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SUM OF SQUARES OF DEGREES IN A GRAPH

BERNARDO M. ÁBREGO, SILVIA FERNÁNDEZ-MERCHANT, MICHAEL G. NEUBAUER, AND WILLIAM WATKINS

DEPARTMENT OF MATHEMATICS
CALIFORNIA STATE UNIVERSITY, NORTHRIDGE
18111 NORDHOFF ST, NORTHRIDGE, CA, 91330-8313, USA.
bernardo.abrego@csun.edu

silvia.fernandez@csun.edu

michael.neubauer@csun.edu

bill.watkins@csun.edu

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ABSTRACT. Let $\mathcal{G}(v,e)$ be the set of all simple graphs with v vertices and e edges and let $P_2(G)=\sum d_i^2$ denote the sum of the squares of the degrees, $d_1,\ldots,d_v$, of the vertices of G.

It is known that the maximum value of $P_2(G)$ for $G\in\mathcal{G}(v,e)$ occurs at one or both of two special graphs in $\mathcal{G}(v,e)$—the quasi-star graph or the quasi-complete graph. For each pair (v,e), we determine which of these two graphs has the larger value of $P_2(G)$. We also determine all pairs (v,e) for which the values of $P_2(G)$ are the same for the quasi-star and the quasi-complete graph. In addition to the quasi-star and quasi-complete graphs, we find all other graphs in $\mathcal{G}(v,e)$ for which the maximum value of $P_2(G)$ is attained. Density questions posed by previous authors are examined.

Key words and phrases: Graph, Degree sequence, Threshold graph, Pell's Equation, Partition, Density.

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1. INTRODUCTION

Let $\mathcal{G}(v,e)$ be the set of all simple graphs with v vertices and e edges and let $P_2(G)=\sum d_i^2$ denote the sum of the squares of the degrees, $d_1,\ldots,d_v$, of the vertices of G. The purpose of this paper is to finish the solution of an old problem:

(1) What is the maximum value of $P_2(G)$, for a graph G in $\mathcal{G}(v,e)$?
(2) For which graphs G in $\mathcal{G}(v,e)$ is the maximum value of $P_2(G)$ attained?

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256-08

Throughout, we say that a graph G is *optimal* in $\mathcal{G}(v,e)$, if $P_2(G)$ is maximum and we denote this maximum value by $\max(v,e)$.

These problems were first investigated by Katz [8] in 1971 and by R. Ahlswede and G.O.H. Katona [2] in 1978. In his review of the paper by Ahlswede and Katona, P. Erdős [4] commented that "the solution is more difficult than one would expect." Ahlswede and Katona were interested in an equivalent form of the problem: they wanted to find the maximum number of pairs of different edges that have a common vertex. In other words, they wanted to maximize the number of edges in the line graph $L(G)$ as G ranges over $\mathcal{G}(v,e)$. That these two formulations of the problem are equivalent follows from an examination of the vertex-edge incidence matrix N for a graph $G \in \mathcal{G}(v,e)$:

$$\begin{aligned}\operatorname{trace}((NN^T)^2) &= P_2(G) + 2e,\\ \operatorname{trace}((N^TN)^2) &= \operatorname{trace}(A_L(G)^2) + 4e,\end{aligned}$$

where $A_L(G)$ is the adjacency matrix of the line graph of G. Thus $P_2(G) = \operatorname{trace}(A_L(G)^2)+2e$. ($\operatorname{trace}(A_L(G)^2)$ is twice the number of edges in the line graph of G.)

Ahlswede and Katona showed that the maximum value $\max(v,e)$ is always attained at one or both of two special graphs in $\mathcal{G}(v,e)$.

They called the first of the two special graphs a *quasi-complete* graph. The quasi-complete graph in $\mathcal{G}(v,e)$ has the largest possible complete subgraph K_k. Let k,j be unique integers such that

$$e = \binom{k+1}{2} - j = \binom{k}{2} + k - j, \text{ where } 1 \le j \le k.$$

The quasi-complete graph in $\mathcal{G}(v,e)$, which is denoted by $\mathrm{QC}(v,e)$, is obtained from the complete graph on the k vertices $1,2,\ldots,k$ by adding $v-k$ vertices $k+1,k+2,\ldots,v$, and the edges $(1,k+1)$, $(2,k+1),\ldots,(k-j,k+1)$.

The other special graph in $\mathcal{G}(v,e)$ is the *quasi-star*, which we denote by $\mathrm{QS}(v,e)$. This graph has as many dominant vertices as possible (a *dominant vertex* is one with maximum degree $v-1$). Perhaps the easiest way to describe $\mathrm{QS}(v,e)$ is to say that it is the graph complement of $\mathrm{QC}(v,e')$, where $e' = \binom{v}{2} - e$.

Define the function $C(v,e)$ to be the sum of the squares of the degree sequence of the quasi-complete graph in $\mathcal{G}(v,e)$, and define $S(v,e)$ to be the sum of the squares of the degree sequence of the quasi-star graph in $\mathcal{G}(v,e)$. The value of $C(v,e)$ can be computed as follows:

Let $e = \binom{k+1}{2} - j$, with $1 \le j \le k$. The degree sequence of the quasi-complete graph in $\mathcal{G}(v,e)$ is

$$d_1 = \cdots = d_{k-j} = k, \quad d_{k-j+1} = \cdots = d_k = k-1, \quad d_{k+1} = k-j, \quad d_{k+2} = \cdots = d_v = 0.$$

Hence

$$C(v,e) = j(k-1)^2 + (k-j)k^2 + (k-j)^2. \tag{1.1}$$

Since $\mathrm{QS}(v,e)$ is the complement of $\mathrm{QC}(v,e')$, it is straightforward to show that

$$S(v,e) = C(v,e') + (v-1)(4e - v(v-1)) \tag{1.2}$$

from which it follows that, for fixed v, the function $S(v,e) - C(v,e)$ is point-symmetric about the middle of the interval $0 \le e \le \binom{v}{2}$. In other words,

$$S(v,e) - C(v,e) = -\left(S(v,e') - C(v,e')\right).$$

It also follows from equation (1.2) that $\mathrm{QC}(v,e)$ is optimal in $\mathcal{G}(v,e)$ if and only if $\mathrm{QS}(v,e')$ is optimal in $\mathcal{G}(v,e')$. This allows us to restrict our attention to values of e in the interval $[0,\binom{v}{2}/2]$

or equivalently the interval $[\binom{v}{2}/2, \binom{v}{2}]$. On occasion, we will do so but we will always state results for all values of e.

As the midpoint of the range of values for e plays a recurring role in what follows, we denote it by

$$m = m(v) = \frac{1}{2}\binom{v}{2}$$

and define $k_0 = k_0(v)$ to be the integer such that

$$\binom{k_0}{2} \le m < \binom{k_0+1}{2}. \tag{1.3}$$

To state the results of [2] we need one more notion, that of the distance from $\binom{k_0}{2}$ to m. Write

$$b_0 = b_0(v) = m - \binom{k_0}{2}.$$

We are now ready to summarize the results of [2]:

Theorem 1.1 ([2, Theorem 2]). $\max(v,e)$ *is the larger of the two values* $C(v,e)$ *and* $S(v,e)$.

Theorem 1.2 ([2, Theorem 3]). $\max(v,e) = S(v,e)$ *if* $0 \le e < m - \frac{v}{2}$ *and* $\max(v,e) = C(v,e)$ *if* $m + \frac{v}{2} < e \le \binom{v}{2}$

Lemma 1.3 ([2, Lemma 8]). *If* $2b_0 \ge k_0$*, or* $2v - 2k_0 - 1 \le 2b_0 < k_0$*, then*

$$C(v,e) \le S(v,e) \textit{ for all } 0 \le e \le m \textit{ and}$$
$$C(v,e) \ge S(v,e) \textit{ for all } m \le e \le \binom{v}{2}.$$

If $2b_0 < k_0$ *and* $2k_0 + 2b_0 < 2v - 1$*, then there exists an* R *with* $b_0 \le R \le \min\{v/2, k_0 - b_0\}$ *such that*

$$C(v,e) \le S(v,e) \textit{ for all } 0 \le e \le m - R$$
$$C(v,e) \ge S(v,e) \textit{ for all } m - R \le e \le m$$
$$C(v,e) \le S(v,e) \textit{ for all } m \le e \le m + R$$
$$C(v,e) \ge S(v,e) \textit{ for all } m + R \le e \le \binom{v}{2}.$$

Ahlswede and Katona pose some open questions at the end of [2]. “Some strange number-theoretic combinatorial questions arise. What is the relative density of the numbers v for which $R = 0$ [$\max(v,e) = S(v,e)$ for all $0 \le e < m$ and $\max(v,e) = C(v,e)$ for all $m < e \le \binom{v}{2}$]?"

This is the point of departure for our paper. Our first main result, Theorem 2.3, strengthens Ahlswede and Katona’s Theorem 2; not only does the maximum value of $P_2(G)$ occur at either the quasi-star or quasi-complete graph in $\mathcal{G}(v,e)$, but all optimal graphs in $\mathcal{G}(v,e)$ are related to the quasi-star or quasi-complete graphs via their so-called diagonal sequence. As a result of their relationship to the quasi-star and quasi-complete graphs, all optimal graphs can be and are described in our second main result, Theorem 2.4. Our third main result, Theorem 2.8, is a refinement of Lemma 8 in [2]. Theorem 2.8 characterizes the values of v and e for which $S(v,e) = C(v,e)$ and gives an explicit expression for the value R in Lemma 8 of [2]. Finally, the “strange number-theoretic combinatorial" aspects of the problem, mentioned by Ahlswede and Katona, turn out to be Pell’s Equation $y^2 - 2x^2 = \pm 1$. Corollary 2.11 answers the density question posed by Ahlswede and Katona. We have just recently learned that Wagner and Wang

[16] have independently answered this question as well. Their approach is similar to ours, as they also find an expression for R in Lemma 8 of [2].

Before stating some new results, we summarize the work on the problem that followed [2].

A generalization of the problem of maximizing the sum of the squares of the degree sequence was investigated by Katz [8] in 1971 and R. Aharoni [1] in 1980. Katz's problem was to maximize the sum of the elements in A^2, where A runs over all $(0,1)$-square matrices of size n with precisely j ones. He found the maxima and the matrices for which the maxima are attained for the special cases where there are k^2 ones or where there are n^2-k^2 ones in the $(0,1)$-matrix. Aharoni [1] extended Katz's results for general j and showed that the maximum is achieved at one of four possible forms for A.

If A is a symmetric $(0,1)$-matrix, with zeros on the diagonal, then A is the adjacency matrix $A(G)$ for a graph G. Now let G be a graph in $\mathcal{G}(v,e)$. Then the adjacency matrix $A(G)$ of G is a $v \times v$ $(0,1)$-matrix with $2e$ ones. But $A(G)$ satisfies two additional restrictions: $A(G)$ is symmetric, and all diagonal entries are zero. However, the sum of all entries in $A(G)^2$ is precisely $\sum d_i(G)^2$. Thus our problem is essentially the same as Aharoni's in that both ask for the maximum of the sum of the elements in A^2. The graph-theory problem simply restricts the set of $(0,1)$-matrices to those with $2e$ ones that are symmetric and have zeros on the diagonal.

Olpp [14], apparently unaware of the work of Ahlswede and Katona, reproved the basic result that $\max(v,e) = \max(S(v,e), C(v,e))$, but his results are stated in the context of two-colorings of a graph. He investigates a question of Goodman [5, 6]: maximize the number of monochromatic triangles in a two-coloring of the complete graph with a fixed number of vertices and a fixed number of red edges. Olpp shows that Goodman's problem is equivalent to finding the two-coloring that maximizes the sum of squares of the red-degrees of the vertices. Of course, a two-coloring of the complete graph on v vertices gives rise to two graphs on v vertices: the graph G whose edges are colored red, and its complement G'. So Goodman's problem is to find the maximum value of $P_2(G)$ for $G \in \mathcal{G}(v,e)$.

Olpp [14] shows that either the quasi-star or the quasi-complete graph is optimal in $\mathcal{G}(v,e)$, but he does not discuss which of the two values $S(v,e), C(v,e)$ is larger. He leaves this question unanswered and does not attempt to identify all optimal graphs in $\mathcal{G}(v,e)$.

In 1999, Peled, Pedreschi, and Sterbini [13] showed that the only possible graphs for which the maximum value is attained are the so-called threshold graphs. The main result in [13] is that all optimal graphs are in one of six classes of threshold graphs. They end with the remark, "Further questions suggested by this work are the existence and uniqueness of the [graphs in $\mathcal{G}(v,e)$] in each class, and the precise optimality conditions."

Also in 1999, Byer [3] approached the problem in yet another equivalent context: he studied the maximum number of paths of length two over all graphs in $\mathcal{G}(v,e)$. Every path of length two in G represents an edge in the line graph $L(G)$, so this problem is equivalent to studying the graphs that achieve $\max(v,e)$. For each (v,e), Byer shows that there are at most six graphs in $\mathcal{G}(v,e)$ that achieve the maximum. These maximal graphs come from among six general types of graphs for which there is at most one of each type in $\mathcal{G}(v,e)$. He also extended his results to the problem of finding the maximum number of monochromatic triangles (or any other fixed connected graph with 3 edges) among two-colorings of the complete graph on v vertices, where exactly e edges are colored red. However, Byer did not discuss how to compute $\max(v,e)$, or how to determine when any of the six graphs is optimal.

In Section 2, we have unified some of the earlier work on this problem by using partitions, threshold graphs, and the idea of a diagonal sequence.

2. STATEMENTS OF THE MAIN RESULTS

2.1. **Threshold graphs.** All optimal graphs come from a class of special graphs called *threshold* graphs. The quasi-star and quasi-complete graphs are just two among the many threshold graphs in $\mathcal{G}(v, e)$. The adjacency matrix of a threshold graph has a special form. The upper-triangular part of the adjacency matrix of a threshold graph is left justified and the number of zeros in each row of the upper-triangular part of the adjacency matrix does not decrease. We will show adjacency matrices using “$+$" for the main diagonal, an empty circle “$\circ$" for the zero entries, and a black dot, “$\bullet$" for the entries equal to one.

For example, the graph G whose adjacency matrix is shown in Figure 2.1(a) is a threshold graph in $\mathcal{G}(8, 13)$ with degree sequence $(6, 5, 5, 3, 3, 3, 1, 0)$.

By looking at the upper-triangular part of the adjacency matrix, we can associate the distinct partition $\pi = (6, 4, 3)$ of 13 with the graph. In general, the *threshold* graph $\mathrm{Th}(\pi) \in \mathcal{G}(v, e)$ corresponding to a distinct partition $\pi = (a_0, a_1, \ldots, a_p)$ of e, all of whose parts are less than v, is the graph with an adjacency matrix whose upper-triangular part is left-justified and contains a_s ones in row s. Thus the threshold graphs in $\mathcal{G}(v, e)$ are in one-to-one correspondence with the set of distinct partitions, Dis(v, e) of e with all parts less than v:

$$\text{Dis}(v, e) = \left\{ \pi = (a_0, a_1, \ldots, a_p) : v > a_0 > a_1 > \cdots > a_p > 0, \sum a_s = e \right\}$$

We denote the adjacency matrix of the threshold graph $\mathrm{Th}(\pi)$ corresponding to the distinct partition π by $\mathrm{Adj}(\pi)$.

Peled, Pedreschi, and Sterbini [13] showed that all optimal graphs in a graph class $\mathcal{G}(v, e)$ must be threshold graphs.

Lemma 2.1 ([13]). *If G is an optimal graph in $\mathcal{G}(v, e)$, then G is a threshold graph.*

Thus we can limit the search for optimal graphs to the threshold graphs.

Actually, a much larger class of functions, including the power functions, $d_1^p + \cdots + d_v^p$ for $p \geq 2$, on the degrees of a graph are maximized only at threshold graphs. In fact, every Schur convex function of the degrees is maximized only at the threshold graphs. The reason is that the degree sequences of threshold graphs are maximal with respect to the majorization order among all graphical sequences. See [11] for a discussion of majorization and Schur convex functions and [10] for a discussion of the degree sequences of threshold graphs.

2.2. **The Diagonal Sequence of a Threshold Graph.** To state the first main theorem, we must now digress to describe the diagonal sequence of a threshold graph in the graph class $\mathcal{G}(v, e)$.

Returning to the example in Figure 2.1(a) corresponding to the distinct partition $\pi = (6, 4, 3) \in$ Dis$(8, 13)$, we superimpose diagonal lines on the adjacency matrix $\mathrm{Adj}(\pi)$ for the threshold graph $\mathrm{Th}(\pi)$ as shown in Figure 2.1(b).

The number of black dots in the upper triangular part of the adjacency matrix on each of the diagonal lines is called the *diagonal sequence* of the partition π (or of the threshold graph $\mathrm{Th}(\pi)$). The diagonal sequence for π is denoted by $\delta(\pi)$ and for $\pi = (6, 4, 3)$ shown in Figure 2.1, $\delta(\pi) = (1, 1, 2, 2, 3, 3, 1)$. The value of $P_2(\mathrm{Th}(\pi))$ is determined by the diagonal sequence of π.

Lemma 2.2. *Let π be a distinct partition in* Dis(v, e) *with diagonal sequence $\delta(\pi) = (\delta_1, \ldots, \delta_t)$. Then $P_2(\mathrm{Th}(\pi))$ is the dot product*

$$P_2(\mathrm{Th}(\pi)) = 2\delta(\pi) \cdot (1, 2, 3, \ldots, t) = 2 \sum_{i=1}^{t} i\delta_i.$$

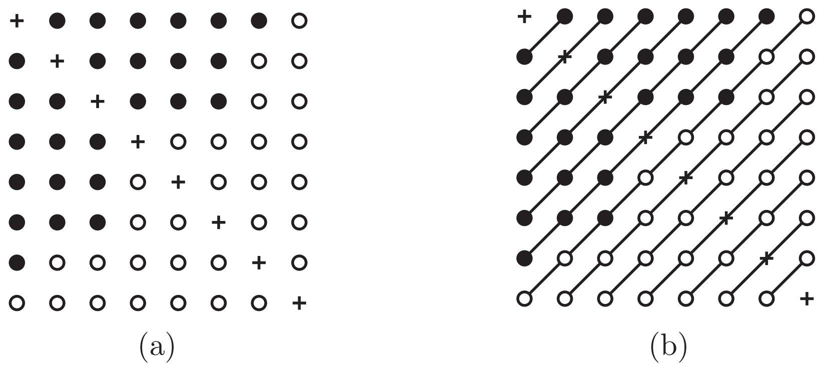


Figure 2.1: The adjacency matrix, $\mathrm{Adj}(\pi)$*, for the threshold graph in* $\mathcal{G}(8,13)$ *corresponding to the distinct partition* $\pi = (6,4,3) \in \mathrm{Dis}(8,13)$ *with diagonal sequence* $\delta(\pi) = (1,1,2,2,3,3,1)$*.*

For example, if $\pi = (6,4,3)$ as in Figure 2.1, then

$$P_2(\mathrm{Th}(\pi)) = 2(1,1,2,2,3,3,1) \cdot (1,2,3,4,5,6,7) = 114,$$

which equals the sum of squares of the degree sequence $(6,5,5,3,3,3,1)$ of the graph $\mathrm{Th}(\pi)$.

Theorem 2 in [2] guarantees that one (or both) of the graphs $\mathrm{QS}(v,e), \mathrm{QC}(v,e)$ must be optimal in $\mathcal{G}(v,e)$. However, there may be other optimal graphs in $\mathcal{G}(v,e)$, as the next example shows.

The quasi-complete graph $\mathrm{QC}(10,30)$, which corresponds to the distinct partition $(8,7,5,4,3,2,1)$ is optimal in $\mathcal{G}(10,30)$. The threshold graph G_2, corresponding to the distinct partition $(9,6,5,4,3,2,1)$ is also optimal in $\mathcal{G}(10,30)$, but is neither quasi-star in $\mathcal{G}(10,30)$ nor quasi-complete in $\mathcal{G}(v,30)$ for any v. The adjacency matrices for these two graphs are shown in Figure 2.2. They have the same diagonal sequence $\delta = (1,1,2,2,3,3,4,4,4,2,2,1,1)$ and both are optimal.

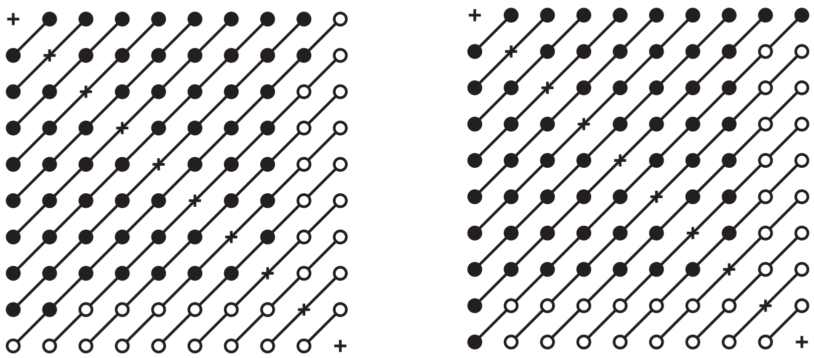


Figure 2.2: Adjacency matrices for two optimal graphs in $\mathcal{G}(10,30)$*,* $\mathrm{QC}(10,30) = \mathrm{Th}(8,7,5,4,3,2,1)$ *and* $\mathrm{Th}(9,6,5,4,3,2,1)$*, having the same diagonal sequence* $\delta = (1,1,2,2,3,3,4,4,4,2,2,1,1)$

We know that either the quasi-star or the quasi-complete graph in $\mathcal{G}(v,e)$ is optimal and that any threshold graph with the same diagonal sequence as an optimal graph is also optimal. In fact, the converse is also true. Indeed, the relationship between the optimal graphs and the quasi-star and quasi-complete graphs in a graph class $\mathcal{G}(v,e)$ is described in our first main theorem.

Theorem 2.3. *Let G be an optimal graph in $\mathcal{G}(v,e)$. Then $G = \mathrm{Th}(\pi)$ is a threshold graph for some partition $\pi \in \mathrm{Dis}(v,e)$ and the diagonal sequence $\delta(\pi)$ is equal to the diagonal sequence of either the quasi-star graph or the quasi-complete graph in $\mathcal{G}(v,e)$.*

Theorem 2.3 is stronger than Lemma 8 of [2] because it characterizes *all* optimal graphs in $\mathcal{G}(v,e)$. In Section 2.3 we describe all optimal graphs in detail.

2.3. **Optimal Graphs.** Every optimal graph in $\mathcal{G}(v,e)$ is a threshold graph, $\mathrm{Th}(\pi)$, corresponding to a partition π in $\mathrm{Dis}(v,e)$. So we extend the terminology and say that the partition π is *optimal* in $\mathrm{Dis}(v,e)$, if its threshold graph $\mathrm{Th}(\pi)$ is optimal in $\mathcal{G}(v,e)$. We say that the partition $\pi \in \mathrm{Dis}(v,e)$ is the *quasi-star partition*, if $\mathrm{Th}(\pi)$ is the quasi-star graph in $\mathcal{G}(v,e)$. Similarly, $\pi \in \mathrm{Dis}(v,e)$ is the *quasi-complete partition*, if $\mathrm{Th}(\pi)$ is the quasi-complete graph in $\mathcal{G}(v,e)$.

We now describe the quasi-star and quasi-complete partitions in $\mathrm{Dis}(v,e)$.

First, the quasi-complete graphs. Let v be a positive integer and e an integer such that $0 \le e \le \binom{v}{2}$. There exists unique integers k and j such that

$$e = \binom{k+1}{2} - j \quad \text{and} \quad 1 \le j \le k.$$

The partition

$$\pi(v,e,\mathrm{qc}) := (k, k-1, \dots, j+1, j-1, \dots, 1) = (k, k-1, \dots, \widehat{j}, \dots, 2, 1)$$

corresponds to the quasi-complete threshold graph $\mathrm{QC}(v,e)$ in $\mathcal{G}(v,e)$. The symbol $\widehat{j}$ means that j is missing.

To describe the quasi-star partition $\pi(v,e,\mathrm{qs})$ in $\mathrm{Dis}(v,e)$, let k', j' be the unique integers such that

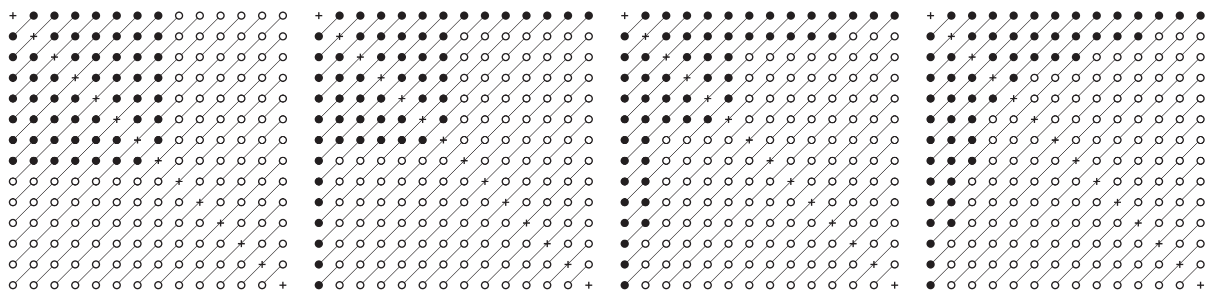
$$e = \binom{v}{2} - \binom{k'+1}{2} + j' \quad \text{and} \quad 1 \le j' \le k'.$$

Then the partition

$$\pi(v,e,\mathrm{qs}) = (v-1, v-2, \dots, k'+1, j')$$

corresponds to the quasi-star graph $\mathrm{QS}(v,e)$ in $\mathcal{G}(v,e)$.

In general, there may be many partitions with the same diagonal sequence as $\pi(v,e,\mathrm{qc})$ or $\pi(v,e,\mathrm{qs})$. For example, if $(v,e) = (14,28)$, then $\pi(14,28,\mathrm{qc}) = (7,6,5,4,3,2,1)$ and all of the partitions in Figure 2.3 have the same diagonal sequence, $\delta = (1,1,2,2,3,3,4,3,3,2,2,1,1)$. However, none of the threshold graphs corresponding to the partitions in Figure 2.3 is



(7,6,5,4,3,2,1) (13,5,4,3,2,1) (13,9,3,2,1) (13,9,5,1)

Figure 2.3: Four partitions with the same diagonal sequence as $\pi(14,28,\mathrm{qc})$

optimal. Indeed, if the quasi-complete graph is optimal in $\mathrm{Dis}(v,e)$, then there are at most three partitions in $\mathrm{Dis}(v,e)$ with the same diagonal sequence as the quasi-complete graph. The same is true for the quasi-star partition. If the quasi-star partition is optimal in $\mathrm{Dis}(v,e)$, then there are at most three partitions in $\text{Dis}(v, e)$ having the same diagonal sequence as the quasi-star partition. As a consequence, there are at most six optimal partitions in $\text{Dis}(v, e)$ and so at most six optimal graphs in $\mathcal{G}(v, e)$. Our second main result, Theorem 2.4, entails Theorem 2.3; it describes the optimal partitions in $\mathcal{G}(v, e)$ in detail. The six partitions described in Theorem 2.4 correspond to the six graphs determined by Byer in [3]. However, we give precise conditions to determine when each of these partitions is optimal.

Theorem 2.4. *Let v be a positive integer and e an integer such that $0 \le e \le \binom{v}{2}$. Let k, k', j, j' be the unique integers satisfying*

$$e = \binom{k+1}{2} - j, \quad \textit{with} \quad 1 \le j \le k,$$

and

$$e = \binom{v}{2} - \binom{k'+1}{2} + j', \quad \textit{with} \quad 1 \le j' \le k'.$$

Then every optimal partition π in $\text{Dis}(v, e)$ is one of the following six partitions:

- **1.1:** $\pi_{1.1} = (v-1, v-2, \ldots, k'+1, j')$*, the quasi-star partition for e,*
- **1.2:** $\pi_{1.2} = (v-1, v-2, \ldots, \widehat{2k'-j'-1}, \ldots, k'-1)$*, if $k'+1 \le 2k'-j'-1 \le v-1$,*
- **1.3:** $\pi_{1.3} = (v-1, v-2, \ldots, k'+1, 2, 1)$*, if $j' = 3$ and $v \ge 4$,*
- **2.1:** $\pi_{2.1} = (k, k-1, \ldots, \widehat{j}, \ldots, 2, 1)$*, the quasi-complete partition for e,*
- **2.2:** $\pi_{2.2} = (2k-j-1, k-2, k-3, \ldots 2, 1)$*, if $k+1 \le 2k-j-1 \le v-1$,*
- **2.3:** $\pi_{2.3} = (k, k-1, \ldots, 3)$*, if $j = 3$ and $v \ge 4$.*

Partitions $\pi_{1.1}$ and $\pi_{2.1}$ always exist and at least one of them is optimal. Furthermore, $\pi_{1.2}$ and $\pi_{1.3}$ (if they exist) have the same diagonal sequence as $\pi_{1.1}$, and if $S(v,e) \ge C(v,e)$, then they are all optimal. Similarly, $\pi_{2.2}$ and $\pi_{2.3}$ (if they exist) have the same diagonal sequence as $\pi_{2.1}$, and if $S(v,e) \le C(v,e)$, then they are all optimal.

A few words of explanation are in order regarding the notation for the optimal partitions in Theorem 2.4. If $k' = v$, then $j' = v, e = 0$, and $\pi_{1.1} = \emptyset$. If $k' = v-1$, then $e = j' \le v-1$, and $\pi_{1.1} = (j')$; further, if $j' = 3$, then $\pi_{1.3} = (2,1)$. In all other cases $k' \le v-2$ and then $\pi_{1.1}$, $\pi_{1.2}$, and $\pi_{1.3}$ are properly defined.

If $j' = k'$ or $j' = k'-1$, then both partitions in 1.1 and 1.2 would be equal to $(v-1, v-2, \ldots, k')$ and $(v-1, v-2, \ldots, k'+1, k'-1)$ respectively. So the condition $k'+1 \le 2k'-j'-1$ merely ensures that $\pi_{1.1} \ne \pi_{1.2}$. A similar remark holds for the partitions in 2.1 and 2.2. By definition the partitions $\pi_{1.1}$ and $\pi_{1.3}$ are always distinct; the same holds for partitions $\pi_{2.1}$ and $\pi_{2.3}$. In general, the partitions $\pi_{i.j}$ described in items 1.1-1.3 and 2.1-2.3 (and their corresponding threshold graphs) are all different. All the exceptions are illustrated in Figure 2.4 and are as follows: For any v, if $e \in \{0,1,2\}$ or $e' \in \{0,1,2\}$ then $\pi_{1.1} = \pi_{2.1}$. For any $v \ge 4$, if $e = 3$ or $e' = 3$, then $\pi_{1.3} = \pi_{2.1}$ and $\pi_{1.1} = \pi_{2.3}$. If $(v,e) = (5,5)$ then $\pi_{1.1} = \pi_{2.2}$ and $\pi_{1.2} = \pi_{2.1}$. Finally, if $(v,e) = (6,7)$ or $(7,12)$, then $\pi_{1.2} = \pi_{2.3}$. Similarly, if $(v,e) = (6,8)$ or $(7,9)$, then $\pi_{1.3} = \pi_{2.2}$. For $v \ge 8$ and $4 \le e \le \binom{v}{2} - 4$, all the partitions $\pi_{i.j}$ are pairwise distinct (when they exist).

In the next section, we determine the pairs (v, e) having a prescribed number of optimal partitions (and hence graphs) in $\mathcal{G}(v, e)$.

2.4. **Pairs (v, e) with a Prescribed Number of Optimal Partitions.** In principle, a given pair (v, e), could have between one and six optimal partitions. It is easy to see that there are infinitely many pairs (v, e) with only one optimal partition (either the quasi-star or the quasi-complete). For example the pair $\left(v, \binom{v}{2}\right)$ only has the quasi-complete partition. Similarly, there are infinitely many pairs with exactly two optimal partitions and this can be achieved in many

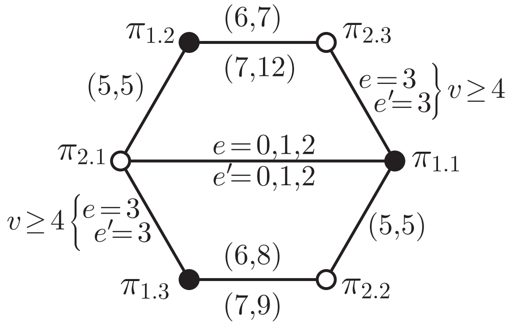


Figure 2.4: Instances of pairs (v, e) where two partitions $\pi_{i.j}$ coincide

different ways. For instance, if $(v, e) = (v, 2v - 5)$ and $v \geq 9$, then $k' = v - 2$, $j' = v - 4 > 3$, and $S(v, e) > C(v, e)$ (c.f. Corollary 2.10). Thus only the partitions $\pi_{1.1}$ and $\pi_{1.2}$ are optimal. The interesting question is the existence of pairs with 3,4,5, or 6 optimal partitions.

Often, both partitions $\pi_{1.2}$ and $\pi_{1.3}$ in Theorem 2.4 exist for the same pair (v, e); however it turns out that this almost never happens when they are optimal partitions. More precisely,

Theorem 2.5. *If $\pi_{1.2}$ and $\pi_{1.3}$ are optimal partitions then $(v, e) = (7, 9)$ or $(9, 18)$. Similarly, if $\pi_{2.2}$ and $\pi_{2.3}$ are optimal partitions, then $(v, e) = (7, 12)$ or $(9, 18)$. Furthermore, the pair $(9, 18)$ is the only one with six optimal partitions, there are no pairs with five. If there are more than two optimal partitions for a pair (v, e), then $S(v, e) = C(v, e)$, that is, both the quasi-complete and the quasi-star partitions must be optimal.*

In the next two results, we describe two infinite families of partitions in $\mathrm{Dis}(v, e)$, and hence graph classes $\mathcal{G}(v, e)$, for which there are exactly three (four) optimal partitions. The fact that they are infinite is proved in Section 9.

Theorem 2.6. *Let $v > 5$ and k be positive integers that satisfy the Pell's Equation*

$$(2v - 3)^2 - 2(2k - 1)^2 = -1 \tag{2.1}$$

and let $e = \binom{k}{2}$. Then (using the notation of Theorem 2.4), $j = k$, $k' = k + 1$, $j' = 2k - v + 2$, and there are exactly three optimal partitions in $\mathrm{Dis}(v, e)$*, namely*

$$\pi_{1.1} = (v - 1, v - 2, \ldots, k + 2, 2k - v + 2)$$
$$\pi_{1.2} = (v - 2, v - 3, \ldots, k)$$
$$\pi_{2.1} = (k - 1, k - 2, \ldots, 2, 1).$$

The partitions $\pi_{1.3}, \pi_{2.2}$, and $\pi_{2.3}$ do not exist.

Theorem 2.7. *Let $v > 9$ and k be positive integers that satisfy the Pell's Equation*

$$(2v - 1)^2 - 2(2k + 1)^2 = -49 \tag{2.2}$$

and $e = m = \frac{1}{2}\binom{v}{2}$. Then (using the notation of Theorem 2.4), $j = j' = 3$, $k = k'$, and there are exactly four optimal partitions in $\mathrm{Dis}(v, e)$*, namely*

$$\pi_{1.1} = (v - 1, v - 2, \ldots, k + 1, 3)$$
$$\pi_{1.3} = (v - 1, v - 2, \ldots, k + 1, 2, 1)$$
$$\pi_{2.1} = (k - 1, k - 2, \ldots, 4, 2, 1)$$
$$\pi_{2.3} = (k - 1, k - 2, \ldots, 4, 3).$$

The partitions $\pi_{1.2}$ and $\pi_{2.2}$ do not exist.

2.5. **Quasi-star versus quasi-complete.** In this section, we compare $S(v,e)$ and $C(v,e)$. The main result of the section, Theorem 2.8, is a theorem very much like Lemma 8 of [2], with the addition that our results give conditions for equality of the two functions.

If $e = 0, 1, 2, 3$, then $S(v,e) = C(v,e)$ for all v. Of course, if $e = 0$, $e = 1$ and $v \geq 2$, or $e \leq 3$ and $v = 3$, there is only one graph in the graph class $\mathcal{G}(v,e)$. If $e = 2$ and $v \geq 4$, then there are two graphs in the graph class $\mathcal{G}(v,2)$: the path P and the partial matching M, with degree sequences $(2,1,1)$ and $(1,1,1,1)$, respectively. The path is optimal as $P_2(P) = 6$ and $P_2(M) = 4$. However, the path is both the quasi-star and the quasi-complete graph in $\mathcal{G}(v,2)$. If $e = 3$ and $v \geq 4$, then the quasi-star graph has degree sequence $(3,1,1,1)$ and the quasi-complete graph is a triangle with degree sequence $(2,2,2)$. Since $P_2(G) = 12$ for both of these graphs, both are optimal. Similarly, $S(v,e) = C(v,e)$ for $e = \binom{v}{2} - j$ for $j = 0,1,2,3$.

Now, we consider the cases where $4 \leq e \leq \binom{v}{4} - 4$. Figures 2.5, 2.6, 2.7, and 2.8 show the values of the difference $S(v,e) - C(v,e)$. When the graph is above the horizontal axis, $S(v,e)$ is strictly larger than $C(v,e)$ and so the quasi-star graph is optimal and the quasi-complete is not optimal. And when the graph is on the horizontal axis, $S(v,e) = C(v,e)$ and both the quasi-star and the quasi-complete graph are optimal. Since the function $S(v,e) - C(v,e)$ is central symmetric, we shall consider only the values of e from 4 to the midpoint, m, of the interval $[0, \binom{v}{2}]$.

Figure 2.5 shows that $S(25,e) > C(25,e)$ for all values of e: $4 \leq e < m = 150$. So, when $v = 25$, the quasi-star graph is optimal for $0 \leq e < m = 150$ and the quasi-complete graph is not optimal. For $e = m(25) = 150$, the quasi-star and the quasi-complete graphs are both optimal.

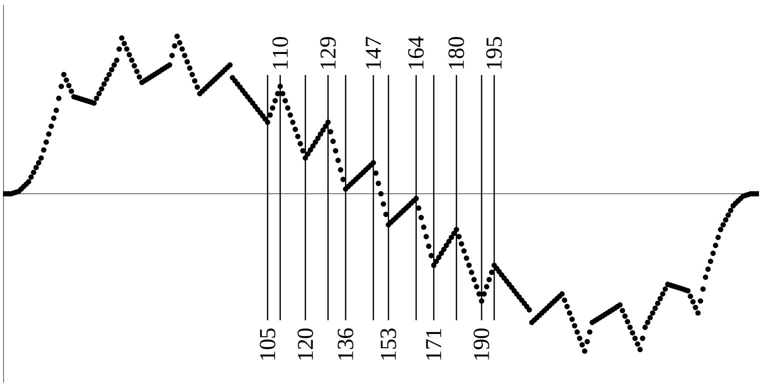


Figure 2.5: $S(25,e) - C(25,e) > 0$ *for* $4 \leq e < m = 150$

Figure 2.6 shows that $S(15,e) > C(15,e)$ for $4 \leq e < 45$ and $45 < e \leq m = 52.5$. But $S(15,45) = C(15,45)$. So the quasi-star graph is optimal and the quasi-complete graph is not optimal for all $0 \leq e \leq 52$ except for $e = 45$. Both the quasi-star and the quasi-complete graphs are optimal in $\mathcal{G}(15,45)$.

Figure 2.7 shows that $S(17,e) > C(17,e)$ for $4 \leq e < 63$, $S(17,64) = C(17,64)$, $S(17,e) < C(17,e)$ for $65 \leq e < m = 68$, and $S(17,68) = C(17,68)$.

Finally, Figure 2.8 shows that $S(23,e) > C(23,e)$ for $4 \leq e \leq 119$, but $S(23,e) = C(23,e)$ for $120 \leq e \leq m = 126.5$.

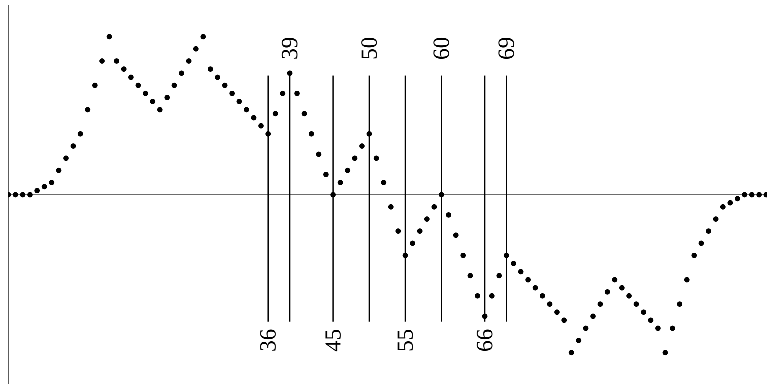


Figure 2.6: $S(15,e) - C(15,e) > 0$ *for* $4 \le e < 45$ *and for* $45 < e \le m = 52.5$

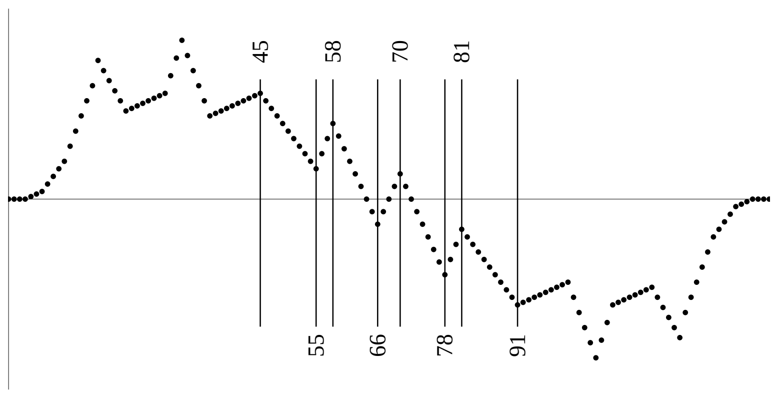


Figure 2.7: $S(17,e) - C(17,e) > 0$ *for* $4 \le e \le 63$.

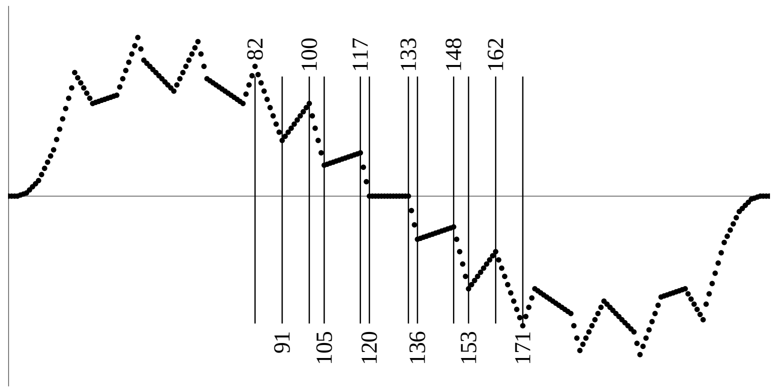


Figure 2.8: $S(23,e) - C(23,e) > 0$ *for* $4 \le e \le 119$*,* $S(23,e) = C(23,e)$ *for* $120 \le e < m = 126.5$

These four examples exhibit the types of behavior of the function $S(v,e) - C(v,e)$, for fixed v. The main thing that determines this behavior is the quadratic function

$$q_0(v) := \frac{1}{4}\left(1 - 2(2k_0 - 3)^2 + (2v - 5)^2\right)$$

(the integer $k_0 = k_0(v)$ depends on v). For example, if $q_0(v) > 0$, then $S(v,e) - C(v,e) \geq 0$ for all values of $e < m$. To describe the behavior of $S(v,e) - C(v,e)$ for $q_0(v) < 0$, we need to define

$$R_0 = R_0(v) = \frac{8(m - e_0)(k_0 - 2)}{-1 - 2(2k_0 - 4)^2 + (2v - 5)^2},$$

where

$$e_0 = e_0(v) = \binom{k_0}{2} = m - b_0$$

Our third main theorem is the following:

Theorem 2.8. *Let v be a positive integer*

(1) *If $q_0(v) > 0$, then*

$$\begin{aligned} &S(v,e) \geq C(v,e) \text{ for all } 0 \leq e \leq m \quad \text{and} \\ &S(v,e) \leq C(v,e) \text{ for all } m \leq e \leq \tbinom{v}{2}. \end{aligned}$$

$S(v,e) = C(v,e)$ if and only if $e, e' \in \{0,1,2,3,m\}$, or $e, e' = e_0$ and $(2v-3)^2 - 2(2k_0-3)^2 = -1, 7$.

(2) *If $q_0(v) < 0$, then*

$$\begin{aligned} &C(v,e) \leq S(v,e) \text{ for all } 0 \leq e \leq m - R_0; \\ &C(v,e) \geq S(v,e) \text{ for all } m - R_0 \leq e \leq m; \\ &C(v,e) \leq S(v,e) \text{ for all } m \leq e \leq m + R_0; \\ &C(v,e) \geq S(v,e) \text{ for all } m + R_0 \leq e \leq \tbinom{v}{2}. \end{aligned}$$

$S(v,e) = C(v,e)$ if and only if $e, e' \in \{0,1,2,3,m - R_0, m\}$.

(3) *If $q_0(v) = 0$, then*

$$\begin{aligned} &S(v,e) \geq C(v,e) \text{ for all } 0 \leq e \leq m \quad \text{and} \\ &S(v,e) \leq C(v,e) \text{ for all } m \leq e \leq \tbinom{v}{2}. \end{aligned}$$

$S(v,e) = C(v,e)$ if and only if $e, e' \in \{0,1,2,3,e_0,...,m\}$.

The conditions in Theorem 2.8 involving the quantity $q_0(v)$ simplify and refine the conditions in [2] involving k_0 and b_0. The condition $2b_0 \geq k_0$ in Lemma 8 of [2] can be removed and the result restated in terms of the sign of the quantity $2k_0 + 2b_0 - (2v-1) = \frac{1}{2}q_0(v)$. While [2] considers only the two cases $q_0(v) \leq 0$ and $q_0(v) > 0$, we analyze the case $q_0(v) = 0$ separately.

It is apparent from Theorem 2.8 that $S(v,e) \geq C(v,e)$ for $0 \leq e \leq m - \alpha v$ if $\alpha > 0$ is large enough. Indeed, Ahlswede and Katona [2, Theorem 3] show this for $\alpha = 1/2$, thus establishing an inequality that holds for all values of v regardless of the sign of $q_0(v)$. We improve this result and show that the inequality holds when $\alpha = 1 - \sqrt{2}/2 \approx 0.2929$.

Corollary 2.9. *Let $\alpha = 1 - \sqrt{2}/2$. Then $S(v,e) \geq C(v,e)$ for all $0 \leq e \leq m - \alpha v$ and $S(v,e) \leq C(v,e)$ for all $m + \alpha v \leq e \leq \binom{v}{2}$. Furthermore, the constant α cannot be replaced by a smaller value.*

Theorem 3 in [2] can be improved in another way. The inequalities are actually strict.

Corollary 2.10. *$S(v,e) > C(v,e)$ for $4 \leq e < m - v/2$ and $S(v,e) < C(v,e)$ for $m + v/2 < e \leq \binom{v}{2} - 4$.*

2.6. **Asymptotics and Density.** We now turn to the questions asked in [2]:

What is the relative density of the positive integers v for which $\max(v,e) = S(v,e)$ for $0 \le e < m$? Of course, $\max(v,e) = S(v,e)$ for $0 \le e \le m$ if and only if $\max(v,e) = C(v,e)$ for $m \le e \le \binom{v}{2}$.

Corollary 2.11. *Let t be a positive integer and let $n(t)$ denote the number of integers v in the interval $[1,t]$ such that*

$$\max(v,e) = S(v,e),$$

for all $0 \le e \le m$. Then

$$\lim_{t\to\infty} \frac{n(t)}{t} = 2 - \sqrt{2} \approx 0.5858.$$

2.7. **Piecewise Linearity of $S(v,e) - C(v,e)$.** The diagonal sequence for a threshold graph helps explain the behavior of the difference $S(v,e) - C(v,e)$ for fixed v and $0 \le e \le \binom{v}{2}$. From Figures 2.5, 2.6, 2.7, and 2.8, we see that $S(v,e) - C(v,e)$, regarded as a function of e, is piecewise linear and the ends of the intervals on which the function is linear occur at $e = \binom{j}{2}$ and $e = \binom{v}{2} - \binom{j}{2}$ for $j = 1, 2, \ldots, v$. We prove this fact in Lemma 6.7. For now, we present an example.

Take $v = 15$, for example. Figure 2.6 shows linear behavior on the intervals $[36, 39]$, $[39, 45]$, $[45, 50]$, $[50, 55]$, $[55, 60]$, $[60, 66]$, and $[66, 69]$. There are 14 binomial coefficients $\binom{j}{2}$ for $2 \le j \le 15$:

$$1, 3, 6, 10, 15, 21, 28, 36, 45, 55, 66, 78, 91, 105.$$

The complements with respect to $\binom{15}{2} = 105$ are

$$104, 102, 99, 95, 90, 84, 77, 69, 60, 50, 39, 27, 14, 0.$$

The union of these two sets of integers coincides with the end points for the intervals on which $S(15,e) - C(15,e)$ is linear. In this case, the function is linear on the 27 intervals with end points:

$$0, 1, 3, 6, 10, 14, 15, 21, 27, 28, 36, 39, 45, 50, 55, 60,$$
$$66, 69, 77, 78, 84, 90, 91, 95, 99, 102, 104, 105.$$

These special values of e correspond to special types of quasi-star and quasi-complete graphs.

If $e = \binom{j}{2}$, then the quasi-complete graph $\mathrm{QC}(v,e)$ is the sum of a complete graph on j vertices and $v - j$ isolated vertices. For example, if $v = 15$ and $j = 9$, and $e = \binom{9}{2} = 36$, then the upper-triangular part of the adjacency matrix for $\mathrm{QC}(15, 21)$ is shown on the left in Figure 2.9. And if $e = \binom{v}{2} - \binom{j}{2}$, then the quasi-star graph $\mathrm{QS}(v,e)$ has j dominant vertices and none of the other $v - j$ vertices are adjacent to each other. For example, the lower triangular part of the adjacency matrix for the quasi-star graph with $v = 15$, $j = 12$, and $e = \binom{14}{2} - \binom{12}{2} = 39$, is shown on the right in Figure 2.9.

As additional dots are added to the adjacency matrices for the quasi-complete graphs with $e = 37, 38, 39$, the value of $C(15,e)$ increases by $18, 20, 22$. And the value of $S(15,e)$ increases by $28, 30, 32$. Thus, the difference *increases* by a constant amount of 10. Indeed, the diagonal lines are a distance of five apart. Hence the graph of $S(15,e) - C(15,e)$ for $36 \le e \le 39$ is linear with a slope of 10. However, for $e = 40$, the adjacency matrix for the quasi-star graph has an additional dot on the diagonal corresponding to 14, whereas the adjacency matrix for the quasi-complete graph has an additional dot on the diagonal corresponding to 24. So $S(15,40) - C(15,40)$ *decreases* by 10. The decrease of 10 continues until the adjacency matrix for the quasi-complete graph contains a complete column at $e = 45$. Then the next matrix for $e = 46$ has an additional dot in the first row and next column and the slope changes again.

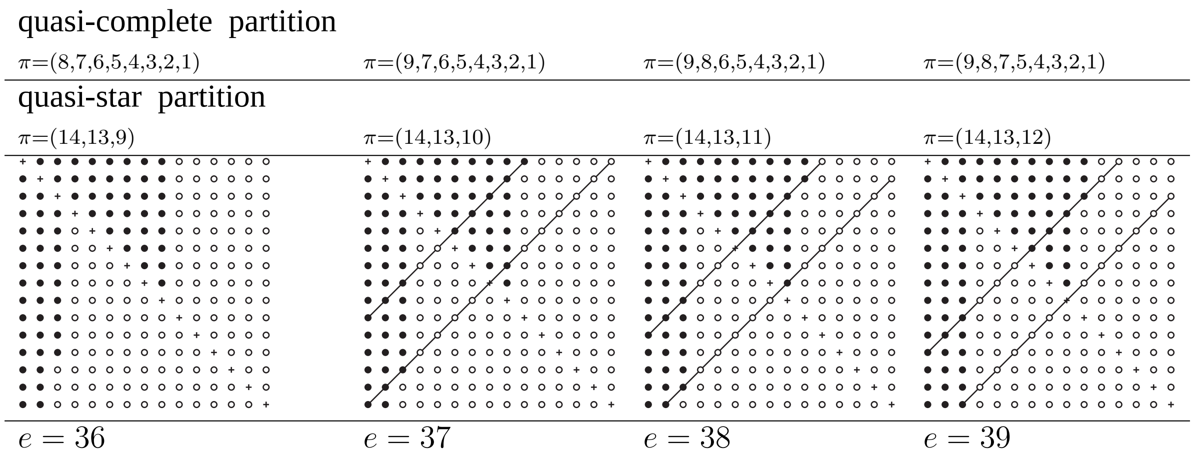


Figure 2.9: Adjacency matrices for quasi-complete and quasi-star graphs with $v = 15$ and $36 \leq e \leq 39$

3. PROOF OF LEMMA 2.2

Returning for a moment to the threshold graph $\mathrm{Th}(\pi)$ from Figure 2.1, which corresponds to the distinct partition $\pi = (6, 4, 3)$, we see the graph complement shown with the white dots. Counting white dots in the rows from bottom to top and from the left to the diagonal, we have 7,5,2,1. These same numbers appear in columns reading from right to left and then top to the diagonal. So if $\mathrm{Th}(\pi)$ is the threshold graph associated with π, then the set-wise complement of π (π^c) in the set $\{1, 2, \ldots, v-1\}$ corresponds to the threshold graph $\mathrm{Th}(\pi)^c$—the complement of $\mathrm{Th}(\pi)$. That is,

$$\mathrm{Th}(\pi^c) = \mathrm{Th}(\pi)^c.$$

The diagonal sequence allows us to evaluate the sum of squares of the degree sequence of a threshold graph. Each black dot contributes a certain amount to the sum of squares. The amount depends on the location of the black dot in the adjacency matrix. In fact all of the dots on a particular diagonal line contribute the same amount to the sum of squares. For $v = 8$, the value of a black dot in position (i, j) is given by the entry in the following matrix:

$$\begin{bmatrix} + & 1 & 3 & 5 & 7 & 9 & 11 & 13 \\ 1 & + & 3 & 5 & 7 & 9 & 11 & 13 \\ 1 & 3 & + & 5 & 7 & 9 & 11 & 13 \\ 1 & 3 & 5 & + & 7 & 9 & 11 & 13 \\ 1 & 3 & 5 & 7 & + & 9 & 11 & 13 \\ 1 & 3 & 5 & 7 & 9 & + & 11 & 13 \\ 1 & 3 & 5 & 7 & 9 & 11 & + & 13 \\ 1 & 3 & 5 & 7 & 9 & 11 & 13 & + \end{bmatrix}$$

This follows from the fact that a sum of consecutive odd integers is a square. So to get the sum of squares $P_2(\mathrm{Th}(\pi))$ of the degrees of the threshold graph associated with the distinct partition π, sum the values in the numerical matrix above that occur in the positions with black dots. Of course, an adjacency matrix is symmetric. So if we use only the black dots in the upper triangular part, then we must replace the (i, j)-entry in the upper-triangular part of the matrix above with the sum of the (i,j)- and the (j,i)-entry, which gives the following matrix:

$$E = \begin{bmatrix} + & 2 & 4 & 6 & 8 & 10 & 12 & 14 \\ & + & 6 & 8 & 10 & 12 & 14 & 16 \\ & & + & 10 & 12 & 14 & 16 & 18 \\ & & & + & 14 & 16 & 18 & 20 \\ & & & & + & 18 & 20 & 22 \\ & & & & & + & 22 & 24 \\ & & & & & & + & 26 \\ & & & & & & & + \end{bmatrix}. \tag{3.1}$$

Thus, $P_2(\mathrm{Th}(\pi)) = 2(1,2,3,\ldots)\cdot\delta(\pi)$. Lemma 2.2 is proved.

4. PROOFS OF THEOREMS 2.3 AND 2.4

Theorem 2.3 is an immediate consequence of Theorem 2.4 (and Lemmas 2.1 and 2.2). Theorem 2.4 can be proved using the following central lemma:

Lemma 4.1. *Let* $\pi = (v-1, c, c-1, \ldots, \widehat{j}, \ldots, 2, 1)$ *be an optimal partition in* Dis(v,e)*, where* $e-(v-1) = 1+2+\cdots+c-j \geq 4$ *and* $1 \leq j \leq c < v-2$*. Then* $j = c$ *and* $2c \geq v-1$ *so that*

$$\pi = (v-1, c-1, c-2, \ldots, 2, 1).$$

We defer the proof of Lemma 4.1 until Section 5 and proceed now with the proof of Theorem 2.4. The proof of Theorem 2.4 is an induction on v.

Proof of Theorem 2.4. Let π be an optimal partition in Dis(v,e), then π^c is optimal in Dis(v,e'). One of the partitions, π, π^c contains the part $v-1$. We may assume without loss of generality that $\pi = (v-1 : \mu)$, where μ is a partition in Dis$(v-1, e-(v-1))$. The cases where μ is a decreasing partition of $0, 1, 2,$ and 3 will be considered later. For now we shall assume that $e-(v-1) \geq 4$. □

Since π is optimal, it follows that μ is optimal and hence by the induction hypothesis, μ is one of the following partitions in Dis$(v-1, e-(v-1))$:

- **1.1a:** $\mu_{1.1} = (v-2, \ldots, k'+1, j')$, the quasi-star partition for $e-(v-1)$,
- **1.2a:** $\mu_{1.2} = (v-2, \ldots, \widehat{2k'-j'}-1, \ldots, k'-1)$, if $k'+1 \leq 2k'-j'-1 \leq v-2$,
- **1.3a:** $\mu_{1.3} = (v-2, \ldots, k'+1, 2, 1)$, if $j' = 3$,
- **2.1a:** $\mu_{2.1} = (k_1, k_1-1, \ldots, \widehat{j_1}, \ldots, 2, 1)$, the quasi-complete partition for $e-(v-1)$,
- **2.2a:** $\mu_{2.2} = (2k_1-j_1-1, k_1-2, k_1-3, \ldots 2, 1)$, if $k_1+1 \leq 2k_1-j_1-1 \leq v-2$,
- **2.3a:** $\mu_{2.3} = (k_1, k_1-1, \ldots, 3)$, if $j_1 = 3$,

where

$$e-(v-1) = 1+2+\cdots+k_1-j_1 \geq 4, \quad \text{with } 1 \leq j_1 \leq k_1.$$

In symbols, $\pi = (v-1, \mu_{i.j})$, for one of the partitions $\mu_{i.j}$ above. For each partition, $\mu_{i.j}$, we will show that $(v-1, \mu_{i.j}) = \pi_{s.t}$ for one of the six partitions, $\pi_{s.t}$, in the statement of Theorem 2.4.

The first three cases are obvious:

$$(v-1, \mu_{1.1}) = \pi_{1.1},$$
$$(v-1, \mu_{1.2}) = \pi_{1.2},$$
$$(v-1, \mu_{1.3}) = \pi_{1.3}.$$

Next suppose that $\mu = \mu_{2.1}, \mu_{2.2}$, or $\mu_{2.3}$. The partitions $\mu_{2.2}$ and $\mu_{2.3}$ do not exist unless certain conditions on k_1, j_1, and v are met. And whenever those conditions are met, the partition

$\mu_{2.1}$ is also optimal. Thus $\pi_1 = (v-1, \mu_{2.1})$ is optimal. Also, since $e-(v-1) \geq 4$, then $k_1 \geq 3$. There are two cases: $k_1 = v-2, k_1 \leq v-3$. If $k_1 = v-2$, then $\mu_{2.2}$ does not exist and

$$(v-1,\mu) = \begin{cases} \pi_{2.1}, \text{ if } \mu = \mu_{2.1}, \\ \pi_{1.1}, \text{ if } \mu = \mu_{2.3}. \end{cases}$$

If $k_1 \leq v-3$, then by Lemma 4.1, $\pi_1 = (v-1, k_1-1, \dots, 2, 1)$, with $j_1 = k_1$ and $2k_1 \geq v-1$. We will show that $k = k_1+1$ and $v-1 = 2k-j-1$. The above inequalities imply that

$$\begin{aligned}\binom{k_1+1}{2} &= 1+2+\cdots+k_1 \leq e \\ &= \binom{k_1+1}{2} - k_1 + (v-1) < \binom{k_1+1}{2} + (k_1+1) = \binom{k_1+2}{2}.\end{aligned}$$

But k is the unique integer satisfying $\binom{k}{2} \leq e < \binom{k+1}{2}$. Thus $k = k_1+1$.

It follows that

$$e = (v-1) + 1 + 2 + \cdots + (k-2) = \binom{k+1}{2} - j,$$

and so $2k-j = v$.

We now consider the cases 2.1a, 2.2a, and 2.3a individually. Actually, $\mu_{2.2}$ does not exist since $k_1 = j_1$. If $\mu = \mu_{2.3}$, then $\mu = (3)$ since $k_1 = j_1 = 3$. This contradicts the assumption that μ is a partition of an integer greater than 3. Therefore

$$\mu = \mu_{2.1} = (k_1, k_1-1, \dots, \widehat{j_1}, \dots, 2, 1) = (k-2, k-3, \dots 2, 1),$$

since $k_1 = j_1$ and $k = k_1+1$. Now since $2k-j-1 = v-1$ we have

$$\pi = (2k-j-1, k-2, k-3, \dots 2, 1) = \begin{cases} \pi_{2.1} \text{ if } e = \binom{v}{2} \text{ or } e = \binom{v}{2} - (v-2), \\ \pi_{2.2} \text{ otherwise.} \end{cases}$$

Finally, if μ is a decreasing partition of $0, 1, 2,$ or 3, then either $\pi = (v-1, 2, 1) = \pi_{1.3}$, or $\pi = (v-1) = \pi_{1.1}$, or $\pi = (v-1, j') = \pi_{1.1}$ for some $1 \leq j' \leq 3$.

Now, we prove that $\pi_{1.2}$ and $\pi_{1.3}$ (if they exist) have the same diagonal sequence as $\pi_{1.1}$ (which always exists). This in turn implies (by using the duality argument mentioned in Section 3) that $\pi_{2.2}$ and $\pi_{2.3}$ also have the same diagonal sequence as $\pi_{2.1}$ (which always exists). We use the following observation. If we index the rows and columns of the adjacency matrix $\mathrm{Adj}(\pi)$ starting at zero instead of one, then two positions (i,j) and (i',j') are in the same diagonal if and only if the sum of their entries are equal, that is, $i+j = i'+j'$. If $\pi_{1.2}$ exists then $2k'-j' \leq v$. Applying the previous argument to $\pi_{1.1}$ and $\pi_{1.2}$, we observe that the top row of the following lists shows the positions where there is a black dot in $\mathrm{Adj}(\pi_{1.1})$ but not in $\mathrm{Adj}(\pi_{1.2})$ and the bottom row shows the positions where there is a black dot in $\mathrm{Adj}(\pi_{1.2})$ but not in $\mathrm{Adj}(\pi_{1.1})$.

$$\begin{array}{lllll} (v-k'-2, v-1) & \dots & (v-k'-t, v-1) & \dots & (v-k'-(k'-j'), v-1) \\ (v-1-k', v-2) & \dots & (v-1-k', v-t) & \dots & (v-1-k', v-(k'-j')). \end{array}$$

Each position in the top row is in the same diagonal as the corresponding position in the second row. Thus the number of positions per diagonal is the same in $\pi_{1.1}$ as in $\pi_{1.2}$. That is, $\delta(\pi_{1.1}) = \delta(\pi_{1.2})$.

Similarly, if $\pi_{1.3}$ exists then $k' \geq j' = 3$. To show that $\delta(\pi_{1.1}) = \delta(\pi_{1.3})$ note that the only position where there is a black dot in $\mathrm{Adj}(\pi_{1.1})$ but not in $\mathrm{Adj}(\pi_{1.3})$ is $(v-1-k', v-1-k'+3)$, and the only position where there is a black dot in $\mathrm{Adj}(\pi_{1.3})$ but not in $\mathrm{Adj}(\pi_{1.1})$ is $(v-k', v-1-k'+2)$. Since these positions are in the same diagonal then $\delta(\pi_{1.1}) = \delta(\pi_{1.3})$.

Theorem 2.4 is proved.

5. PROOF OF LEMMA 4.1

There is a variation of the formula for $P_2(\mathrm{Th}(\pi))$ in Lemma 2.2 that is useful in the proof of Lemma 4.1. We have seen that each black dot in the adjacency matrix for a threshold graph contributes a summand, depending on the location of the black dot in the matrix E in (3.1). For example, if $\pi = (3,1)$, then the part of $(1/2)E$ that corresponds to the black dots in the adjacency matrix $\mathrm{Adj}(\pi)$ for π is

$$\mathrm{Adj}((3,1)) = \begin{bmatrix} + & \bullet & \bullet & \bullet \\ & + & \bullet & \circ \\ & & + & \circ \\ & & & + \end{bmatrix}, \qquad \begin{bmatrix} + & 1 & 2 & 3 \\ & + & 3 & \\ & & + & \\ & & & + \end{bmatrix}.$$

Thus $P_2(\mathrm{Th}(\pi)) = 2(1+2+3+3) = 18$. Now if we index the rows and columns of the adjacency matrix starting with zero instead of one, then the integer appearing in the matrix $(1/2)E$ at entry (i,j) is just $i+j$. So we can compute $P_2(\mathrm{Th}(\pi))$ by adding all of the positions (i,j) corresponding to the positions of black dots in the upper-triangular part of the adjacency matrix of $\mathrm{Th}(\pi)$. What are the positions of the black dots in the adjacency matrix for the threshold graph corresponding to a partition $\pi = (a_0, a_1, \ldots, a_p)$? The positions corresponding to a_0 are

$$(0,1), (0,2), \ldots, (0, a_0)$$

and the positions corresponding to a_1 are

$$(1,2), (1,3), \ldots, (1, 1+a_1).$$

In general, the positions corresponding to a_t in π are

$$(t, t+1), (t, t+2), \ldots, (t, t+a_t).$$

We use these facts in the proof of Lemma 4.1.

Let $\mu = (c, c-1, \ldots, \widehat{j}, \ldots, 2, 1)$ be the quasi-complete partition in $\mathrm{Dis}(v, e-(v-1))$, where $1 \le j \le c < v-2$ and $1+2+\cdots+c-j \ge 4$. We deal with the cases $j=1$, $j=c$, and $2 \le j \le c-1$ separately. Specifically, we show that if $\pi = (v-1 : \mu)$ is optimal, then $j = c$ and

$$\pi = (v-1, c-1, \ldots, 2, 1), \tag{5.1}$$

with $2c \ge v-1$.

Arguments for the cases are given below.

5.1. $j = 1 : \mu = (c, c-1, \ldots, 3, 2)$. Since $2+3+\cdots+c \ge 4$ then $c \ge 3$. We show that $\pi = (v-1 : \mu)$ is not optimal. In this case, the adjacency matrix for π has the following form:

$$\begin{array}{c|cccccccccc}
 & 0 & 1 & 2 & \cdots & & c & & & \cdots & v-1 \\
\hline
0 & + & \bullet & \bullet & \cdots & & \bullet & \bullet & \bullet & \cdots & \bullet \\
1 & & + & \bullet & \cdots & & \bullet & \bullet & \circ & \cdots & \circ \\
2 & & & + & & & & & & & \\
\vdots & & & & \ddots & & & & & & \\
c-1 & & & & & + & \bullet & \bullet & \circ & \cdots & \circ \\
c & & & & & & + & \circ & \circ & \cdots & \circ \\
c+1 & & & & & & & + & \circ & \cdots & \circ \\
\vdots & & & & & & & & \ddots & & \vdots \\
 & & & & & & & & & & \circ \\
v-1 & & & & & & & & & & +
\end{array}$$

5.1.1. $2c \leq v - 1$. Let

$$\pi' = (v - 1, 2c - 1, c - 2, c - 3, \ldots, 3, 2).$$

The parts of π' are distinct and decreasing since $2c \leq v - 1$. Thus $\pi' \in \text{Dis}(v, e)$.

The adjacency matrices $\text{Adj}(\pi)$ and $\text{Adj}(\pi')$ each have e black dots, many of which appear in the same positions. But there are differences. Using the fact that $c - 1 \geq 2$, the first row of the following list shows the positions in which a black dot appears in $\text{Adj}(\pi)$ but not in $\text{Adj}(\pi')$. And the second row shows the positions in which a black dot appears in $\text{Adj}(\pi')$ but not in $\text{Adj}(\pi)$:

$$\begin{array}{ccccc} (2, c+1) & (3, c+1) & \cdots & (c-1, c+1) & (c-1, c) \\ (1, c+2) & (1, c+3) & \cdots & (1, 2c-1) & (1, 2c) \end{array}$$

For each of the positions in the list, except the last ones, the sum of the coordinates for the positions is the same in the first row as it is in the second row. But the coordinates of the last pair in the first row sum to $2c - 1$ whereas the coordinates of the last pair in the second row sum to $2c + 1$. It follows that $P_2(\pi') = P_2(\pi) + 4$. Thus, π is not optimal.

5.1.2. $2c > v - 1$. Let $\pi' = (v - 2, c, c - 1, \ldots, 3, 2, 1)$. Since $c < v - 2$, the partition π' is in $\text{Dis}(v, e)$. The positions of the black dots in the adjacency matrices $\text{Adj}(\pi)$ and $\text{Adj}(\pi')$ are the same but with only two exceptions. There is a black dot in position $(0, v - 1)$ in π but not in π', and there is a black dot in position $(c, c + 1)$ in π' but not in π. Since $c + (c + 1) > 0 + (v - 1)$, π is not optimal.

5.2. $j = c : \mu = (c - 1, \ldots, 2, 1)$**.** Since $1 + 2 + \cdots + (c - 1) \geq 4$, then $c \geq 4$. We will show that if $2c \geq v - 1$, then π has the same diagonal sequence as the quasi-complete partition. And if $2c < v - 1$, then π is not optimal.

The adjacency matrix for π is of the following form:

$$\begin{array}{c|cccccccc} & 0 & 1 & 2 & \cdots & c & & \cdots & v-1 \\ \hline 0 & + & \bullet & \bullet & \cdots & \bullet & \bullet & \cdots & \bullet \\ 1 & & + & \bullet & & \bullet & \circ & & \circ \\ \vdots & & & \ddots & & & & & \\ & & & & + & \bullet & \circ & \cdots & \circ \\ c & & & & & + & \circ & \cdots & \circ \\ & & & & & & + & \cdots & \circ \\ & & & & & & & \ddots & \\ v-1 & & & & & & & & + \end{array}$$

5.2.1. $2c \geq v - 1$. The quasi-complete partition in $\mathcal{G}(v, e)$ is $\pi' = (c + 1, c, \ldots, \widehat{k}, \ldots, 2, 1)$, where $k = 2c - v + 2$. To see this, notice that

$$1 + 2 + \cdots + c + (c + 1) - k = 1 + 2 + \cdots + (c - 1) + (v - 1)$$

for $k = 2c - v + 2$. Since $2c \geq v - 1$ and $c < v - 2$, then $1 \leq k < c$ and $\pi' \in \text{Dis}(v, e)$.

To see that π and π' have the same diagonal sequence, we again make a list of the positions in which there is a black dot in $\text{Adj}(\pi)$ but not in $\text{Adj}(\pi')$ (the top row below), and the positions in which there is a black dot in $\mathrm{Adj}(\pi')$ but not in $\mathrm{Adj}(\pi)$ (the bottom row below):

$$\begin{array}{cccccc} (0,c+2) & (0,c+3) & \cdots & (0,c+t+1) & \cdots & (0,v-1) \\ (1,c+1) & (2,c+1) & \cdots & (t,c+1) & \cdots & (v-c-2,c+1). \end{array}$$

Each position in the top row is in the same diagonal as the corresponding position in the bottom row, that is, $0+(c+t+1)=t+(c+1)$. Thus the diagonal sequences $\delta(\pi)=\delta(\pi')$.

5.2.2. $2c < v-1$. In this case, let $\pi'=(v-1,2c-2,c-3,\dots,3,2)$. And since $2c-2\le v-3$, the parts of π' are distinct and decreasing. That is, $\pi'\in$ Dis(v,e).

Using the fact that $c-2\ge 2$, we again list the positions in which there is a black dot in $\mathrm{Adj}(\pi)$ but not in $\mathrm{Adj}(\pi')$ (the top row below), and the positions in which there is a black dot in $\mathrm{Adj}(\pi')$ but not in $\mathrm{Adj}(\pi)$:

$$\begin{array}{ccccc} (2,c) & (3,c) & \cdots & (c-1,c) & (c-2,c-1) \\ (1,c+1) & (1,c+2) & \cdots & (1,2c-2) & (1,2c-1). \end{array}$$

All of the positions but the last in the top row are on the same diagonal as the corresponding position in the bottom row: $t+c=1+(c-1+t)$. But in the last positions we have $(c-2)+(c-1)=2c-3$ and $1+(2c-1)=2c$. Thus $P_2(\pi')=P_2(\pi)+6$ and so π is not optimal.

5.3. $1<j<c:\mu=(c,c-1,\dots,\widehat{j},\dots,2,1)$. We will show that $\pi=(v-1,c,c-1,\dots,\widehat{j},\dots,2,1)$ is not optimal. The adjacency matrix for π has the following form:

$$\begin{array}{l|ccccccccccc}
 & 0 & 1 & 2 & \cdots & c-1 & c & c+1 & c+2 & \cdots & v-1 \\ \hline
0 & + & \bullet & \bullet & \cdots & & \bullet & \bullet & \bullet & \cdots & \bullet \\
1 & & + & \bullet & & & \bullet & \bullet & \circ & & \circ \\
\vdots & & & & & & & & & & \\
c-j & & & & & & \bullet & \bullet & \circ & \cdots & \circ \\
c-j+1 & & & & \ddots & & \bullet & \circ & \circ & \cdots & \circ \\
\vdots & & & & & & & & & & \\
c-1 & & & & & + & \bullet & \circ & \circ & \cdots & \circ \\
c & & & & & & + & \circ & \circ & \cdots & \circ \\
c+1 & & & & & & & + & \circ & \cdots & \circ \\
\vdots & & & & & & & & + & & \\
 & & & & & & & & & \ddots & \\
v-1 & & & & & & & & & & +
\end{array}$$

There are two cases.

5.3.1. $2c > v-1$. Let $\pi'=(v-r,c,c-1,\dots,\widehat{j+1-r},\dots,2,1)$, where $r=\min(v-1-c,j)$. Then $r>1$ because $j>1$ and $c<v-2$. We show that $\pi'\in$ Dis(v,e) and $P_2(\pi')>P_2(\pi)$.

In order for π' to be in Dis(v,e), the sum of the parts in π' must equal the sum of the parts in π:

$$1+2+\cdots+c+(v-r)-(j+1-r)=1+2+\cdots+c+(v-1)-j.$$

And the parts of π' must be distinct and decreasing:

$$v-r>c>j+1-r>1.$$

The first inequality holds because $v - 1 - c \geq r$. The last two inequalities hold because $c > j > r > 1$. Thus $\pi' \in \mathrm{Dis}(v, e)$.

The top row below lists the positions where there is a black dot in $\mathrm{Adj}(\pi)$ but not in $\mathrm{Adj}(\pi')$; the bottom row lists the positions where there is a black dot in $\mathrm{Adj}(\pi')$ but not in $\mathrm{Adj}(\pi)$:

$$\begin{array}{lllll} (0, v-1) & \cdots & (0, v-t) & \cdots & (0, v-r+1) \\ (c-j+r-1, c+1) & \cdots & (c-j+r-t, c+1) & \cdots & (c-j+1, c+1). \end{array}$$

Since $r > 1$, the lists above are non-empty. Thus, to ensure that $P_2(\pi') > P_2(\pi)$, it is sufficient to show that for each $1 \leq t \leq r-1$, position $(0, v-t)$ is in a diagonal to the left of position $(c-j+r-t, c+1)$. That is,

$$0 < [(c-j+r+1-t) + (c+1)] - [0 + (v-t)] = 2c + r - v - j,$$

or equivalently,

$$v - 2c + j - 1 \leq r = \min(v - 1 - c, j).$$

The inequality $v - 2c + j \leq v - 1 - c$ holds because $j < c$, and $v - 2c + j \leq j$ holds because $v - 1 < 2c$. It follows that π is not an optimal partition.

5.3.2. $2c \leq v - 1$. Again we show that $\pi = (v-1, c, c-1, \ldots, \widehat{j}, \ldots, 2, 1)$ is not optimal. Let

$$\pi' = (v-1, 2c-2, c-2, \ldots, \widehat{j-1}, \ldots, 2, 1).$$

The sum of the parts in π equals the sum of the parts in π'. And the partition π' is decreasing:

$$1 \leq j - 1 \leq c - 2 < 2c - 2 < v - 1.$$

The first three inequalities follow from the assumption that $1 < j < c$. And the fourth inequality holds because $2c \leq v - 1$. So $\pi' \in \mathrm{Dis}(v, e)$.

The adjacency matrices $\mathrm{Adj}(\pi)$ and $\mathrm{Adj}(\pi')$ differ as follows. The top rows of the following two lists contain the positions where there is a black dot in $\mathrm{Adj}(\pi)$ but not in $\mathrm{Adj}(\pi')$; the bottom row lists the positions where there is a black dot in $\mathrm{Adj}(\pi')$ but not in $\mathrm{Adj}(\pi)$.

$$\begin{array}{llllll} \text{List 1} & (2, c+1) & \cdots & (t, c+1) & \cdots & (c-j, c+1) \\ & (1, c+2) & \cdots & (1, c+t) & \cdots & (1, 2c-j) \\ \\ \text{List 2} & (c-j+1, c) & \cdots & (c-j+t, c) & \cdots & (c-1, c) \\ & (1, 2c-j+1) & \cdots & (1, 2c-j+t) & \cdots & (1, 2c-1). \end{array}$$

Each position, $(t, c+1)$ ($t = 2, \ldots, c-j$), in the top row in List 1 is in the same diagonal as the corresponding position, $(1, c+t)$, in the bottom row of List 1. Each position, $(c-j+t, c)$ ($t = 1, \ldots, j-1$), in the top row of List 2 is in a diagonal to the left of the corresponding position, $(1, 2c-j+t)$ in the bottom row of List 2. Indeed, $(c-j+t)+c = 2c-j+t < 2c-j+t+1 = 1 + (2c-j+t)$. And since $1 < j$, List 2 is not empty. It follows that $P_2(\pi') > P_2(\pi)$ and so π is not a optimal partition.

The proof of Lemma 4.1 is complete.

6. PROOF OF THEOREM 2.8 AND COROLLARIES 2.9 AND 2.10

The notation in this section changes a little from that used in Section 1. In Section 1, we write $e = \binom{k+1}{2} - j$, with $1 \leq j \leq k$. Here, we let $t = k - j$ so that

$$e = \binom{k}{2} + t, \tag{6.1}$$

with $0 \leq t \leq k - 1$. Then Equation (1.1) is equivalent to

$$C(v, e) = C(k, t) = (k-t)(k-1)^2 + tk^2 + t^2 = k(k-1)^2 + t^2 + t(2k-1). \tag{6.2}$$

Before proceeding, we should say that the abuse of notation in $C(v,e) = C(k,t)$ should not cause confusion as it will be clear which set of parameters (v,e) *vs.* (k,t) are being used. Also notice that if we were to expand the range of t to $0 \le t \le k$, that is allow $t = k$, then the representation of e in Equation (6.1) is not unique:

$$e = \binom{k}{2} + k = \binom{k+1}{2} + 0.$$

But the value of $C(v,e)$ is the same in either case:

$$C(k,k) = C(k+1,0) = (k+1)k^2.$$

Thus we may take $0 \le t \le k$.

We begin the proofs now. At the beginning of Section 2.5, we showed that $S(v,e) = C(v,e)$ for $e = 0,1,2,3$. Also note that, when m is an integer, $\mathrm{Diff}(v,m) = 0$. We now compare $S(v,e)$ with $C(v,e)$ for $4 \le e < m$. The first task is to show that $S(v,e) > C(v,e)$ for all but a few values of e that are close to m. We start by finding upper and lower bounds on $S(v,e)$ and $C(v,e)$.

Define

$$U(e) = e\left(\sqrt{8e+1} - 1\right) \quad \text{and}$$
$$U(k,t) = \left(\binom{k}{2} + t\right)\left(\sqrt{(2k-1)^2 + 8t} - 1\right).$$

The first lemma shows that $U(e)$ is an upper bound for $C(v,e)$ and leads to an upper bound for $S(v,e)$. The arguments used here to obtain upper and lower bounds are similar to those in [12].

Lemma 6.1. *For* $e \ge 2$,

$$C(v,e) \le U(e) \quad \textit{and}$$
$$S(v,e) \le U(e') + (v-1)(4e - v(v-1)).$$

It is clearly enough to prove the first inequality. The second one is trivially obtained from Equation (1.2) on linking the values of $S(v,e)$ and $C(v,e)$.

Proof. We prove the inequality in each interval $\binom{k}{2} \le e \le \binom{k+1}{2}$ and so fix $k \ge 2$ for now. We make yet another change of variables to remove the square root in the above expression of $U(k,t)$.

Set $t(x) = (x^2 - (2k-1)^2)/8$, for $2k-1 \le x \le 2k+1$. Then

$$U(k,t(x)) - C(k,t(x)) = \frac{1}{64}(x-(2k-1))((2k+1)-x)\left(x^2 + 4(k-2)(k+x) - 1\right),$$

which is easily seen to be positive for all $k \ge 2$ and all $2k-1 \le x \le 2k+1$. □

Now define

$$L(e) = e\left(\sqrt{8e+1} - 1.5\right) \quad \text{and}$$
$$L(k,t) = \left(\binom{k}{2} + t\right)\left(\sqrt{(2k-1)^2 + 8t} - 1.5\right).$$

The next lemma shows that $L(e)$ is a lower bound for $C(v,e)$ and leads to a lower bound for $S(v,e)$.

Lemma 6.2. *For* $e \geq 3$

$$C(v,e) \geq L(e) \quad \textit{and}$$
$$S(v,e) \geq L(e') + (v-1)(4e - v(v-1)).$$

Proof. As above, set $t(x) = (x^2 - (2k-1)^2)/8$, $2k-1 \leq x \leq 2k+1$, and $x(k,b) = 2k+b$, $-1 \leq b \leq 1$. Then

$$C(k,t(x(k,b))) - L(k,t(x(k,b))) = \frac{1}{64}b^2(b+4k-4)^2 + \frac{1}{32}(4k-7)\left(b + \frac{2(k+1)}{4k-7}\right)^2 + \frac{4k(22k-49)+13}{64(4k-7)}$$

This expression is easily seen to be positive for $k \geq 3$. □

We are now ready to prove that $S(v,e) > C(v,e)$ for $0 \leq e \leq m$ for all but a few small values and some values close to m.

Lemma 6.3. *Assume* $v \geq 5$. *For* $4 \leq e < v$ *we have* $C(v,e) < S(v,e)$.

Proof. As we showed above in Lemma 6.1, $e\left(\sqrt{8e+1}-1\right)$ is an upper bound on $C(v,e)$ for all $1 \leq e \leq \binom{v}{2}$. Furthermore, it is easy to see that for $1 \leq e < v$ we have $S(v,e) = e^2 + e$. In fact, the quasi-star graph is optimal for $1 \leq e < v$. The rest is then straightforward. For $4 \leq e$, we have

$$0 < (e-3)(e-1) = (e+2)^2 - (8e+1).$$

Taking square roots and rearranging some terms proves the result. □

Lemma 6.4. *Assume* $v \geq 5$. *For* $v \leq e \leq m - 0.55v$ *we have*

$$S(v,e) > C(v,e).$$

Proof. Assume that $0 \leq e \leq m$. Let $e = m - d$ with $0 \leq d \leq m$. By Lemmas 6.1 and 6.2, we have

$$\begin{aligned} S(v,e) - C(v,e) &\geq L(e') + (v-1)(4e - v(v-1)) - U(e) \\ &= (m+d)\sqrt{8(m+d)+1} - (m-d)\sqrt{8(m-d)+1} \\ &\quad - \left(\left(4(v-1) + \frac{5}{2}\right)d + \frac{m}{2}\right). \end{aligned}$$

We focus on the first two terms. Set

$$h(d) = (m+d)\sqrt{8(d+m)+1} - (m-d)\sqrt{8(m-d)+1}.$$

By considering a real variable d, it is easy to see that $h'(d) > 0$, $h^{(2)}(0) = 0$, and $h^{(3)}(d) < 0$ on the interval in question. Thus $h(d)$ is concave down on $0 \leq d \leq m$. We are comparing $h(d)$ with the line $(4(v-1) + 5/2)d + m/2$ on the interval $[0.55v, m-v]$. The concavity of $h(d)$ allows us to check only the end points. For $d = m - v$, we need to check

$$\frac{1}{2}v\left((v-3)\sqrt{4v^2 - 12v + 1} - 2\sqrt{8v+1}\right) > \frac{1}{4}v\left(4v^2 - 21v + 7\right).$$

It is messy, but elementary to verify this inequality for $v \geq 9$.

For $d = 0.55v$ we need to check

$$\left(\frac{v^2}{4} + 0.3v\right)\sqrt{2v^2 + 2.4v + 1} - \left(\frac{v^2}{4} - 0.8v\right)\sqrt{2v^2 - 6.4v + 1} > v(2.325v - 0.95).$$

This inequality holds for $v \geq 29$. This time the calculations are rather messier, yet still elementary. For $4 < v \leq 28$, we verify the result directly by calculation. □

In Section 2, we introduced the value $e_0 = \binom{k_0}{2}$.
We now define

$$e_1 = \binom{k_0 - 1}{2},$$
$$f_1 = \binom{v}{2} - \binom{k_0 + 1}{2},$$
$$f_2 = \binom{v}{2} - \binom{k_0 + 2}{2}.$$

The next lemma shows that those binomial coefficients and their complements are all we need to consider.

Lemma 6.5. $e_1, f_2 < m - 0.55v$.

As a consequence, $S(v,e) > C(v,e)$ for all $4 \le e \le \max\{e_1, f_2\}$. We need a small result on the relationship between k_0 and v first. The upper bound will be used later in this section.

Lemma 6.6. $\frac{\sqrt{2}}{2}\left(v - \frac{1}{2}\right) - \frac{1}{2} < k_0 < \frac{\sqrt{2}}{2} v + \frac{1}{2}$.

Proof. Since $\binom{k_0}{2} \le m \le \binom{k_0+1}{2} - \frac{1}{2}$, we have

$$2k_0(k_0 - 1) \le v^2 - v \le 2k_0(k_0 + 1) - 2.$$

Thus

$$2(k_0 - 1/2)^2 \le (v - 1/2)^2 + 1/4 \le 2(k_0 + 1/2)^2 - 2.$$

That is,

$$\frac{\sqrt{2}}{2}\sqrt{\left(v - \frac{1}{2}\right)^2 + \frac{9}{4}} - \frac{1}{2} \le k_0 \le \frac{\sqrt{2}}{2}\sqrt{\left(v - \frac{1}{2}\right)^2 + \frac{1}{4}} + \frac{1}{2}.$$

The result follows using $(v - 1/2)^2 < (v - 1/2)^2 + 9/4$ and $(v - 1/2)^2 + 1/4 < v^2$. $\square$

Proof of Lemma 6.5. Note that $e_1 = e_0 - (k_0 - 1) \le m - (k_0 - 1)$ and $f_2 = f_1 - (k_0 + 1) < m - (k_0 + 1) < m - (k_0 - 1)$. Hence, it is enough to show that $0.55v < (k_0 - 1)$. This follows from the previous lemma for $v \ge 12$. For $5 \le v \le 11$, we verify the statement by direct calculation. $\square$

Next, we show that the difference function

$$\mathrm{Diff}(v,e) = S(v,e) - C(v,e)$$

is piecewise linear on the intervals induced by the binomial coefficients $\binom{k}{2}$, $2 \le k \le v$, and their complements $\binom{v}{2} - \binom{k}{2}$, $2 \le k \le v$. In Section 2.7, we show a specific example.

Lemma 6.7. *As a function of e, the function $\mathrm{Diff}(v,e)$ is linear on the interval*

$$\max\left\{\binom{k}{2}, \binom{v}{2} - \binom{l+1}{2}\right\} \le e \le \min\left\{\binom{k+1}{2}, \binom{v}{2} - \binom{l}{2}\right\}.$$

The line has the slope

$$-\frac{1}{4}\left(1 - (2k-3)^2 - (2l-3)^2 + (2v-5)^2\right). \tag{6.3}$$

Proof. If $e = \binom{k+1}{2} - j$ with $1 \leq j \leq k$, then it is easy to see from Equation (1.1) that

$$C(v, e+1) - C(v, e) = 2e - 2\binom{k}{2} + 2k = 2e - k(k-3).$$

Using Equations (1.2) and (6.2), we find that, if $e' = \binom{l}{2} + c$, $1 \leq c \leq l$, then

$$S(v, e+1) - S(v, e) = 2e + 4(v-1) - 2\binom{v}{2} - 2l + 2\binom{l}{2} + 2.$$

We now have

$$\begin{aligned}
&(S(v, e+1) - C(v, e+1)) - (S(v, e) - C(v, e)) \\
&= k(k-3) + l(l-3) - (v-1)(v-4) + 2 \\
&= -\frac{1}{4}\left(1 - (2k-3)^2 - (2l-3)^2 + (2v-5)^2\right).
\end{aligned}$$

The conclusion follows. □

Since we already know that $\mathrm{Diff}(v, e) > 0$ for $4 \leq e \leq \max\{e_1, f_2\}$, and $\mathrm{Diff}(v, e) = 0$ for $e = 0, 1, 2, 3,$ or m, we can now focus on the interval $I_1 = (\max\{e_1, f_2\}, m)$. The only binomial coefficients or complements of binomial coefficients that can fall into this interval are e_0 and f_1.

There are two possible arrangements we need to consider

(1) $e_1, f_2 < e_0 \leq f_1 < m$ and
(2) $f_1 < e_0 \leq m$.

The next result deals with the first arrangement.

Lemma 6.8. *If $e_0 \leq f_1 < m$, then $q_0(v) > 0$. Furthermore, $S(v, e) \geq C(v, e)$ for $0 \leq e \leq m$ with equality if and only if $e = 0, 1, 2, 3,$ or m; or $e = e_0$ and $(2v-3)^2 - 2(2k_0 - 1)^2 = -1, 7$.*

Proof. $e_0 \leq f_1$ implies $e_0 \leq m - k_0/2$. By Lemma 6.6, we conclude that for $v > 12$,

$$\begin{aligned}
4q_0(v) &= 1 - 2(2k_0 - 3)^2 + (2v-5)^2 \\
&= 16(m - e_0) - 16(v - k_0) + 8 \\
&\geq 24k_0 - 16v + 8 \\
&\geq 24\left(\sqrt{2}/2(v - 1/2) - 1/2\right) - 16v + 8 \\
&= \left(12\sqrt{2} - 16\right)v - \left(6\sqrt{2} + 4\right) \\
&> 0.
\end{aligned}$$

For smaller values, we verify that $q_0(v) > 0$ by direct calculation.

If $e = f_1$ in Equation (6.2), and since $e_0 \leq f_1 < m$, then $k = k_0$ and $t = f_1 - \binom{k_0}{2}$. Using Equation (1.2), $\mathrm{Diff}(v, f_1) = (m - f_1)q_0(v) > 0$. Similarly, since $f_2 < e_0 \leq f_1$, then for $e = e_0'$ in Equation (6.2), we have $k = k_0 + 1$ and $t = e_0' - \binom{k_0+1}{2}$. Again, using Equation (1.2),

$$\begin{aligned}
\mathrm{Diff}(v, e_0) &= (v^2 - 3v - 2k_0^2 + 2k_0 + 2)(v^2 - 3v - 2k_0^2 + 2k_0)/4 \\
&= ((2v-3)^2 - 2(2k_0-1)^2 + 1)((2v-3)^2 - 2(2k_0-1)^2 - 7)/64. \qquad (6.4)
\end{aligned}$$

Notice that $\mathrm{Diff}(v, e_0) \geq 0$ since both factors in (6.4) are even and differ by 2. Equality occurs if and only if $(2v-3)^2 - 2(2k_0-1)^2 = -1$ or 7. Finally, observe that $\mathrm{Diff}(v, e_1) > 0$ and $\mathrm{Diff}(v, f_2) > 0$ by Lemmas 6.4 and 6.5, and e_1 and f_2 are both less than f_1. Hence $\mathrm{Diff}(v, e) \geq 0$ for $e \in [\max\{e_1, f_2\}, m]$ follows from the piecewise linearity of $\mathrm{Diff}(v, e)$. The rest follows from Lemma 6.4. □

Now we deal with the case $f_1 < e_0$. There are three cases depending on the sign of $q_0(v)$. All these cases require the following fact. If $f_1 < e_0$, then for $e_0 \le e \le m$ in Equation (6.2), $k = k_0$ and $t = e - \binom{k_0}{2}$. Since $f_1 < e \le m$, for e' in Equation (6.2), $k = k_0$ and $t = e' - \binom{k_0}{2}$. Thus, using Equation (1.2),

$$\mathrm{Diff}(v, e) = (m - e)q_0(v) \tag{6.5}$$

whenever $f_1 < e_0 \le e \le m$. This automatically gives the sign of $\mathrm{Diff}(v, e)$ near m. By the piecewise linearity of $\mathrm{Diff}(v, e)$ given by Lemma 6.7, the only thing remaining is to investigate the sign of $\mathrm{Diff}(v, f_1)$.

Lemma 6.9. *Assume $f_1 < e_0$ and $q_0(v) > 0$. Then $S(v, e) \ge C(v, e)$ for $0 \le e \le m$, with equality if and only if $e = 0, 1, 2, 3, m$.*

Proof. First, note that $e_1 \le f_1 < e_0 < m$, since $e_1 > f_1$ occurs only if $m = e_0$ and thus $q_0(v) = 2 - 4(v - k_0) < 0$. For $e_0 \le e < m$, by Equation (6.5), $\mathrm{Diff}(v, e) = (m - e)q_0(v) > 0$. Furthermore, if $e = f_1$ in Equation (6.2), then $k = k_0 - 1$ and $t = f_1 - \binom{k_0-1}{2}$. Thus, by Equation (1.2),

$$\mathrm{Diff}(v, f_1) = (-4k_0^4 + 16k_0^3 + 4v^2k_0^2 - 12vk_0^2 - 8v^2k_0 + 4k_0 - v^4 + 6v^3 + v^2 - 6v)/4,$$

and

$$\mathrm{Diff}(v, f_1) - \mathrm{Diff}(v, e_0) = (2k_0^2 - v^2 + v)(-2 - 2k_0^2 + 8k_0 + v^2 - 5v)/2.$$

The first factor is positive because $f_1 < e_0$. The second factor is positive for $v \ge 15$. This follows from the fact that $v < \sqrt{2}k_0 + (\sqrt{2}+1)/2$ by Lemma 6.6, and $-2-2k_0^2+2k_0+v^2-v \ge 0$ because $e_1 \le f_1$. For $v \ge 15$,

$$\begin{aligned} -2 - 2k_0^2 + 8k_0 + v^2 - 5v &= (-2 - 2k_0^2 + 2k_0 + v^2 - v) + 2(3k_0 - 2v) \\ &\ge 2(3k_0 - 2v) \\ &> 0. \end{aligned}$$

Since $\mathrm{Diff}(v, e_0) > 0$, then $\mathrm{Diff}(v, f_1) > 0$ for $v \ge 15$. The only case left to verify satisfying the conditions of this lemma is $v = 14$. In this case, $f_1 = 36$ and $\mathrm{Diff}(14, 36) = 30 > 0$. ☐

The previous two lemmas provide a proof of part 1 of Theorem 2.8.

Lemma 6.10. *Assume $f_1 < e_0$ and $q_0(v) = 0$. Then $S(v, e) \ge C(v, e)$ for $0 \le e \le m$ with equality if and only if $e = 0, 1, 2, 3, e_0, e_0 + 1, \ldots, m$.*

Proof. For $e_0 \le e \le m$, by Equation (6.5), $\mathrm{Diff}(v, e) = (m - e)q_0(v) = 0$. As in the previous lemma, for $v \ge 15$

$$\mathrm{Diff}(v, f_1) - \mathrm{Diff}(v, e_0) = (2k_0^2 - v^2 + v)(-2 - 2k_0^2 + 8k_0 + v^2 - 5v)/2 > 0$$

and thus $\mathrm{Diff}(v, f_1) > 0$. The only value of $v < 15$ satisfying the conditions of this lemma is $v = 6$ with $f_1 = 5$, and $\mathrm{Diff}(6, 5) = 4 > 0$. ☐

The previous lemma provides a proof for part 3 of Theorem 2.8.

Lemma 6.11. *Assume $f_1 < e_0 \le m$ and $q_0(v) < 0$. Then $S(v, e) \ge C(v, e)$ for $0 \le e \le m - R_0$ and $S(v, e) \le C(v, e)$ for $m - R_0 \le e \le m$ with equality if and only if $e = 0, 1, 2, 3, m - R_0, m$.*

Proof. For $e_0 \le e < m$, by Equation (6.5), $\mathrm{Diff}(v, e) = (m - e)q_0(v) < 0$. This time it is possible that $f_1 < e_1$. In this case, by Lemmas 6.4 and 6.5, we know that $\mathrm{Diff}(v, f_1), \mathrm{Diff}(v, e_1) > 0$. Also, $m = e_0$ and $R_0 = 0$, implying $\mathrm{Diff}(v, e_0) = 0$ and $\mathrm{Diff}(v, e) > 0$ for all $e_1 \le e < e_0 = m - R_0 = m$.

If $e_1 \le f_1$, by Lemma 6.7, $\mathrm{Diff}(v,e)$ is linear as a function of e on the interval $[f_1, e_0]$. Let $-q_1(v)$ be the slope of this line. Since $e_1 < f_1 < e_0 \le m$, then $k = k_0$ and $l = k_0$ in Lemma 6.7. Thus $q_1(v) = (-1 - 2(2k_0 - 4)^2 + (2v-5)^2)/4 = q_0(v) + 2k_0 - 4$ and $\mathrm{Diff}(v, f_1) = (m - e_0)q_0(v) + (e_0 - f_1)q_1(v)$. The line through the two points $(e_0, \mathrm{Diff}(v, e_0))$ and $(f_1, \mathrm{Diff}(v, f_1))$ crosses the x-axis at $m - R_0$. We now show that $f_1 < m - R_0 < e_0$, which in turn proves that $\mathrm{Diff}(v, f_1) > 0$.

We have

$$m - R_0 = e_0 + (m - e_0)\frac{q_0(v)}{q_1(v)} \tag{6.6}$$

$$= m - (m - e_0)\frac{2k_0 - 4}{q_1(v)}. \tag{6.7}$$

Since $e_0 \le m$ and $v > 4$, then

$$k_0 \le \frac{1}{2} + \sqrt{\binom{v}{2} + \frac{1}{4}} < 2 + \sqrt{\binom{v-2}{2}}, \tag{6.8}$$

which is equivalent to $q_1(v) > 0$. Thus $m - R_0 < e_0$ by Equation (6.6). To prove $f_1 < m - R_0$, according to Equation (6.7), we need to show

$$(m - e_0)\frac{2k_0 - 4}{q_1(v)} < \binom{k_0 + 1}{2} - m.$$

After multiplying by $q_1(v)$, the last inequality becomes

$$\left(m - \binom{k_0+1}{2} + \frac{k_0}{2}\right)(2k_0 - 4) < \left(\binom{k_0+1}{2} - m\right)\left((v-2)(v-3) - 2(k_0-2)^2\right),$$

which is equivalent to

$$\frac{k_0}{2}(2k_0 - 4) < \left(\binom{k_0+1}{2} - m\right)\left((v-2)(v-3) - 2(k_0-2)(k_0-3)\right).$$

Since $f_1 < e_0$ we know that $k_0/2 < \binom{k_0+1}{2} - m$. Also, Inequality (6.8) is equivalent to $2k_0 - 4 < (v-2)(v-3) - 2(k_0-2)(k_0-3)$. Multiplying these two inequalities yields the result. $\square$

The previous lemma provides a proof of part 2 of Theorem 2.8.

The expression for $m - R_0$ is sometimes an integer. Those $v < 1000$ for which $m - R_0$ is an integer are 14, 17, 21, 120, 224, 309, 376, 393, 428, 461, 529, 648, 697, and 801.

In the remaining part of this section, we prove Corollaries 2.9 and 2.10.

Lemma 6.12. *Assume that $v > 4$ and $q_0(v) < 0$. Then $R_0 \le \alpha v$ where $\alpha = 1 - \sqrt{2}/2$.*

Proof. We show that $R_0 \le \alpha v$ for $v > 4$. Recall that

$$R_0 = \frac{(m - e_0)(2k_0 - 4)}{q_1(v, k_0)}.$$

Thus we need to show

$$\alpha v q_1(v, k_0) - (m - e_0)(2k_0 - 4) > 0.$$

Define the function $h(x) = \alpha v q_1(v, x) - \left(m - \binom{x}{2}\right)(2x - 4)$. The interval for x is limited by the condition that $q_0(v) < 0$ which implies that

$$i_1 := \frac{\sqrt{2}}{2}v - \frac{5\sqrt{2}}{4} + \frac{3}{2} < k_0.$$

Furthermore, since $e_0 \le m$, we know that $i_2 := (\sqrt{2}/2)v + 1/2 > k_0$. We show that $h(x)$ is increasing on $I := [i_1, i_2]$. Note that, since $v > 4$,

$$h''(x) = -6 - \left(4 - 2\sqrt{2}\right) v + 6x > 0$$

for $x \in I$. Hence $h(x)$ is concave up on I. Furthermore

$$h'(i_1) = \left(3 - 2\sqrt{2}\right) v^2 + \left(-10 + \frac{11}{2}\sqrt{2}\right) v - \frac{15}{4}\sqrt{2} + \frac{73}{8} > 0$$

for $v \ge 11$, and hence

$$\begin{aligned} h(x) &> h(i_1) \\ &= \frac{1}{32}\left(\left(-72 + 58\sqrt{2}\right) v + 23\left(6 - 5\sqrt{2}\right)\right) > 0 \end{aligned}$$

for $v \ge 11$. The only values of v greater than 4 and smaller than 11 for which $q_0(v) < 0$ are $v = 7, 10$. The result is easily verified in those two cases. □

How good is the bound $R_0 \le \alpha v$? Suppose there is a parameter β such that $R_0 \le \beta v$ with $\beta < \alpha$. Assume that $q_0(v) = -2$. There are infinitely many values of v for which this is true (see Section 9). In all of those cases $k_0(v) = 1/2\sqrt{(9 + (2v-5)^2)/2} + 3/2$. We have the following

$$(\beta v q_1(v) - (m - e_0)(2k_0 - 4))/v^2 \to \sqrt{2}\beta - \sqrt{2} + 1 \ge 0$$

as $v \to \infty$. Thus $\beta \ge \alpha$ and hence α is the greatest number for which the bound on R_0 holds.

Since $S(v, e) \ge C(v, e)$ for all $1 \le e \le m - R_0$, we have proved Corollary 2.9.

To prove Corollary 2.10, we need to investigate the other non-trivial case of equality in Theorem 2.8. It occurs when $e = e_0$ and $(2v - 3)^2 - 2(2k_0 - 1)^2 = -1, 7$. Notice that this implies

$$\begin{aligned} m - e_0 &= \frac{1}{16}\left((2v - 1)^2 - 2(2k_0 - 1)^2 + 1\right) \\ &= \frac{v}{2} \quad \text{or} \quad \frac{v - 1}{2}. \end{aligned}$$

There are infinitely many values of v such that $(2v - 3)^2 - 2(2k_0 - 1)^2 = -1$, and infinitely many values of v such that $(2v - 3)^2 - 2(2k_0 - 1)^2 = 7$ (see Section 9). Thus the most we can say is that $S(v, e) > C(v, e)$ for all $4 \le e < m - v/2$, and Corollary 2.10 is proved.

7. PROOF OF COROLLARY 2.11

Recall that for each v, $k_0(v) = k_0$ is a unique positive integer such that

$$\binom{k_0}{2} \le \frac{1}{2}\binom{v}{2} < \binom{k_0 + 1}{2}.$$

It follows that

$$\text{(7.1)} \qquad -1 \le (2v - 1)^2 - 2(2k_0 - 1)^2, \quad \text{and} \quad (2v - 1)^2 - 2(2k_0 + 1)^2 \le -17.$$

Let us restrict our attention to the parts of the hyperbolas

$$H_{\text{low}} : (2v - 1)^2 - 2(2k - 1)^2 = -1, \quad H_{\text{high}} : (2v - 1)^2 - 2(2k + 1)^2 = -17$$

that occupy the first quadrant as shown in Figure 7.1. Then each lattice point, (v, k_0) is in the closed region bounded by H_{low} below and H_{high} above. Furthermore, the sign of the quadratic form $(2v - 5)^2 - 2(2k - 3)^2 + 1$ determines whether the quasi-star graph is optimal in $\mathcal{G}(v, e)$ for all $0 \le e \le m$. By Theorem 2.8, if $(2v - 5)^2 - 2(2k - 3)^2 + 1 \ge 0$, then $S(v, e) \ge C(v, e)$

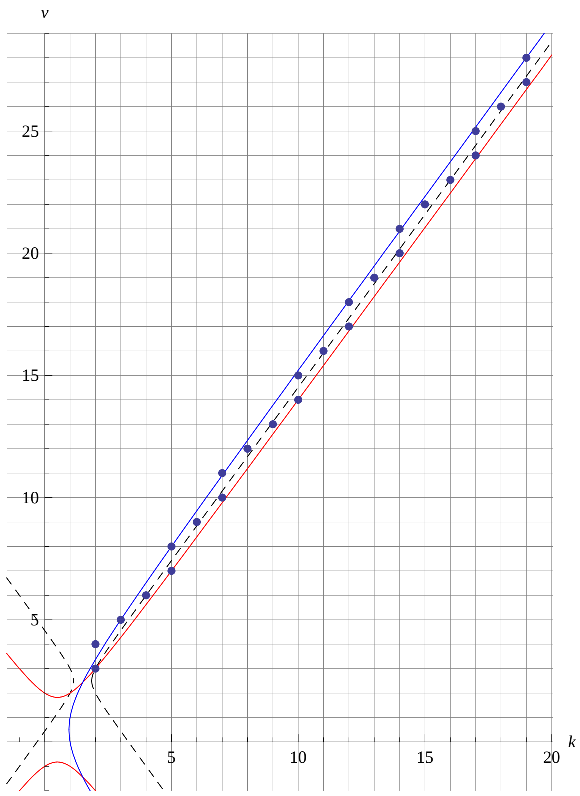


Figure 7.1: Hyperbolas $(2v-1)^2-2(2k-1)^2=-1$, $(2v-1)^2-2(2k+1)^2=-17$, $(2v-5)^2-2(2k-3)^2=-1$

(and the quasi-star graph is optimal) for $0 \le e \le m$. Thus, if the lattice point (v,k) is between H_{high} and the hyperbola

$$H : (2v-5)^2 - 2(2k-3)^2 = -1,$$

then the quasi-star graph is optimal in $\mathcal{G}(v,e)$ for all $0 \le e \le m$. But if the lattice point (v,k_0) is between H and H_{low}, then there exists a value of e in the interval $4 \le e \le m$ such that the quasi-complete graph is optimal and the quasi-star graph is not optimal. Of course, if the lattice point (v,k_0) is on H, then the quasi-star graph is optimal for all $0 \le e \le m$ but the quasi-complete graph is also optimal for $\binom{k_0}{2} \le e \le m$. Apparently, the density limit

$$\lim_{v\to\infty} \frac{n(v)}{v}$$

from Corollary 2.11 depends on the density of lattice points (v,k) in the region between H_{high} and H.

We can give a heuristic argument to suggest that the limit is $2-\sqrt{2}$. The asymptotes for the three hyperbolas are

$$A : v - \frac{5}{2} = \sqrt{2}\left(k - \frac{3}{2}\right),$$

$$A_{\text{low}} : v - \frac{1}{2} = \sqrt{2}\left(k - \frac{1}{2}\right),$$

$$A_{\text{high}} : v - \frac{1}{2} = \sqrt{2}\left(k + \frac{1}{2}\right),$$

and intersect the k-axis at

$$k = \frac{6-5\sqrt{2}}{4},$$
$$k_{\text{low}} = \frac{2-\sqrt{2}}{4},$$
$$k_{\text{high}} = \frac{-2-\sqrt{2}}{4}.$$

The horizontal distance between A_{high} and A_{low} is

$$k_{\text{low}} - k_{\text{high}} = 1$$

and the horizontal distance between A_{high} and A is

$$k - k_{\text{high}} = 2 - \sqrt{2}.$$

To make the plausibility argument rigorous, we need a theorem of Weyl [15, Satz 13, page 334], [9, page 92]:

For any real number r, let $\langle r\rangle$ denote the fractional part of r. That is, $\langle r\rangle$ is the unique number in the half-open interval $[0,1)$ such that $r - \langle r\rangle$ is an integer. Now let β be an irrational real number. Then the sequence $\langle n\beta\rangle$, $n = 1,2,3,\ldots$, is uniformly distributed on the interval $[0,1)$.

In our problem, the point (v,k_0) is between the hyperbolas H_{low} and H_{high} and, with few exceptions, (v,k_0) is also between the asymptotes A_{low} and A_{high}. To be precise, suppose that (v,k_0) satisfies Inequalities (7.1). We need an easy fact from number theory here. Namely that $y^2 - 2x^2 \equiv -1 \pmod 8$ for all odd integers x, y. Thus

$$2(2k_0-1)^2 < (2v-1)^2 < 2(2k_0+1)^2,$$

unless $(2v-1)^2 - 2(2k_0-1)^2 = -1$ (these are the exceptions). But for all other points (v,k_0) we have

$$\sqrt{2}\left(k_0 - \frac{1}{2}\right) < v - \frac{1}{2} < \sqrt{2}\left(k_0 + \frac{1}{2}\right).$$

Thus

$$0 < \frac{\sqrt{2}}{2}\left(v - \frac{1}{2}\right) + \frac{1}{2} - k_0 < 1$$

and so

$$\frac{\sqrt{2}}{2}\left(v - \frac{1}{2}\right) + \frac{1}{2} - k_0 = \left\langle \frac{\sqrt{2}}{2}\left(v - \frac{1}{2}\right) + \frac{1}{2}\right\rangle.$$

Next, consider the condition $q_0(v,k_0) \geq 0$, which is equivalent to

$$(2v-5)^2 - 2(2k_0-3)^2 \geq -1.$$

Unless $(2v-5)^2 - 2(2k_0-3)^2 = -1$, $q_0(v,k_0) \geq 0$ is equivalent to

$$\left\langle \frac{\sqrt{2}}{2}\left(v - \frac{1}{2}\right) + \frac{1}{2}\right\rangle > \sqrt{2} - 1.$$

To summarize, if (v,k_0) does not satisfy either of these Pell's Equations

$$(2v-1)^2 - 2(2k_0-1)^2 = -1, \quad (2v-5)^2 - 2(2k_0-3)^2 = -1,$$

then $q_0(v,k_0) \geq 0$ if and only if

$$\sqrt{2} - 1 < \left\langle \frac{\sqrt{2}}{2}\left(v - \frac{1}{2}\right) + \frac{1}{2}\right\rangle < 1.$$

From Weyl's Theorem, we know that the fractional part in the above inequality is uniformly distributed in the interval $[0, 1)$. Since the density of the values of v for which (v, k_0) is a solution to one of the Pell's Equations above is zero, then $\lim_{v\to\infty} n(v)/v = 1 - (\sqrt{2} - 1) = 2 - \sqrt{2}$. The proof of Corollary 2.11 is complete.

8. PROOFS OF THEOREMS 2.5, 2.6, AND 2.7

We first prove Theorem 2.5. If $\pi_{1.2}$ and $\pi_{1.3}$ are optimal partitions, then according to Theorem 2.4, $j' = 3$, $k' \geq j' + 2 = 5$, and so $v \geq 2k' - j' \geq 7$. In addition, the quasi-star partition is optimal, that is, $S(v, e) \geq C(v, e)$. Thus by Corollary 2.10, either $e \geq \binom{v}{2} - 3$ or $e \leq m + v/2 = \binom{v}{2}/2 + v/2$. If $e \geq \binom{v}{2} - 3$ and since $j' = 3$, then $k' \leq 3$, contradicting $k' \geq 5$. Thus $e \leq \frac{1}{2}\binom{v}{2} + \frac{v}{2}$. Since $2k' - 3 \leq v$ and $e = \binom{v}{2} - \binom{k'+1}{2} + 3$, then

$$3 + \frac{1}{2}\binom{v}{2} \leq \binom{k'+1}{2} + \frac{v}{2} \leq \binom{(v+3)/2 + 1}{2} + \frac{v}{2}.$$

Therefore $7 \leq v \leq 13$. In this range of v, the only pairs (v, e) that satisfy all the required inequalities are $(v, e) = (7, 9)$ or $(9, 18)$.

Using the relation between a graph and its complement described below, Equation (1.2), we conclude that if $\pi_{2.2}$ and $\pi_{2.3}$ are optimal partitions, then $(v, e) = (7, 12)$ or $(9, 18)$.

As a consequence, we see that the pair $(9, 18)$ is the only candidate to have six different optimal partitions. This in fact is the case. The six graphs and partitions are depicted in Figure 8.1. We note here that Byer [3] also observed that the pair $(v, e) = (9, 18)$ yields six different optimal graphs. Another consequence is that the pairs $(7, 9)$ and $(7, 12)$ are the only candidates to have five different optimal partitions. For the pair $(7, 9)$, the partitions $\pi_{1.1}, \pi_{1.2}, \pi_{1.3}, \pi_{2.1}$ and $\pi_{2.2}$ all exist and are optimal. However, $\pi_{1.3} = \pi_{2.2}$. Thus the pair $(7, 9)$ only has four distinct optimal partitions. Similarly, for the pair $(7, 12)$ the partitions $\pi_{1.1}, \pi_{1.2}, \pi_{2.1}, \pi_{2.2}$ and $\pi_{2.3}$ all exist and are optimal, but $\pi_{1.2} = \pi_{2.3}$. So there are no pairs with five optimal partitions, and thus all other pairs have at most four optimal partitions. Moreover, $S(v, e) = C(v, e)$ is a necessary condition to have more than two optimal partitions, since any pair other than $(7, 9)$ or $(7, 12)$ must satisfy that both $\pi_{1.1}$ and $\pi_{2.1}$ are optimal. The proof of Theorem 2.5 is complete.

In Theorem 2.6, $e = \binom{k}{2} = \binom{k+1}{2} - k$ and thus $j = k$. Note that, if $v > 5$ and k satisfy Equation (2.1), then $k + 2 < v < 2k - 1$, and so $k \geq 4$. Thus $e = \binom{v}{2} - \binom{k+2}{2} + (2k + 2 - v)$ with $4 \leq 2k + 2 - v \leq k + 1$, that is, $k' = k + 1$ and $j' = 2k + 2 - v$. Hence, $\pi_{1.1} = (v - 1, v - 2, \ldots, k + 2, 2k + 2 - v)$ and $\pi_{2.1} = (k - 1, ..., 1)$ (which always exist) are different because $2k + 2 - v \geq 4 > 1$. The partition $\pi_{1.2} = (v - 2, ..., k)$ exists because $k \leq v - 3$, and it is different to $\pi_{2.1}$ because $k \geq 4 > 1$ ($\pi_{1.2} \neq \pi_{1.1}$ by definition). Finally, the partitions $\pi_{1.3}, \pi_{2.2}$, and $\pi_{2.3}$ do not exist because $j' = 2k + 2 - v \geq 4, k + 1 > k - 1 = 2k - j - 1$, and $j = k \geq 4$, respectively. Theorem 2.6 is proved.

Now, if v and k satisfy Equation (2.2), then $\frac{1}{2}\binom{v}{2} = \binom{k+1}{2} - 3$. Moreover, since $v > 9$, then $k > (v+3)/2$. Hence, in Theorem 2.7, $e = m = \frac{1}{2}\binom{v}{2} = \binom{k+1}{2} - 3 = \binom{v}{2} - \binom{k+1}{2} + 3$, with $k \geq 3$ because $v > 1$. That is, $k = k'$ and $j = j' = 3$. Thus $\pi_{1.1} = (v - 1, v - 2, ..., k + 1, 3), \pi_{1.3} = (v - 1, v - 2, ..., k + 1, 2, 1), \pi_{2.1} = (k - 1, k - 2, ..., 4, 3)$, and $\pi_{2.3} = (k - 1, k - 2, ..., 4, 2, 1)$ all exist and are different because $k = v$ does not yield a solution to (2.2). Also $\pi_{1.2}$ and $\pi_{2.2}$ do not exist because $2k - j - 1 = 2k' - j' - 1 = 2k - 4 > v - 1$. Theorem 2.7 is proved.

9. PELL'S EQUATION

Pell's Equation

$$V^2 - 2J^2 = P, \tag{9.1}$$

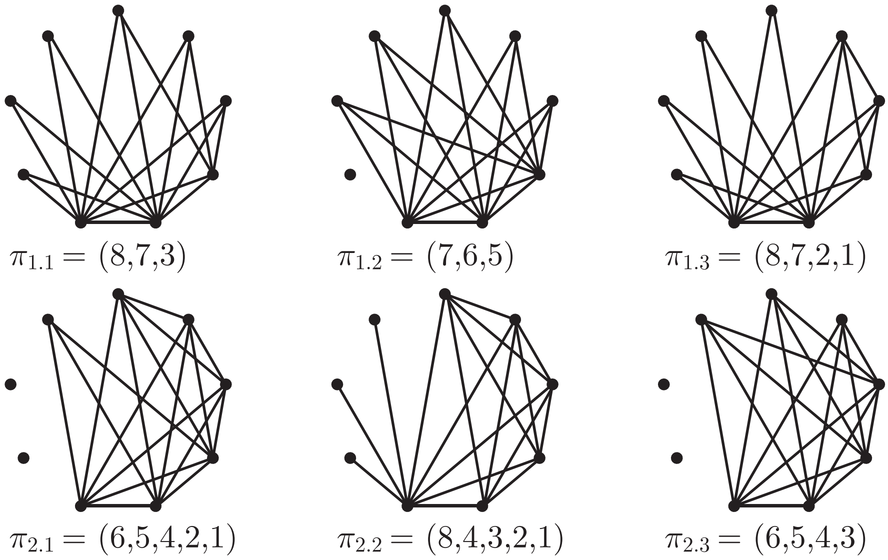


Figure 8.1: $(v,e) = (9,18)$ *is the only pair with six different optimal graphs. For all graphs,* $P_2(\mathrm{Th}(\pi_{i.j})) = \max(v,e) = C(v,e) = S(v,e) = 192$

where $P \equiv -1 \pmod 8$, appears several times in this paper. For example, a condition for the equality of $S(v,e)$ and $C(v,e)$ in Theorem 2.8 involves the Pell's Equation $(2v-5)^2 - 2(2k_0 - 3)^2 = -1$. And in Theorem 2.7, we have $(2v-1)^2 - 2(2k+1)^2 = -49$. There are infinitely many solutions to each of these equations. In each instance, V and J in Equation (9.1) are positive odd integers and $P \equiv -1 \pmod 8$. The following lemma describes the solutions to the fundamental Pell's Equation.

Lemma 9.1 ([7])**.** *All positive integral solutions of*

$$V^2 - 2J^2 = -1 \tag{9.2}$$

are given by

$$V + J\sqrt{2} = (1+\sqrt{2})(3+2\sqrt{2})^n,$$

where n is a nonnegative integer.

It follows from the lemma that if (V,J) is a solution to Equation (9.2), then both V and J are odd. We list the first several solutions to Equation (9.2):

V	1	7	41	239	1393
J	1	5	29	169	985

Now let us consider the equation $(2v-3)^2 - 2(2k-1)^2 = -1$ from Theorem 2.6. Since all of the positive solutions (V,J) consist of odd integers, the pair (v,k) defined by

$$v = \frac{V+3}{2}, \qquad k = \frac{J+1}{2}$$

are integers and satisfy Equation (2.1). Thus there is an infinite family of values for $v > 5$ such that there are exactly 3 optimal partitions in Dis(v,e), where $e = \binom{k}{2}$. The following is a list of the first three values of v, k, e in this family:

v	22	121	698
k	15	85	493
e	105	3570	121278

Next, consider Equation (2.2) from Theorem 2.7 and the corresponding Pell's Equation:

$$V^2 - 2J^2 = -49.$$

A simple argument using the norm function, $N(V + J\sqrt{2}) = V^2 - 2J^2$ shows that all positive integral solutions are given by

$$V + J\sqrt{2} = (1 + 5\sqrt{2})(3 + 2\sqrt{2})^n, \quad (7 + 7\sqrt{2})(3 + 2\sqrt{2})^n, \quad \text{or} \quad (17 + 13\sqrt{2})(3 + 2\sqrt{2})^n,$$

where n is a nonnegative integer. The first several solutions are

V	1	7	17	23	49	103	137
J	5	7	13	17	35	73	97

Thus the pairs (v, k), defined by

$$v = \frac{V+1}{2}, \qquad k = \frac{J-1}{2}$$

satisfy Equation (2.2). The first three members, (v, k, e) of this infinite family of partitions Dis(v, e) with $v > 9$, $e = \binom{v}{2}/2$, and exactly 4 optimal partitions are:

v	12	25	52	69
k	8	17	36	48
e	33	150	663	1173

The Pell's Equation

$$4q_0(v) = (2v-5)^2 - 2(2k_0 - 3)^2 + 1 = 0 \tag{9.3}$$

appears in Theorem 2.8. Here again there are infinitely many solutions to the equation $(2v - 5)^2 - 2(2k-3)^2 = -1$ starting with:

v	2	2	3	3	6	23	122
k	1	2	1	2	4	16	86

The proof of Corollary 2.9 requires infinitely many solutions to the equation $q_0(v) = -2$, which is equivalent to the Pell's Equation

$$(2v-5)^2 - 2(2k-3)^2 = -9. \tag{9.4}$$

All its positive integral solutions are given by

$$v = \frac{V+5}{2}, \qquad k = \frac{J+3}{2}, \qquad V + J\sqrt{2} = (3 + 3\sqrt{2})(3 + 2\sqrt{2})^n,$$

where n is a nonnegative integer. The first several solutions are

v	3	12	63	360	2091
k	2	8	44	254	1478

The proof of Corollary 2.10 requires infinitely many solutions to the Pell's Equation

$$(2v-3)^2 - 2(2k-1)^2 = 7, \tag{9.5}$$

and infinitely many solutions to the Pell's Equation

$$(2v-3)^2 - 2(2k-1)^2 = -1. \tag{9.6}$$

All positive integral solutions to (9.5) are given by

$$v = \frac{V+3}{2}, \qquad k = \frac{J+1}{2}, \qquad V + J\sqrt{2} = (3+\sqrt{2})(3+2\sqrt{2})^n, \qquad (5+3\sqrt{2})(3+2\sqrt{2})^n,$$

where n is a nonnegative integer. The first several solutions are

v	3	4	8	15	39	80
k	1	2	5	10	27	56

We have shown that Equation (9.6) has infinitely many solutions, as it is the same equation that appears in Theorem 2.6. However, in Corollary 2.10, k must be k_0, the unique integer that satisfies Inequality (1.3). This condition is also necessary for Equations (9.3), (9.4), and (9.5). In other words, we must show that for v large enough, every solution (v, k) to one of the Equations (9.3), (9.4), or (9.5), satisfies Inequality (1.3). We do this only for Equation (9.3) as all other cases are similar.

Lemma 9.2. *Let (v, k) be a positive integral solution to Equation (9.3) with $v > 3$. Then (v, k) satisfies Inequality (1.3). That is, $k = k_0$.*

Proof. Suppose that (v, k) is a solution to Equation (9.3) with $v > 3$. Then $k < v < 2k$. Inequality (1.3) consists of two parts, the first of which is

$$\binom{k}{2} \leq \frac{1}{2}\binom{v}{2}.$$

To prove this part, we compute

$$\begin{aligned}\frac{1}{2}\binom{v}{2} - \binom{k}{2} &= \frac{1}{2}\binom{v}{2} - \binom{k}{2} - \left((2v-5)^2 - 2(2k-3)^2 + 1\right)/16 \\ &= (v-k) - \frac{1}{2} > 0.\end{aligned}$$

The second part of Inequality (1.3) is

$$\frac{1}{2}\binom{v}{2} \leq \binom{k+1}{2}.$$

This time, we have

$$\begin{aligned}\binom{k+1}{2} - \frac{1}{2}\binom{v}{2} &= \binom{k+1}{2} - \frac{1}{2}\binom{v}{2} + \left((2v-5)^2 - 2(2k-3)^2 + 1\right)/16 \\ &= 2k - v + \frac{1}{2} > 0.\end{aligned}$$

□

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