{n^3} + \frac{276}{n^4} - \frac{144}{n^5}\right).$$

The Maple code that produced this table (for m up to 10) is given in the next section and the output of the code is in the section after that.

Cycles	Coefficients of n											
	n^{-0}	n^{-1}	n^{-2}	n^{-3}	n^{-4}	n^{-5}	n^{-6}	n^{-7}	n^{-8}	n^{-9}	n^{-10}	n^{-11}
3	1	-6	9									
4	1	-8	20	-16								
5	1	-10	35	-50	25							
3,3	1	-12	54	-108	81							
6	1	-12	54	-112	105	-36						
3,4	1	-14	77	-208	276	-144						
7	1	-14	77	-210	294	-196	49					
3,5	1	-16	104	-350	640	-600	225					
8	1	-16	104	-352	660	-672	336	-64				
4,4	1	-16	104	-352	656	-640	256					
3,3,3	1	-18	135	-540	1215	-1458	729					
3,6	1	-18	135	-544	1263	-1674	1161	-324				
9	1	-18	135	-546	1287	-1782	1386	-540	81			
4,5	1	-18	135	-546	1285	-1760	1300	-400				
3,3,4	1	-20	170	-796	2217	-3672	3348	-1296				
3,7	1	-20	170	-798	2247	-3850	3871	-2058	441			
5,5	1	-20	170	-800	2275	-4000	4250	-2500	625			
10	1	-20	170	-800	2275	-4004	4290	-2640	825	-100		
4,6	1	-20	170	-800	2273	-3980	4180	-2400	576			
3,3,5	1	-22	209	-1118	3676	-7590	9585	-6750	2025			
3,8	1	-22	209	-1120	3708	-7800	10308	-8128	3408	-576		
3,4,4	1	-22	209	-1120	3704	-7744	10000	-7296	2304			
5,6	1	-22	209	-1122	3740	-8006	10985	-9310	4425	-900		
11	1	-22	209	-1122	3740	-8008	11011	-9438	4719	-1210	121	
4,7	1	-22	209	-1122	3738	-7980	10857	-9016	4116	-784		
3,3,3,3	1	-24	252	-1512	5670	-13608	20412	-17496	6561			
3,3,6	1	-24	252	-1516	5742	-14148	22572	-22356	12393	-2916		
3,9	1	-24	252	-1518	5778	-14418	23661	-24894	15795	-5346	729	
3,4,5	1	-24	252	-1518	5776	-14384	23452	-24040	14100	-3600		
5,7	1	-24	252	-1520	5814	-14686	24724	-27300	18865	-7350	1225	
12	1	-24	252	-1520	5814	-14688	24752	-27456	19305	-8008	1716	-144
6,6	1	-24	252	-1520	5814	-14688	24748	-27408	19089	-7560	1296	
4,8	1	-24	252	-1520	5812	-14656	24544	-26752	17984	-6656	1024	
4,4,4	1	-24	252	-1520	5808	-14592	24128	-25344	15360	-4096		

B.1 Maple code used to produce cycle data.

```
# This file generates the data given in an appendix of my thesis
with(linalg)

`To generate the data all I need is the coefficients in a list`,
C  = proc(k,A)
A  = vector(k),
for i from 0 to k-1 do
A[i+1]  = (k/(k-i))*(-1)^i * binomial(2*k-i-1,i),
od,
end

# multiply two arrays
Pmult  = proc (a1,a2,rval)
local n1,n2,n,k,i,j
n1  = vectdim(a1)
n2  = vectdim(a2)
n  = n1 + n2
k  = 1
rval  = vector(n-1)
for i to n-1 do rval[i]  = 0  od
for i from 1 to n1 do
for j from 1 to n2 do
k  = i+j-1
rval[k]  = rval[k] + a1[i] * a2[j]
od
od
end


C(3,c3)  C(4,c4)  C(5,c5)  C(6,c6)
C(7,c7)  C(8,c8)  C(9,c9)  C(10,c10)
Pmult (c3,c3,  r33)  Pmult (c3,c4,  r34)
Pmult (c3,c5,  r35)  Pmult (c4,c4,  r44)
Pmult (c3,r33, r333)  Pmult (c3,c6,  r36)
Pmult (c4,c5,  r45)  Pmult (c3,r34, r334)
Pmult (c3,c7,  r37)  Pmult (c5,c5,  r55)
Pmult (c4,c6,  r46)
```

```
M := 13;
amp := ' &';
en := '\\\\';
inb := cat ('\\hline ',en);

p := proc(ind,r)
t := cat (ind,' ', amp);
n := vectdim(r);
for i to n do
t := cat (t, ' ', r[i], amp);
od;
for j from i to M do t := cat (t,amp); od;
t := cat (t, en);
end;


p('3',c3), inb,
p('4',c4), inb,
p('5',c5), inb,
p('3,3',r33), p('6',c6), inb,
p('3,4',r34), p('7', c7), inb,
p('3,5',r35), p('8', c8), inb,
p('3,3,3',r333), p('3,6',r36), p('9', c9), inb,
p('3,3,4',r334), p('3,7',r37), p('5,5',r55), p('10',c10), p('4,6',r46), inb,
```

B.2 Maple output for cycle data

```
    |\^/|     Maple V Release 2 (University of Victoria)
._|\|   |/|_. Copyright (c) 1981-1992 by the University of Waterloo.
 \  MAPLE  /  All rights reserved. MAPLE is a registered trademark of
 <____ ____>  Waterloo Maple Software.
      |       Type ? for help.
> read(`cyc_app.maple`);

             3  & 1 & -6 & 9 &  &  &  &  &  &  &  &  &  &  & \\

            4  & 1 & -8 & 20 & -16 &  &  &  &  &  &  &  &  & \\

           5  & 1 & -10 & 35 & -50 & 25 &  &  &  &  &  &  &  & \\

         3,3  & 1 & -12 & 54 & -108 & 81 &  &  &  &  &  &  &  & \\
        6  & 1 & -12 & 54 & -112 & 105 & -36 &  &  &  &  &  &  & \\

        3,4  & 1 & -14 & 77 & -208 & 276 & -144 &  &  &  &  &  &  & \\
        7  & 1 & -14 & 77 & -210 & 294 & -196 & 49 &  &  &  &  &  & \\

      3,5  & 1 & -16 & 104 & -350 & 640 & -600 & 225 &  &  &  &  &  & \\
     8  & 1 & -16 & 104 & -352 & 660 & -672 & 336 & -64 &  &  &  &  & \\

    3,3,3  & 1 & -18 & 135 & -540 & 1215 & -1458 & 729 &  &  &  &  &  & \\
   3,6  & 1 & -18 & 135 & -544 & 1263 & -1674 & 1161 & -324 &  &  &  &  & \\
   9  & 1 & -18 & 135 & -546 & 1287 & -1782 & 1386 & -540 & 81 &  &  &  & \\

 3,3,4  & 1 & -20 & 170 & -796 & 2217 & -3672 & 3348 & -1296 & & & & & & \\
3,7  & 1 & -20 & 170 & -798 & 2247 & -3850 & 3871 & -2058 & 441 & & & & & \\
5,5  & 1 & -20 & 170 & -800 & 2275 & -4000 & 4250 & -2500 & 625 & & & & & \\
10  & 1 & -20 & 170 & -800 & 2275 & -4004 & 4290 & -2640 & 825 & -100 & & & & \\
4,6  & 1 & -20 & 170 & -800 & 2273 & -3980 & 4180 & -2400 & 576 & & & & & \\
```

Appendix C

Polynomials for Path Components

The table below shows the coefficients for the polynomials of some small paths. The top row gives the i^{th} exponent for n and the complete formula is obtained by multiplying the given polynomial by n^{n-2}. For example, the graph P_3 has polynomial

$$n^{n-2}\left(1 - \frac{6}{n} + \frac{10}{n^2} - \frac{4}{n^3}\right)$$

These polynomials were derived with Maple in a manner similar to that used for the cycle data above.

Path	Coefficients of n											
	n^{-0}	n^{-1}	n^{-2}	n^{-3}	n^{-4}	n^{-5}	n^{-6}	n^{-7}	n^{-8}	n^{-9}	n^{-10}	n^{-11}
3	1	-4	3									
4	1	-6	10	-4								
5	1	-8	21	-20	5							
6	1	-10	36	-56	35	-6						
7	1	-12	55	-120	126	-56	7					
8	1	-14	78	-220	330	-252	84	-8				
9	1	-16	105	-364	715	-792	462	-120	9			

Appendix D

Special Cases: Maple output

```
    |\^/|     Maple V Release 2 (University of Victoria)
._|\|   |/|_. Copyright (c) 1981-1992 by the University of Waterloo.
 \  MAPLE  /  All rights reserved. MAPLE is a registered trademark of
 <____ ____>  Waterloo Maple Software.
      |       Type ? for help.
> A := k -> (x^(2*k)-1);
                                        (2 k)
                              A := k -> x      - 1

> B := k -> (x^k + (-1)^(k+1))^2;
                                         k       (k + 1) 2
                          B := k -> (x  + (-1)       )

> a2 := A(2);
                                         4
                                 a2 := x  - 1

> a3 := A(3);
                                         6
                                 a3 := x  - 1

> a4 := A(4);
                                         8
                                 a4 := x  - 1
```

```
> b3 := B(3);
                                          3     2
                                  b3 := (x  + 1)

>
> a := factor(simplify(b3*a3*a2 - a4^2));
               3   2          4    3      2                  2        2
         a := x  (x  + 1) (2 x  - x  + 2 x  - x + 2) (x - 1)  (x + 1)

> b := factor(simplify(b3*a2^3 - a3^3));
                   3      2           2         2        3        3
             b := x  (2 x  + x + 2) (x  - x + 1)  (x - 1)  (x + 1)

> c := factor(simplify(b3*a2^2 - a4*a3));
                       3   2        2                 2        2
               c := 2 x  (x  + 1) (x  - x + 1) (x - 1)  (x + 1)

>
> latex(a);
x^{3}\left (x^{2}+1\right )\left (2\,x^{4}-x^{3}+2\,x^{2}-x+2\right )
\left (x-1\right )^{2}\left (x+1\right )^{2}
> latex(b);
x^{3}\left (2\,x^{2}+x+2\right )\left (x^{2}-x+1\right )^{2}\left (x-1
\right )^{3}\left (x+1\right )^{3}
> latex(c);
2\,x^{3}\left (x^{2}+1\right )\left (x^{2}-x+1\right )\left (x-1
\right )^{2}\left (x+1\right )^{2}
>
> quit
```

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Title of Thesis:

Maximizing Spanning Trees in Almost Complete Graphs

Author: [redacted]

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Sept 28/95

Date