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Reliable network topologies in a model with node failures

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RELIABLE NETWORK TOPOLOGIES
IN A MODEL WITH NODE FAILURES

by

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Abstract

RELIABLE NETWORK TOPOLOGIES
IN A MODEL WITH NODE FAILURES

by

Olga Salizkiy

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In the study of network reliability, one is interested in the effects of node and line failures on the communication capabilities of a network. The vulnerability of a network may be gauged by whether or not the network remains connected after such failures. Herein we consider a probabilistic model with node failures. In particular, we wish to study network topologies which are optimal in their invulnerability to disconnection in this model.

Let a network with n nodes and e lines be represented by a graph G with n vertices and e edges. Assume that lines never fail. If all the nodes in the network have an equal and independent probability of failure q and if ℓ_i is the number of disconnecting node sets of size i, then the probability that the network represented by G is disconnected due to node failure is given by the *unreliability polynomial*

$$P_n(G,q) = \sum_{i=1}^{n} \ell_i q^i (1-q)^{n-i}.$$

Of interest are network topologies with a fixed cost of n nodes and e lines which minimize the unreliability polynomial. It has been shown that such optimal networks may not exist for certain n and e since different topologies may be optimal for different q. However, for a fixed q, n, and e, an optimal topology can always be found. To that end, we examine the cases with large q.

For sufficiently large q, (n,e)-graphs which minimize the term $\ell_{n-3}q^{n-3}(1-q)^3$ minimize the unreliability polynomial. Such graphs have the maximum number of induced connected subgraphs on 3 vertices. The number of such subgraphs is given by

$$\sum_{i=1}^{n}\binom{d_i}{2} - 2\tau(G)$$

where τ is the number of triangles in G and d_i is the degree of vertex v_i. Graphs which maximize the above expression for a fixed n and e are called *3-optimal.*

There are few known results on 3-optimal graphs. Boesch, Li, Stivaros, and Suffel have found all 3-optimal graphs with n vertices and $n-1 \le e \le 2n-4$ and $n(n-1)/2 - 2n \le e \le n(n-1)/2$ edges. We have found all 3-optimal graphs for the cases $2n-3 \le e \le 3n-10$ and, along with Bloom, Stivaros, and Suffel, we have shown that $K_{n1,n2}$ is 3-optimal.

We have also found several properties of 3-optimal graphs which make them useful topologies for networks. For example, we have shown that 3-optimal graphs have diameter ≤ 3. We have also shown that the distance from a node with maximum degree in the network to any other node is is no more than 2. Several other results pertaining to circuits and cutpoints have been proved.

ACKNOWLEDGEMENTS

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CHAPTER 1

INTRODUCTION TO NETWORK VULNERABILITY AND RELIABILITY

One concern in the construction of networks is choice of topology. In particular, given a fixed cost of n nodes and e lines, one is interested in topologies which are best able to withstand node and line failures. In the study of network vulnerability and reliability, the effects of such failures are examined on the communication capabilities of networks.

A graph serves as a natural model of a communication network, with vertices representing nodes and edges representing communication lines. Two approaches may be taken in the study of component failures in a network: deterministic and probabilistic. In the deterministic approach, one studies graph properties which indicate how much the functioning of a network is disrupted by component failures. In the probabilistic approach, a probability of failure is associated with every node or line and one is interested in the probability that a given network is functional. Frank Boesch [5] initiated the terminology which refers to the deterministic approach as *network vulnerability* and the probabilistic approach as *network* *reliability*. We will use this terminology.

In both network vulnerability and reliability, it is of interest to establish results which lead to the construction of optimal network topologies. This is referred to as the *synthesis problem* [5]. In this chapter, we briefly survey results in network vulnerability, particularly those which have a bearing on network reliability. We then examine two models in network reliability. The first involves line failures and the second involves node failures. It is an instance of the latter model which is the main focus of this paper. We will discuss this case in the remaining chapters and present new results pertaining to it.

1.1 GRAPH THEORY

As mentioned earlier, graphs serve as natural models of network topologies. Therefore, before we begin our discussion of results in network vulnerability and reliability, we need to present some basic concepts in graph theory.

A *graph* G is a pair of sets, G = (V,E), where V is the finite *vertex set* and E is the *edge set*. Each *edge* is defined as an unordered pair of distinct vertices in V, the *endpoints* of the edge. Note that the edges in our graph are not directed. Also, our definition of graph forbids multiple edges between vertices as well as edges between a vertex and itself. A graph G with n vertices and e edges is called an (n,e) graph, G(n,e).

An edge is said to be *incident* to its endpoints. Edges incident to the same vertex are *adjacent*. Vertices that have an edge between them are *adjacent*. The number of edges incident to a vertex v is the *degree* of v. A *pendant edge* is an edge one of whose endpoints has degree 1. The largest degree in a graph G is denoted Δ and the smallest degree in G is denoted δ. A graph is said to be *regular* if all of its vertices have the same degree. The *degree sequence* of a graph with n vertices is a sequence of n integers $\{d_i\}$ with $d_1 \geq d_2 \geq d_3 \geq \ldots \geq d_n$ such that each d_i is the degree of a distinct vertex in V. We write the degree sequence $d_0d_1d_2 \ldots d_n$ with $(d_i)^k$ denoting the occurrence of degree d_i k times. The *complement* of a graph G = (V,E) is the graph $G^c = (V,E^c)$ in which two vertices are adjacent if and only if they are not adjacent in G.

A sequence of n adjacent edges starting at a vertex v_0 and ending at a vertex v_n in which all vertices are distinct is a *path* of *length* n. A path of length at least 2 from v_1 to v_n plus the edge $\{v_1,v_n\}$ is a *circuit* of *length* n. A graph is *connected* if any two of its distinct vertices are connected by a path. A connected graph consists of one *component*; a disconnected graph consists of several connected components. In a connected graph, the *distance* between vertices v_1 and v_2 is the length of a shortest path between them, denoted $d(v_1,v_2)$. The *diameter* of a connected graph is the maximum distance in the graph.

A *subgraph* of $G = (V,E)$ is a graph $H = (V',E')$ in which $V \supseteq V'$ and $E \supseteq E'$ and all endpoints of edges in E' lie in V'. An *induced subgraph* of G is a subgraph of G in which all edges in E with endpoints in V' are in E'. A *spanning subgraph* of G is a subgraph in which $V' = V$.

Let L be a subset of edges of G. Then G-L denotes the subgraph of G obtained by removing the edges in L. If G is connected but G-L is not connected, then L is a *disconnecting edge set*. The size of a smallest disconnecting edge set is the *edge connectivity* of G and is denoted $\lambda(G)$ or simply λ. A single edge whose removal disconnects a graph is a *bridge*.

Similarly, vertices may be removed from G. However, when a vertex is removed from a graph, its incident edges are removed as well. Thus if K is a subset of vertices of G, then G-K denotes the subgraph obtained by removing the vertices in K. If G is connected and G-K is not connected or consists of a single vertex (the *trivial graph*), then K is a *disconnecting vertex set*. The size of a smallest disconnecting vertex set is the *vertex connectivity* or simply *connectivity* of G, denoted $\kappa(G)$ or simply κ. A single vertex whose removal disconnects a graph is a *cutpoint*

A *tree* is a connected graph which has no circuits. A tree with n vertices has $e = n-1$ edges. A *spanning tree* of a connected graph G is a subgraph of G which is a tree and contains all of the vertices of G. A graph on n vertices which consists of a path is denoted P_n. A *complete graph* on n vertices, denoted K_n, is a graph in which all vertices are adjacent. The graph K_3 is called a *triangle*. A *bipartite graph* is a graph in which the vertex set V can be partitioned into two subsets, V_1 and V_2, so that all edges lie between vertices in V_1 and V_2. A *complete bipartite graph*, denoted K_{n_1,n_2}, is a bipartite graph in which every one of the n_1 vertices in V_1 is adjacent to every one of the n_2 vertices in V_2. The graph $K_{1,n-1}$ is a *star*. A *regular complete k-partite graph*, denoted $K(m^k)$, is a graph on n = km vertices such that the vertices are partitioned into k parts of m vertices each and each vertex is adjacent to all of the vertices in the remaining k-1 parts.

Two graphs G = (V,E), G' = (V',E') are said to be *isomorphic* if there is a bijective function $\phi: V \to V'$ which preserves adjecency, i.e., vertices v_1 and v_2 are adjacent in G if and only if vertices $\phi(v_1)$ and $\phi(v_2)$ are adjacent in G'. The function ϕ is an *isomorphism*. An *automorphism* is an isomorphism from a graph G onto itself.

A more thorough discussion of the above topics may be found in Harary's text [18] or in any other graph theory text.

1.2 NETWORK VULNERABILITY

Recall that in network vulnerability, we are interested in graph properties which can be used to gauge the effects of node and line failures on the functioning of a network. Of obvious interest is the case in which component failures cause the network to become disconnected or trivial. Clearly the surviving nodes in the network cannot all communicate and so the network is not functional. If there is only one node left, we will consider this case as representing a non-functioning network. The properties of interest here are the connectivity and edge connectivity of the underlying graph.

There exist many other vulnerability criteria. In this section we will discuss primarily results dealing with connectivity and edge connectivity. Other vulnerability measure will be briefly discussed at the end of this section.

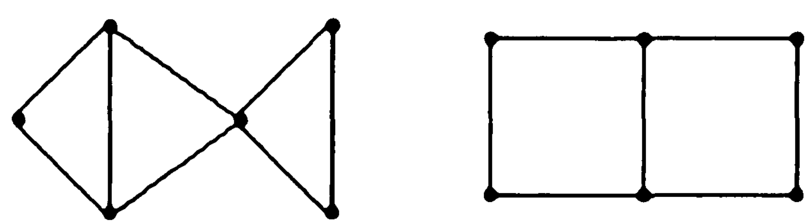
1.2.1 Max-λ and Max-κ Graphs

One of the earliest results on connectivity is due to Harary (1962). His theorem gives an upper bound for the connectivities of a graph with n vertices and e edges. For convenience, we combine his result with a theorem of Whitney (1932). Both theorems may be found in [18]. Recall that $\lceil x \rceil$ denotes the smallest integer not less than x; similarly, $\lfloor x \rfloor$ denotes the greatest integer not greater than x.

<u>Theorem 1.1</u> Let G be a connected graph with n vertices and e edges. Then $\kappa \leq \lambda \leq \delta \leq \lfloor 2e/n \rfloor$.

Clearly a graph can be disconnected by removing the edges incident to a vertex of degree δ. Thus, we have $\lambda \le \delta$. Removing some of the endpoints from the edges in a disconnecting set of size λ also disconnects the graph. At most one endpoint from each edge needs to be removed. This gives us $\kappa \le \lambda$. The last inequality is due to the fact that $\delta \le \frac{1}{n}\sum_{i=1}^{n} d_i = \frac{2e}{n}$, where d_i denotes the degree of vertex v_i. Note that if G is regular of degree δ, the summation equals $n\delta$ and so $2e/n$ is an integer.

From Theorem 1.1, it is easy to see that graphs with $\kappa = \lambda = \delta = \lfloor 2e/n \rfloor$ have the largest connectivities possible for a fixed n and e. Graphs which have $\lambda = \delta = \lfloor 2e/n \rfloor$ are called *max-λ* graphs; graphs which have $\kappa = \lambda = \delta = \lfloor 2e/n \rfloor$ are called *max-κ* graphs. The max-κ property implies the max-λ property. Graph (a) in Figure 1.1 is max-λ only; graph (b) is max-κ and max-λ.



(a) $\lfloor 2e/n \rfloor = \delta = \lambda = 2, \kappa = 1$ (b) $\lfloor 2e/n \rfloor = \delta = \lambda = \kappa = 2$

Figure 1.1. Connectivities in graphs.

Clearly max-λ and max-κ graphs are of interest in network vulnerability. For e = n-1, any tree has $\kappa = \lambda = \delta = \lfloor 2e/n \rfloor = 1$ so all trees are max-κ. For $e \geq n$, there are many graphs which attain the maximum connectivity $\kappa = \lambda = \delta = \lfloor 2e/n \rfloor$. One such family of graphs is the *elementary Harary graphs* .

Using the notation of Boesch in [5], we construct the elementary Harary graph H(n,k) on n vertices as follows: Label the vertices 0, 1, 2, ...n-1. Make each vertex i adjacent to vertices i+1, i+2, ..., $i + \lfloor k/2 \rfloor \pmod{n}$. If k is odd, we have in addition each node i, $0 \leq i \leq \lfloor (n-1)/2 \rfloor$, adjacent to $i + \lfloor n/2 \rfloor$. See Figure 1.2 for examples of H(n,k).

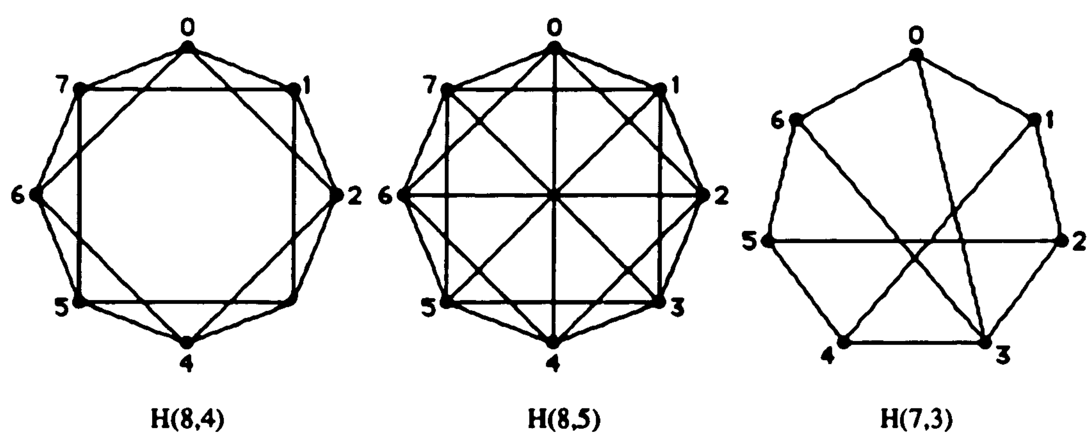
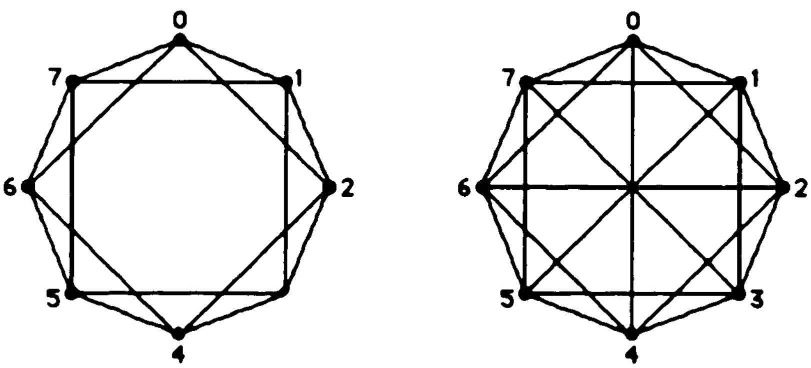


Figure 1.2. Elementary Harary Graphs.

The elementary Harary graphs are max-κ. These graphs also possess several other interesting properties. Unless n and k are both odd, $H(n,k)$ is regular of degree k. If n and k are both odd, $H(n,k)$ has one vertex of degree k+1 and the remaining vertices have degree k. Other properties of elementary Harary graphs of importance to vulnerability will be discussed later.

In [2], the authors give a simple method for constructing max-κ graphs for any n and e, $e \geq n$, based on elementary Harary graphs. Let $2e = an+b$ so that a and b are non-negative integers and $0 \leq b < n$. Construct the elementary Harary graph $H(n,a)$. This graph will have $\kappa = \lambda = \delta = a = \lfloor 2e/n \rfloor$ and $\lceil na/2 \rceil$ edges. Add the remaining edges to the graph at random. It can be shown that this will not alter the connectivity and will use up the desired number of edges.

A class of graphs which are related to Harary graphs and have been extensively studied, particularly with respect to their connectivity properties, are *circulants*. A circulant with n vertices is denoted by $C_n< a_1, a_2, ...a_k >$, where the a_i are *jumps*. The jump sequence is a sequence of integers which satisfies $0 < a_1 < a_2 <...< a_k < (n+1)/2$. The vertices in $C_n< a_1, a_2, ..., a_k >$ are labelled 0,1,2,...n. The vertex i is joined to vertices $i + a_1, i + a_2, ..., i + a_k \pmod{n}$. See Figure 1.3 for examples of circulants. The elementary Harary graph $H(n,k)$ is the circulant $C_n<1,2,3,...k/2>$ when k is even. When n is even and k is odd, $H(n,k)$ is $C_n<1,2,3,...\lfloor k/2 \rfloor, n/2>$. For example, $C_8<1,2,4>$ in Figure 1.3 is $H(8,5)$. $H(n,k)$ for n and k odd is not a circulant. Regular complete bipartite graphs, and more generally, regular complete k-partite graphs are circulants.



$C_8\langle 1,2 \rangle$ $C_8\langle 1,2,4 \rangle$

Figure 1.3. Circulant Graphs.

The circulant $C_n\langle a_1, a_2, \ldots a_k \rangle$ is regular of degree 2k if $a_k \neq n/2$. If $a_k = n/2$, then n must be even and the circulant is regular of degree 2k-1 because of diagonal jumps. Circulants need not be connected. A circulant $C_n\langle a_1, a_2, \ldots a_k \rangle$ is connected if and only if $\gcd(n, a_1, a_2, \ldots, a_k) = 1$, where gcd denotes greatest common divisor. A thorough discussion of circulants can be found in [12].

Circulants are highly symmetric. To be precise, they are *point-symmetric*. A graph G = (V,E) is point-symmetric if for every pair of vertices v_1 and v_2 in V, there is an automorphism $\phi: V \to V$ such that $\phi(v_1) = v_2$. An interesting result due to Turner[24] states that every point-symmetric graph with a prime number of vertices is a circulant. The point-symmetry of circulants is pertinent to connectivity because of a theorem of Mader[21] which we state here as Theorem 1.2:

Theorem 1.2 A connected point-symmetric graph is max-λ.

Thus, since all circulants are point-symmetric, connected circulants are max-λ. In fact, since $C_n<a_1, a_2, \ldots a_k>$ is regular, 2e/n is an integer, and we have $\lambda = \delta = 2e/n$.

As it turns out, circulants need not be max-κ. That is, it is possible for $\kappa < \lambda = \delta$. This is the case with $C_{15}<1,4,5,6>$ which has as one of its disconnecting vertex sets {1,4,6,9,11,14} so that $\delta=8$ but $\kappa=6$. A result due to Boesch and Tindell[12] gives necessary and sufficient conditions for a circulant to have $\kappa < \delta$. We state it here as Theorem 1.3:

Theorem 1.3 The circulant $C_n< a_1, a_2, \ldots a_k >$ has $\kappa < \delta$ if and only if for some proper divisor d of n, the number of distinct positive residues mod d of the numbers $a_1, a_2, \ldots, a_k$, $n-a_k, n-a_{k-1}, \ldots, n-a_1$ is less than the minimum of d-1 and $\delta d/n$.

The observation can be made that there is a relationship between maximum connectivity and symmetry in graphs. There is, for example, Mader's theorem for point-symmetric graphs (Theorem

1.2). Another result deals with *line-symmetric* graphs. A graph G is line-symmetric if for every pair of edges e and e' in G there is an automorphism $\phi: V \rightarrow V'$ which maps e to e'. That is, the endpoints v_1 and v_2 of e will map to the endpoints v_1' and v_2' of e'. The following result is attributed to Watkins[25] and Mader[21]:

Theorem 1.4 A connected line-symmetric graph is max-κ.

In [11], Boesch and Tindell address the issue of connectivity and symmetry in graphs. It turns out that while symmetries imply maximum connectivity values, symmetry is not necessary for maximum connectivity in a graph. In fact, there are *identity graphs* which are maximally connected. An identity graph is a graph whose only automorphism is the *identity mapping*, i.e. the trivial isomorphism $\phi: V \rightarrow V$ such that $\phi(v) = v$.

1.2.2 Super-λ and Super-κ Graphs

Max-λ and max-κ graphs require that the maximum number of edges and vertices be removed, relative to n and e, for the graph to become disconnected. We have not yet considered the structure of the disconnected graph. In a network, it is important to consider the components which arise when λ edges are removed or when κ vertices are removed. For instance, it may be more catastrophic to split a network in half that it is to simply isolate one node in the network from the others. Figure 1.4 illustrates this idea. In (a), the network is split in half. In (b), except for the isolated node, all of the nodes in the disrupted network can still communicate.

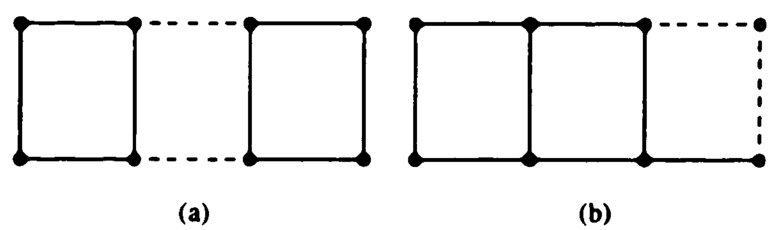


Figure 1.4. Two λ-size disconnecting edge sets.

Super-λ graphs are those max-λ graphs in which the removal of any λ-size disconnecting edge set isolates exactly one vertex. That is, one of the two components which result is the trivial graph and the rest of the graph remains connected. Recall that in a max-λ graph we have $\lambda = \delta$. It is precisely the vertices of degree δ that will become disconnected. Thus, all of the minimum size disconnecting edge sets consist of edges incident to a vertex of degree δ. The graph in Figure 1.4 is not super-λ; the circulants in Figure 1.3 are both super-λ. We will see later that super-λ graphs are important in network reliability.

Bauer et al. show that elementary Harary graphs with $e > n$

edges are super-λ in [2]. However, not all circulants are super-λ. Two exceptions are given in a result of Boesch and Wang[13]. We combine these results in Theorem 1.5:

Theorem 1.5

(a) The elementary Harary graphs with $e > n$ are super-λ.

(b) The only connected circulants which are not super-λ are $C_n< a >$ and $C_{2n}< 2,4,6,\ldots,n-1,n >$ for odd n.

Analogous to super-λ graphs, we have *super-κ* graphs. A super-κ graph is a max-κ graph in which every κ-size disconnecting vertex set isolates a single vertex. Thus all minimum size disconnecting vertex sets consist of the vertices adjacent to a vertex of degree δ. Note that unlike the case with super-λ graphs, more than two components may result when such vertices are removed from the graph. This is the case with $K_{2,3}$. The problem of finding super-κ graphs appears to be more difficult than that of finding super-λ graphs [5]. Smith and Doty[23], Doty[16], and Hakimi and Amin[17] have obtained results on super-κ graphs.

1.2.3 Other Vulnerability Measures

Connectivity properties are of interest in network reliability because they determine when a network can no longer function as a result of line and node failures. However, the loss of lines and nodes in a network can adversely affect its functioning without necessarily causing the network to become disconnected. A parameter which can be used to gauge more subtle effects of line and node removal is the diameter of the underlying graph. It is important to maintain a small diameter in a communication network in order to minimize the distance a message must travel from one point to another in the network. The shorter the distance, the faster it is that messages can travel from source to destination. Thus, graphs with small diameter are desirable, and in particular, those in which the diameter is not greatly increased by vertex and edge removal.

Using the diameter as a measure of network vulnerability, Boesch and Kabell give various results for the *persistence* and *line-persistence* of a graph in [8]. The persistence of a graph is the minimum number of vertices that must be removed from a graph in order to increase the diameter or yield the trivial graph. Analogously, the line-persistence of a graph is the minimum number of edges which must be removed from a graph in order to increase the diameter or yield a graph all of whose components are trivial.

It is unfortunate that graphs with maximum connectivity like Harary graphs and circulants tend to have large diameters. While there are some results on the diameters of graphs with maximum connectivities[5], at least one class of graphs constructed specifically to have a small diameter has proved to have maximum connectivity. In [1], Amar shows that certain *(Δ,d)-graphs* constructed by Memmi and Reillard have $\kappa = \lambda = \delta$. A ($\Delta$,d)-graph is a graph with maximum degree Δ and diameter d. A problem in designing networks is to maximize the number of vertices in a (Δ,d)-graph while minimizing the diameter d for a fixed Δ. We will show later that in a particular instance of our reliability model, optimal graphs always have diameter ≤ 3.

1.3 NETWORK RELIABILITY

In network reliability, nodes and lines in the network are assumed to fail with a given probability. We are interested in the probability that a given network is functional, i.e. that it is connected. Network topologies for which the probability of disconnection is minimum are clearly of interest. We will consider two probabilistic models. In one, the nodes will be reliable but the lines will have an equal probability of failure. In the other, the lines will be reliable but the nodes will have an equal probability of failure. Both models are surveyed by Boesch in [4]. An excellent source on network reliability is the monograph by Colbourn[15].

1.3.1 A Reliability Model With Line Failures

We begin with the model in which lines fail. Let $G(n,e)$ be the graph underlying a network with n nodes and e lines. Assume that nodes never fail and that lines fail with equal and independent probability q. Thus edges will be removed from G. We consider the network functioning if what remains is a connected subgraph of G. This model is hierarchical in that a subset of a non-functioning state is also non-functioning. That is, if edge failures cause the network to become disconnected, additional edge failures will not change the state of the network.

The probability that a given disconnecting set of i edges, and only those i edges, fail in G is given by $q^i(1-q)^{e-i}$. Let m_i be the number of disconnecting edge sets of size i in G. The probability that G is disconnected by the failure of any disconnecting set of i edges is $m_i q^i(1-q)^{e-i}$. Finally, the probability that G is disconnected due to edge failures is given by the *unreliability polynomial*

$$P_e(G,q) = \sum_{i=1}^{e} m_i q^i(1-q)^{e-i}.$$

The subscript e on $P_e(G,q)$ indicates that we are dealing with edge failures. Note that for $i < \lambda$, $m_i = 0$ since λ is the size of the smallest disconnecting edge set. Therefore, we may rewrite the unreliability polynomial as:

$$P_e(G,q) = \sum_{i=\lambda}^{e} m_i q^i (1-q)^{e-i}.$$

If p is the probability that a given edge in G survives, i.e., $p = 1-q$, the *reliability* of G is $R_e(G,p) = 1 - P_e(G,q)$, i.e., the probability that G remains connected in the face of edge failures.

We compute the unreliability polynomial for the graph in Figure 1.5 with $n = 4$, $e = 5$, and edge connectivity $\lambda = 2$. The coefficients m_i are $m_2 = 2$, $m_3 = \binom{5}{3} = 10$, $m_4 = \binom{5}{4} = 5$, $m_5 = \binom{5}{5} = 1$. The resulting unreliability polynomial is

$$P_e(G,q) = 2q^2(1-q)^3 + 10q^3(1-q)^2 + 5q^4(1-q)^1 + 2q^5(1-q)^0.$$

It turns out that the terms in the unreliability polynomial past $i = e-n+1$ depend only on n and e and do not depend on G. In G(n,e), $e-n+1$ is the number of edges which must be removed in order to obtain a spanning tree. If more than $e-n+1$ edges are removed, G will be disconnected regardless of which edges are chosen. Therefore,

$$m_i = \binom{e}{i} \text{ for } i > e-n+1.$$

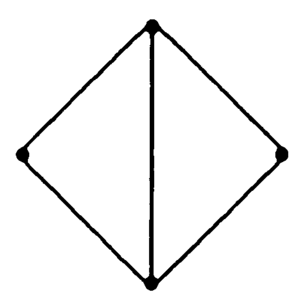


Figure 1.5. G(4,5) with $\lambda = 2$.

We are interested in finding graphs which minimize $P_e(G,q)$ for a fixed n and e. Given two (n,e) graphs, one graph may do better than the other depending on q. However, if q is fixed, then the problem is one of finding an optimal graph among the finitely many (n,e) graphs. We will examine cases with extreme values of q in the remainder of this section.

If q is sufficiently small, then the polynomial $P_e(G,q)$ is dominated by the first term $m_\lambda q^\lambda(1-q)^{e-\lambda}$ since

$$q^i(1-q)^{e-i} > q^{i+1}(1-q)^{e-(i+1)}.$$

To minimize $P_e(G,q)$, we therefore need to minimize $m_\lambda q^\lambda(1-q)^{e-\lambda}$. It turns out that this is accomplished by finding graphs which maximize λ and minimize m_λ. Note that if the $m_{\lambda+k}$ are very large compared with m_λ, q would have to be very small in order to offset the effect of the large $m_{\lambda+k}$. Another problem occurs in determining the order of the minimization and maximization of m_λ and λ, respectively. Both issues are resolved by Bauer et al. in [3]. We present the version of their results given in [4] as Theorems 1.6 and 1.7.

__Theorem 1.6__ Given any two (n,e) graphs G_1 and G_2, there is a $q_0(G_1,G_2)$ such that for all $0 < q < q_0$, if $\{ \lambda(G_1) < \lambda(G_2) \}$ or $\{ [\lambda(G_1) = \lambda(G_2)]$ and $[m_\lambda(G_1) > m_\lambda(G_2)] \}$, then $P_e(G_2,q) < P_e(G_1,q)$.

Thus, in constructing a graph which minimizes $P_e(G,q)$ for fixed n, e, and sufficiently small q, we must first maximize λ and then minimize m_λ. The graph we want must be *λ-optimal.* A λ-optimal graph is an (n,e) graph which has the minimum value of m_λ over all (n,e) max-λ graphs. Theorem 1.7 assures us that any λ-optimal graph will be more reliable than a graph which is not λ-optimal for a fixed n, e, and sufficiently small q.

<u>**Theorem 1.7**</u> Let G_1, G_2, and G be (n,e) graphs such that G_1 and G_2 are λ-optimal but G is not. Then for any $\varepsilon > 0$, there is a q'(n,e) such that for all q, $0 < q < q'(n,e)$

$$P_e(G,q) > P_e(G_1,q) \text{ and } P_e(G,q) > P_e(G_2,q)$$

$$\text{and} \quad \frac{|P_e(G_1,q)-P_e(G_2,q)|}{P_e(G_2,q)} < \varepsilon.$$

We now turn our attention to λ-optimal graphs. First of all, such graphs are max-λ. Recall that this means $\lambda = \delta = \lfloor 2e/n \rfloor$ and that, for example, the elementary Harary graphs and connected circulants have maximum λ. We need to determine which of these graphs minimize m_λ. Recall that in max-λ graphs, the edges incident to a vertex of degree δ comprise a λ-size disconnecting edge set. So, clearly m_λ, the number of disconnecting edge sets of size λ, is greater than or equal to the number of vertices of degree δ. In a super-λ

graph, the only disconnecting edge sets are the edges incident to a vertex of degree δ so m_λ equals the number of vertices of degree δ. This means that the λ-optimal graphs are precisely those super-λ graphs which minimize the number of vertices of degree δ.

Theorem 1.5 states that the elementary Harary graphs are super-λ. More generally, the construction of maximally connected (n,e) graphs based on elementary Harary graphs given in 1.2.1 can be used to construct super-λ graphs. In order to obtain a λ-optimal graph, the edges added to the elementary Harary graph must be placed so that the number of vertices of degree δ is reduced as much as possible[2].

Given n and e, if 2e/n is an integer, then it is possible to construct a regular graph on n vertices of degree 2e/n = a. If such a graph is maximally connected, $\lambda = \delta = 2e/n$. Now m_λ in a maximally connected regular graph is at least n. In super-λ graphs, the number of disconnecting edge sets of size λ is equal to the number of vertices of degree δ. For regular super-λ graphs, this is n. Therefore, all super-λ circulants are λ-optimal. Theorem 1.5, presented earlier, gives a characterization of super-λ circulants.

For large q, a similar argument can be made for minimizing $P_e(G,q)$. The last term in the polynomial which depends on G is $i = e-n+1$ and it is this term which dominates the summation in the case of large q. To minimize $m_i q^i (1-q)^{e-i}$ with $i = e-n+1$, we need to find (n,e) graphs which minimize m_{e-n+1}. In this case we are leaving n-1 edges in G. Therefore, $m_{e-n+1} = \binom{e}{e-n+1} - t(G)$ where t(G) is the number of spanning trees in G. So we need to maximize t(G). A graph G with n vertices and e edges is *t-optimal* if it has the maximum t(G) for all (n,e) graphs. Very few t-optimal graphs have been found. Kelmans and Chelnokov[19], and Shier[22] independently obtained a class of t-optimal graphs constructed by deleting certain edges in complete graphs. Another result is due to Cheng[14]. We combine these results in Theorem 1.8:

Theorem 1.8

Let G^* be the graph obtained by deleting $k \leq n/2$ mutually non-adjacent edges (a *matching*) in K_n. Then, G^* is t-optimal for n vertices and $n(n-1)/2 - k$ edges.

For $n = mk$ and $e = m^2k(k-1)/2$, the unique t-optimal graph is the regular complete k-partite graph $K(m^k)$.

It is of interest to consider graphs which might be *uniformly edge reliable* . That is, for a given n and e, such graphs would minimize $P_e(G,q)$ regardless of q. It it possible that for certain n and e such graphs may not exist. If they do exist, uniformly edge reliable graphs would have to be both λ-optimal and t-optimal. Boesch and Li[9] have found uniformly edge reliable graphs for n vertices and $n-1 \leq e \leq n+2$ edges.

1.3.2 A Reliability Model With Node Failures

We now consider the analogous reliability model with node failures. Let G(n,e) be the graph underlying a network with n nodes and e lines. Assume that lines never fail and that nodes fail with equal and independent probability q. Thus vertices will be removed from G. We consider the network still functioning if we are left with a connected, non-trivial subgraph of G.

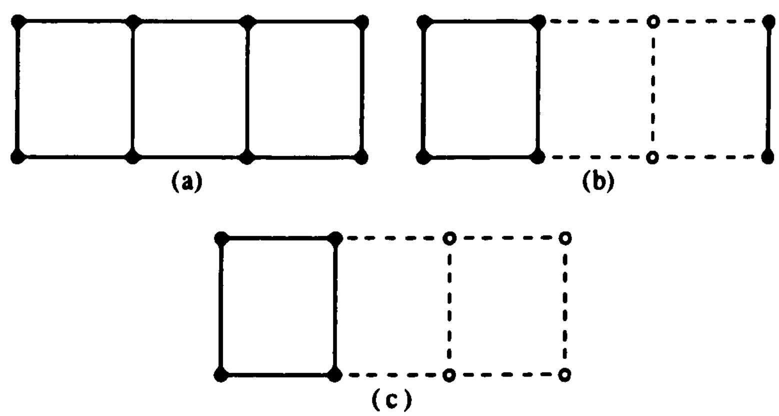


Figure 1.6. A non-hierarchical situation with node failures.

Unlike the edge failure case, this model is not hierarchical in that a superset of a non-functioning state can be functioning. That is, if node failures cause the network to become disconnected, additional node failures may change the non-functioning state of the network to a functioning state. In Figure 1.6, the network in (a) becomes disconnected and hence non-functioning in (b) after two node failures. However, two additional node failures cause the network to become functioning in (c).

The probability that a given disconnecting set of i vertices, and only those i vertices, fail in G is given by $q^i(1-q)^{n-i}$. Let ℓ_i be the number of disconnecting vertex sets of size i in G. The probability that G is disconnected by the failure of any disconnecting set of i vertices is $\ell_i q^i(1-q)^{n-i}$. Finally, the probability that G is disconnected due to vertex failures is given by the *unreliability polynomial*

$$P_n(G,q) = \sum_{i=1}^{n} \ell_i q^i(1-q)^{n-i}.$$

The subscript n on $P_n(G,q)$ indicates that we are dealing with vertex failures. Note that for $i < \kappa$, $\ell_i = 0$ since κ is the size of the smallest disconnecting vertex set. Therefore, we may rewrite the unreliability polynomial as:

$$P_n(G,q) = \sum_{i=\kappa}^{n} \ell_i q^i(1-q)^{n-i}.$$

We compute the unreliability polynomial for the graph in Figure 1.5 with $n = 4$, $e = 5$, and edge connectivity $\kappa = 2$. The coefficients ℓ_i are $\ell_2 = 1$, $\ell_3 = \binom{4}{3} = 4$, $\ell_4 = \binom{4}{4} = 1$. The resulting unreliability polynomial is

$$P_n(G,q) = 1q^2(1-q)^2 + 4q^3(1-q)^1 + 1q^4(1-q)^0.$$

We may also compute the reliability of G, $R_n(G,p) = 1 - P_n(G,q)$, where $p = 1-q$ is the probability that a node survives. Let s_i be the number of connected induced subgraphs in G which have i vertices. Note that $\binom{n}{i} - s_i = \ell_{n-i}$. Then the probability that G remains connected in the face of node failures is

$$R_n(G,p) = \sum_{i=1}^{n} s_i p^i (1-p)^{n-i}.$$

It turns out that the last three terms in the unreliability polynomial depend only on n and e and not on G. When i = n, we have $\ell_n = 1$ since there is only one way to remove all n vertices and clearly, the resulting graph does not represent a functioning network. When $i = n-1$, $\ell_{n-1} = n$ since there are n ways to remove n-1 vertices from G and in each case, the result will be the trivial graph. If we remove n-2 vertices from G, the remaining subgraph containing 2 vertices will be connected in the event that we are left with an edge. Therefore, $\ell_{n-2} = \binom{n}{2} - e$.

Similar to the model with unreliable edges, we are interested in finding graphs which minimize $P_n(G,q)$ for fixed n, e, and q. Here again we can expect to find different optimal (n,e) graphs for different q. We examine the cases when q is small and when q is large.

For small q, the unreliability polynomial $P_n(G,q) = \sum_{i=\kappa}^{n} \ell_i q(1-q)^{n-i}$ is dominated by the first term $\ell_\kappa q^\kappa (1-q)^{n-\kappa}$. Therefore, to minimize the unreliability polynomial in this case, we need to find graphs which minimize $\ell_\kappa q^\kappa(1-q)^{n-\kappa}$ by first making κ as large as possible and then making ℓ_κ as small as possible. This is accomplished by κ-*optimal* graphs. A κ-optimal graph G is an (n,e) graph which has the minimum value of ℓ_κ over all max-κ (n,e) graphs. The following theorem of Boesch in [6] is analogous to Theorem 1.7 and guarantees that any κ-optimal graph solves the problem of minimizing $P_n(G,q)$ for a fixed n, e, and small q.

Theorem 1.9 Let G_1, G_2, and G be (n,e) graphs such that G_1 and G_2 are κ-optimal but G is not. Then for any $\varepsilon > 0$, there is a q'(n,e) such that for all q, $0 < q < q'(n,e)$

$$P_n(G,q) > P_n(G_1,q) \text{ and } P_n(G,q) > P_n(G_2,q)$$

$$\text{and} \quad \frac{|P_n(G_1,q)-P_n(G_2,q)|}{P_n(G_2,q)} < \varepsilon.$$

Unlike the case for λ-optimal graphs, a κ-optimal graph need not be super-κ. This was demonstrated by Hakimi and Amin in [17]. Doty obtains a class of κ-optimal graphs in [16] Another result is due to Boesch and Feltzer[7]:

Theorem 1.10 The complete k-partite graphs, $K(m^k)$, are κ-optimal

For large q, a similar argument can be made for minimizing $P_n(G,q)$. The last term in the polynomial which depends on G is $i = n-3$. Consider the difference $P_n(H,q) - P_n(G,q)$ for two graphs with n vertices and e edges:

$$P_n(H,q) - P_n(G,q) =$$

$$q^n\left(\frac{1-q}{q}\right)^3\left[[\ell_{n-3}(H)-\ell_{n-3}(G)] + \sum_{i=\kappa}^{n-4}[\ell_i(H)-\ell_i(G)]\left(\frac{1-q}{q}\right)^{n-i-3}\right].$$

Suppose $\ell_{n-3}(G) < \ell_{n-3}(H)$. For sufficiently large q, we have

$$\left|\sum_{i=\kappa}^{n-4}[\ell_i(H)-\ell_i(G)]\left(\frac{1-q}{q}\right)^{n-i-3}\right| < \ell_{n-3}(H)-\ell_{n-3}(G).$$

Thus, the difference is positive and G is more reliable than H.

Therefore, to minimize the unreliability polynomial, we need to find (n,e) graphs which minimize ℓ_{n-3}. Recall that s_i is the number of induced connected subgraphs in G having i vertices. So we may write $\ell_{n-i} = \binom{n}{i} - s_i$. Thus, $\ell_{n-3} = \binom{n}{3} - s_3$, where s_3 is the number if connected induced subgraphs in G with 3 vertices. Minimizing ℓ_{n-3} is equivalent to maximizing s_3. Graphs which have the maximum value of s_3 for a given n and e are *3-optimal*. It is the 3-optimal graphs which will be the focus of the remainder of this paper. In Chapter 2, we will discuss the computation of s_3 for a graph and some early results on 3-optimal graphs. In Chapter 3, we will present properties of 3-optimal graphs. Finally, in Chapter 4, we will present our main result on which graphs are 3-optimal.

We conclude this chapter by mentioning that, as in the edge failure model, we are interested in graphs which might be *uniformly vertex reliable*. That is, for a given n and e, such graphs would minimize $P_n(G,q)$ regardless of q. It it possible that for certain n and e such graphs may not exist. If they do exist, uniformly optimally reliable graphs would have to be both κ-optimal and 3-optimal. Stivaros and Suffel have shown that the graphs obtained by removing the edges in a matching from K_n are uniformly optimally reliable. Their results are known to us by private communication. Our results will show cases in which no uniformly vertex reliable graphs exist.

CHAPTER 2

EARLY RESULTS ON 3-OPTIMAL GRAPHS

Recall that s_3 is the number of induced connected subgraphs of G having 3 vertices. We wish to find (n,e) graphs for which s_3 is maximum. Such graphs are said to be 3-optimal. In this chapter, we first discuss the s_3 value of a graph, including methods for its computation. We then present some early results on 3-optimal graphs. These results will serve as motivation for the properties of 3-optimal graphs discussed in Chapter 3.

2.1 COMPUTING $s_3(G)$

The s_3 value of a graph is the number of induced connected subgraphs in G having 3 vertices. There are only two such subgraphs: a path on 3 vertices, P_3, and a triangle, K_3. See Figure 2.1. Let $\tau(G)$ be the number of induced triangles in G. Let $\pi(G)$ be the number of induced paths on 3 vertices in G. Then

$$s_3(G) = \tau(G) + \pi(G).$$

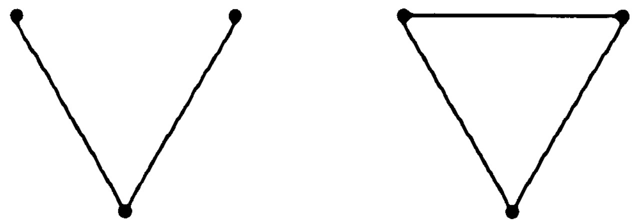


Figure 2.1. Induced connected subgraphs on 3 vertices.

Let d_i be the degree of vertex v_i. The quantity $\binom{d_i}{2}$ counts all possible pairs of adjacent edges at the vertex v_i. If we now sum up all possible $\binom{d_i}{2}$, we will be counting all paths on three vertices once. However, triangles will be counted three times since they will be counted at each of their vertices. So we have

$$\sum_{i=1}^{n}\binom{d_i}{2} = \pi(G) + 3\tau(G).$$

Combining the above expression with $s_3(G) = \tau(G) + \pi(G)$, we get the formula for s_3 obtained by Boesch in [6]:

$$(2.1) \qquad s_3(G) = \pi(G) + \tau(G) = \sum_{i=1}^{n}\binom{d_i}{2} - 2\tau(G).$$

In a 3-optimal graph, s_3 is the maximum possible for the given n and e. The quantities $\sum_{i=1}^{n}\binom{d_i}{2}$ and $\tau(G)$ are clearly dependent. For example, the smallest number of triangles a graph can have is $\tau(G) = 0$. But it turns out that some 3-optimal graphs have triangles, even though for the given n and e it is possible to construct a graph without triangles. On the other hand, if we wish to maximize $\sum_{i=1}^{n} \binom{d_i}{2}$, the graphs we get may not be 3-optimal. Kennedy and Quintas [20] provide a construction for graphs which maximize $\sum_{i=1}^{n} \binom{d_i}{2}$. Essentially one obtains a degree sequence in which Δ is the maximum possible and the number of vertices with degree Δ is maximized. Related results have been obtained by Tindell and Burr and are known to us from private communications.

Another interesting characteristic of the s_3 value of a graph involves the complement of the graph. Let G be an (n,e) graph and let G^c be the complement of G. Any 3 vertices induce a connected subgraph either in G or G^c and the subgraph in G is connected if and only if the corresponding induced subgraph in G^c is disconnected. Thus the following is true:

$$s_3(G) + s_3(G^c) = \binom{n}{3}.$$

So, as $s_3(G)$ increases, $s_3(G^c)$ decreases. As a matter of fact, G is 3-optimal if and only if G^c is *3-worst*.

It turns out, however, that as $\sum_{i=1}^{n} \binom{d_i}{2}$ increases in G, the corresponding summation increases in G^c as well. Indeed,

$\sum_{i=1}^{n}\binom{d_i}{2} = 1/2\sum_{i=1}^{n} d_i^2$ - e increases if and only if $\sum_{i=1}^{n} d_i^2$ increases. In G^c, the degree of vertex v_i is $d^c_i = n - 1 - d_i$. So

$$\sum_{i=1}^{n}\binom{d^c_i}{2} = 1/2\sum_{i=1}^{n}(d^c_i)^2 - 1/2\sum_{i=1}^{n} d^c_i$$

$$= 1/2\sum_{i=1}^{n}(n-1-d_i)^2 - 1/2\sum_{i=1}^{n}(n-1-d_i)$$

$$= 1/2\sum_{i=1}^{n} d_i^2 + n(n-1)^2/2 - n(n-1)/2 + e.$$

Thus we see that in G^c, $\sum_{i=1}^{n}\binom{d^c_i}{2}$ increases if $\sum_{i=1}^{n} d_i^2$ increases, as is the case with G.

An alternative formula for $s_3(G)$ is due to Satyanarayana and was obtained by private communication. Consider the set N(v) of vertices adjacent to v in the graph G. Let IN(v) be the number of edges incident to exactly one endpoint in N(v) in the graph G-v. We first consider the contribution of a vertex v with degree d to $s_3(G)$. Clearly, we need to count all P_3 which have v as a central vertex as well as all triangles which contain v. The number of such paths and triangles is $\binom{d}{2}$. We now need to consider all induced P_3 which have v as an end vertex. Each such path has one edge incident to v and the other incident to exactly one vertex in N(v). Thus the number of such paths is IN(v), the number of edges not incident to v with exactly one endpoint in N(v). We get the following expression for s_3:

$$(2.2) \qquad s_3(G) = s_3(G\text{-}v) + IN(v) + \binom{d}{2}$$

We have obtained a formula for $s_3(G)$ which uses the *point degree of an edge*. The point degree of an edge is the number of vertices adjacent to the endpoints of the edge, excluding the endpoints themselves. We denote the point degree of e as d_e.

For every edge e, we denote the endpoints as u and v. Let d_u and d_v be the degrees of u and v, respectively. Consider the following:

$$\sum_{i=1}^{n} d_i^2 = \sum_{e} (d_u + d_v)$$

$$= \sum_{e} (|N(u)| + |N(v)|)$$

$$= \sum_{e} (|N(u) \cup N(v)| + |N(u) \cap N(v)|)$$

$$= \sum_{e} (|N(u) \cup N(v)|) + 3\tau.$$

Note that if we sum up $|N(u) \cap N(v)|$ over all edges, we will be counting triangles 3 times, once for every edge in the triangle. Now, for an edge e, $|N(u) \cup N(v)| = dp_e + 2$. So we get

$$\sum_{i=1}^{n} d_i^2 = \sum_{e} (|N(u) \cup N(v)|) + 3\tau$$

$$= \sum_{e} (d_e + 2) + 3\tau$$

$$= \sum_{e} d_e + 2e + 3\tau.$$

Using equation (2.1), we get

$$s_3(G) = \sum_{i=1}^{n} \binom{d_i}{2} - 2\tau$$

$$= 1/2\sum_{i=1}^{n} d_i^2 - 1/2\sum_{i=1}^{n} d_i - 2\tau$$

$$= 1/2(\sum_{e} d_e + 2e + 3\tau) - e - 2\tau$$

$$= 1/2(\sum_{e} d_e - \tau).$$

So,

$$s_3(G) = 1/2(\sum_{e} d_e - \tau).$$

2.2 SOME 3-OPTIMAL GRAPHS

We begin with preliminary results which are due to Boesch [6]. One deals with the case $e = n-1$, that is, 3-optimal trees. The other deals with the case $e = n$. We present both results as Theorem 2.1.

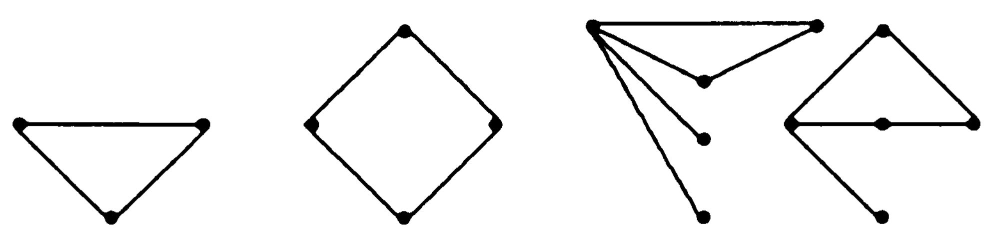


Figure 2.2. The 3-optimal graphs for $e = n \leq 5$.

Theorem 2.1 For $e = n-1$, the star is the unique 3-optimal graph. For $e = n$, $n > 5$, the star plus one edges is the unique 3-optimal graph. For $3 \leq n \leq 5$, the 3-optimal graphs are shown in Figure 2.2.

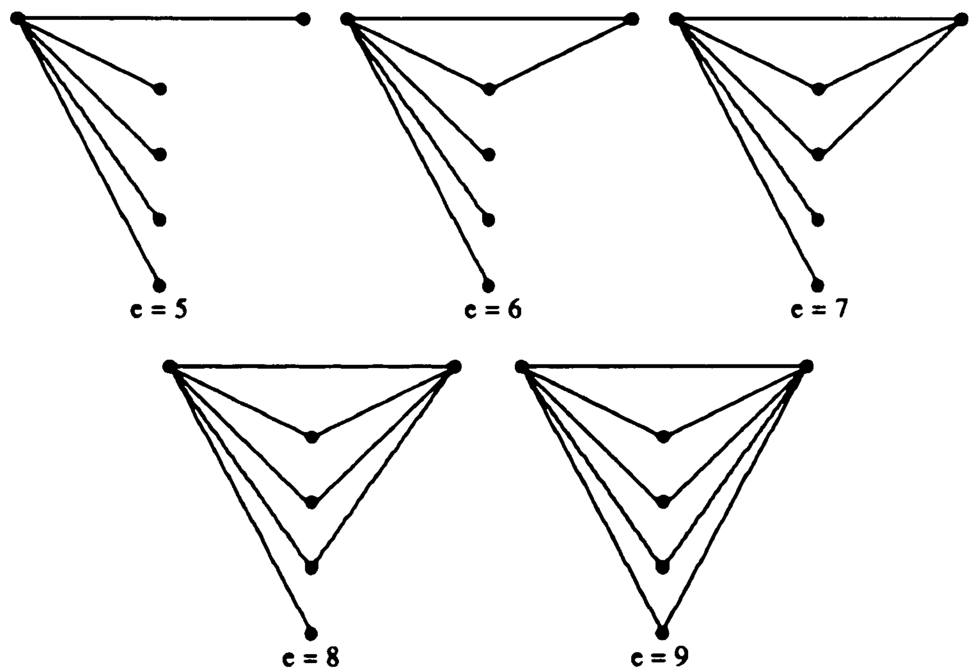


Figure 2.3. The graph $G_A(n,e)$ for $n = 6$.

We introduce some notation. Let $G_A(n,e)$ denote the graph on n vertices and e edges, $n-1 \leq e \leq 2n-3$, obtained by constructing a bipartite graph with vertices v_1 and v_2 in one part, v_1 adjacent to $n-2$ vertices, v_2 adjacent to $e-(n-1)$ vertices, plus an edge between v_1 and v_2. The 3-optimal graphs of Theorem 2.1, with the exception of some of the graphs in Figure 2.2, are in fact $G_A(n,n-1)$ and $G_A(n,n)$. Figure

2.3 shows $G_A(n,e)$ for n = 6 and all possible e.

In [6], Boesch conjectured which graphs would be 3-optimal for e = n+1. We proved his conjecture and also found all 3-optimal graphs for e = n+2. We present these results as Theorems 2.2a and 2.2b.

Theorem 2.2a For n vertices and e = n+1 edges, n > 7, the unique 3-optimal graph is $G_A(n,n+1)$. For smaller n, the 3-optimal graphs are shown in Figure 2.4.

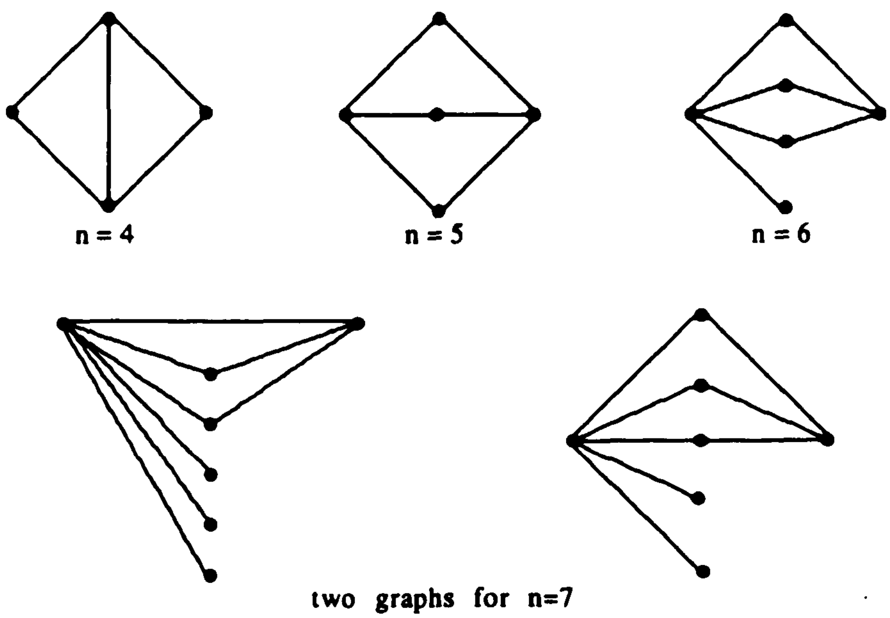


Figure 2.4. The 3-optimal graphs for e = n + 1, n ≤ 7.

Theorem 2.2b For n vertices and e = n+2 edges, n > 9, the unique 3-optimal graph is $G_A(n,n+2)$. The 3-optimal graphs for smaller n are shown in Figure 2.5.

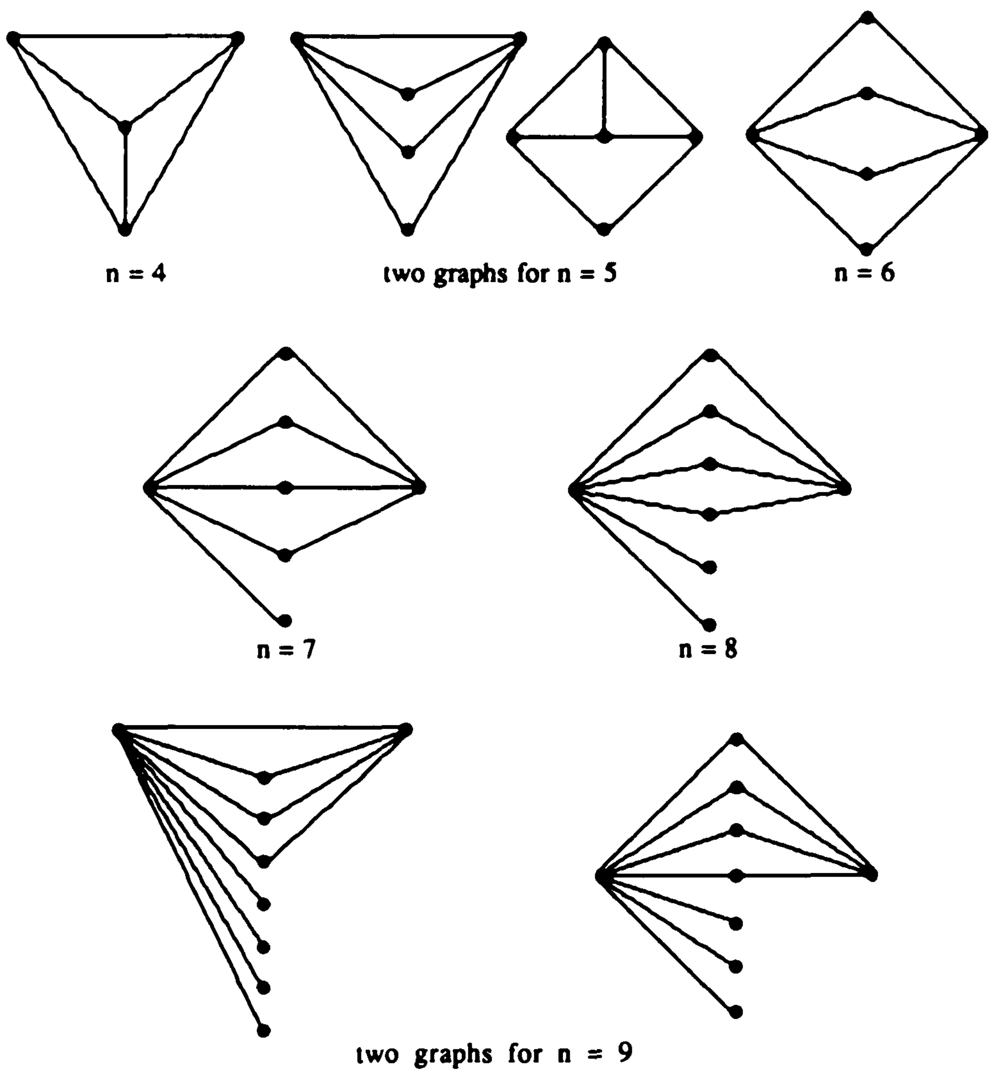
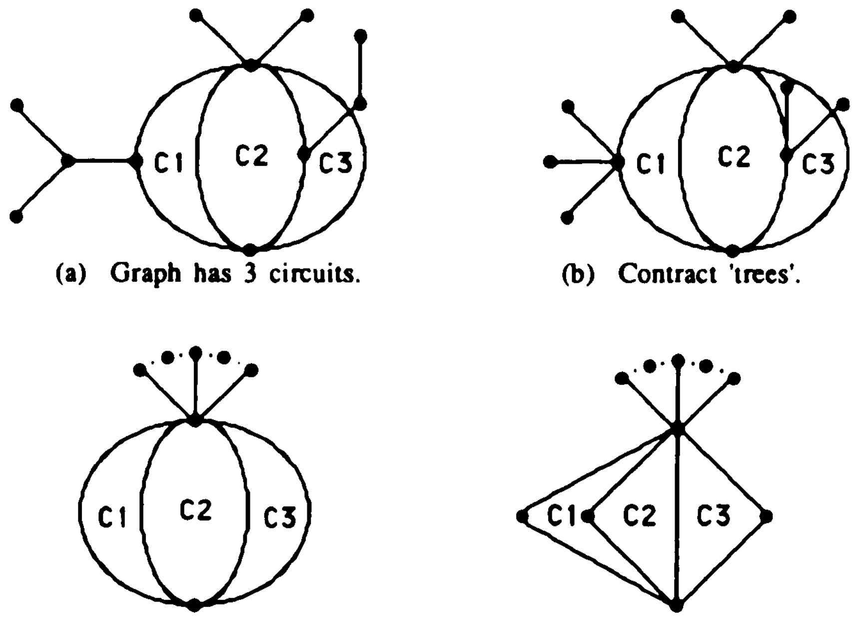


Figure 2.5. The 3-optimal graphs for e = n+2, n ≤ 9.



(a) Graph has 3 circuits.
(b) Contract 'trees'.
(c) Form a single star
(d) Contract circuits.

Figure 2.6. Typical transformations used in Theorem 2.2b.

The proofs of Theorems 2.2a and 2.2b are given in detail in the Appendix. The proofs involve a series of transformations on a given graph which cause an increase in its s_3 value. The transformations terminates either with $G_A(n,e)$ or with a graph which has a smaller s_3 value than $G_A(n,e)$. We briefly outline the proof for one of the cases with $e = n+2$. The steps described can be followed in Figure 2.6.

We begin with the graph in Figure 2.6(a). The graph contains 3 circuits. In addition, there may be "trees" attached at any vertex. First, all the trees are contracted to stars. See Figure 2.6(b). Next, the stars are combined to form one large star. This combined star is centered at a vertex with maximum degree. See Figure 2.6(c).

Finally, edges on circuits are contracted until all remaining non-pendant edges lie on triangles. The removed edges and vertices are added to the star. We are left with $G_A(n,n+2)$ as shown in Figure 2.6(d).

Note that for small n, with $e \leq 2n-4$, whenever $G_A(n,e)$ is not uniquely 3-optimal, a bipartite graph with two vertices in one part is 3-optimal. Observe that one vertex has degree n-2 in that graph. Call such a bipartite graph $G_B(n,e)$. Figure 2.7 shows the graph $G_B(n,e)$ for n = 7 and all possible e.

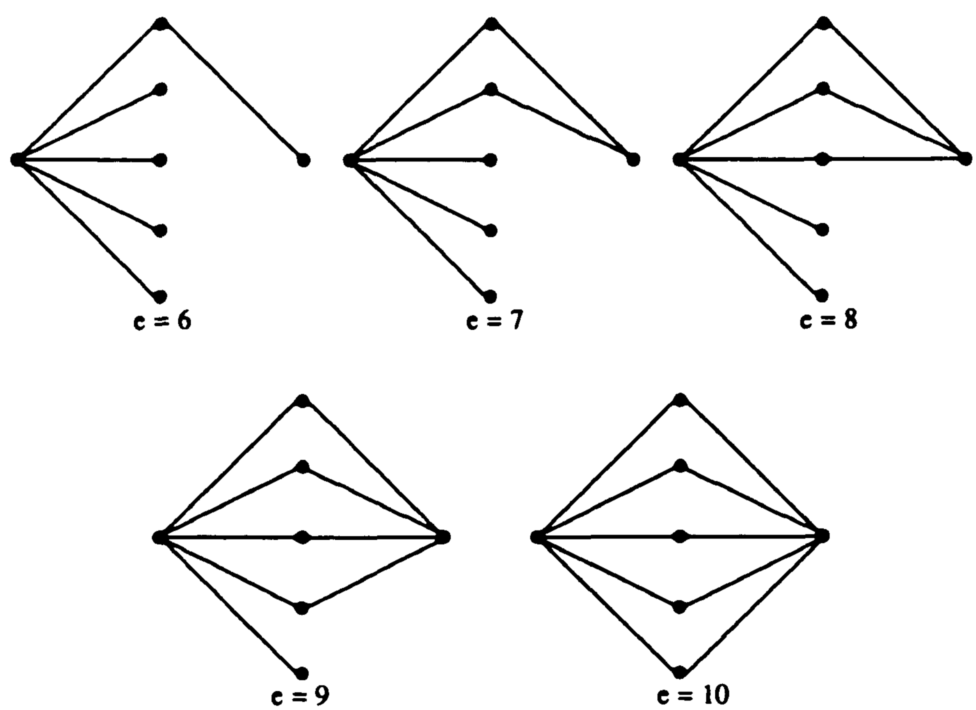


Figure 2.7. The graph $G_B(n,e)$ for n = 7.

It turns out that for the cases with n vertices and $n-1 \leq e \leq 2n-4$ edges, either G_A or G_B or both graphs are 3-optimal. This result was proved by Boesch, Li, Stivaros, and Suffel[10]. We state it here as Theorem 2.3.

Theorem 2.3 Let $e = n+a$ with $-1 \leq a \leq n-4$ so that $n-1 \leq e \leq 2n-4$. Let $n \geq 3$. Then the following are the only 3-optimal graphs:

If $n \geq 5+2a$, G_A is 3-optimal.

If $n \leq 5+2a$, then G_B is 3-optimal.

Note that the graph $G_A(n,e)$ can be viewed as $K_{1,n-1}$ with added edges and that $G_B(n,e)$ can be viewed as $K_{2,n-2}$ with some edges deleted. In a sense, bipartite graphs serve as a kind of basis for the construction of 3-optimal graphs in this case. We will show in Chapter 4 that this pattern is repeated for $2n-3 \leq e \leq 3n-9$.

We now present some results on complete bipartite graphs. Our first result deals with the case of regular and *nearly regular* complete bipartite graphs. The degrees of the vertices in a nearly regular graph differ by at most 1.

Theorem 2.4 $K_{n,n}$ and $K_{n,n-1}$ are 3-optimal.

Proof: Consider the complements of $K_{n,n}$ and $K_{n,n-1}$, namely $K_n \cup K_n$ and $K_n \cup K_{n-1}$, respectively. We will show that $K_n \cup K_n$ and $K_n \cup K_{n-1}$ have the smallest s_3 in their class, thereby proving that $K_{n,n}$ and $K_{n,n-1}$ are 3-optimal.

For any graph with degree sequence {di}, we have

$$s_3(G) \geq 1/3\sum_{i=1}^{n}\binom{d_i}{2}$$

For the graphs $K_n \cup K_n$ and $K_n \cup K_{n-1}$ we have equality in the above expression. Any graph in the same class as $K_n \cup K_n$ or $K_n \cup K_{n-1}$ with a degree sequence $\{d_j\}$ such that

$$\sum_{i=1}^{n}\binom{d_j}{2} > \sum_{i=1}^{n}\binom{d_i}{2}$$

will have a larger s_3 than

$$1/3\sum_{i=1}^{n}\binom{d_i}{2}$$

So, the only graphs to consider are those in the same class as $K_n \cup K_n$ and $K_n \cup K_{n-1}$ for which a smaller $\sum_{i=1}^{n}\binom{d_i}{2}$ is produced. However, since the terms in the degree sequences of $K_n \cup K_n$ and $K_n \cup K_{n-1}$ are as equal as possible, $\sum_{i=1}^{n}\sum\Big($ is as small as possible.

#

These results were generalized by Bermond and were obtained by private communication by us. Bermond showed the following:

Theorem 2.5 Regular and almost regular complete k-partite graphs are 3-optimal.

We end this chapter with a result on complete bipartite graphs. Along with the members of the SITGTG, we have shown that the complete bipartite graphs are 3-optimal. This result was later strengthened to show that these graphs are uniquely 3-optimal in their class. Several elegant proofs have been obtained. We give the original proof.

Theorem 2.6 The graph K_{n_1,n_2} is 3-optimal.

Proof: Assume on the contrary that there is a 3-optimal graph G in the same class as K_{n_1,n_2} and that $s_3(G) > s_3(K_{n_1,n_2})$. We will show that the complement of G is not 3-worst.

Let d_i be the degree of vertex v_i in K_{n_1,n_2}. Since K_{n_1,n_2} has no triangles, $\tau = 0$ and so

$$s_3(K_{n_1,n_2}) = \sum_{i=1}^{n} \binom{d_i}{2}$$

Let $d_i(G)$ be the degree of vertex v_i in G. Then, since $s_3(G) > s_3(K_{n_1,n_2})$,

$$\sum_{i=1}^{n} \binom{d_i(G)}{2} > \sum_{i=1}^{n} \binom{d_i}{2}$$

The complement of K_{n_1,n_2} is $K_{n_1} \cup K_{n_2}$. Let $d^c{}_i$ be the degree of vertex v_i in $K_{n_1} \cup K_{n_2}$. Then

$$s_3(K_{n_1} \cup K_{n_2}) = 1/3 \sum_{i=1}^{n} \binom{d^c{}_i}{2}$$

because all induced three vertex subgraphs of $K_{n_1} \cup K_{n_2}$ are triangles.

Let G^c be the complement of G and let $d_i(G^c)$ be the degree of vertex v_i in G^c. Recall our discussion on the relationship between the degrees in a graph and its complement in the previous section. Then from the previous inequality, we must have

$$1/3 \sum_{i=1}^{n} \binom{d_i(G^c)}{2} > 1/3 \sum_{i=1}^{n} \binom{d^c{}_i}{2}$$

But $s_3(G^c) \geq 1/3 \sum_{i=1}^{n} \binom{d_i(G^c)}{2}$. So it must be that $s_3(G^c) > s_3(K_{n_1} \cup K_{n_2})$.

This means that G^c is not 3-worst.

#

CHAPTER 3

PROPERTIES OF 3-OPTIMAL GRAPHS

In this chapter, we discuss structural properties of 3-optimal graphs. Our motivation for these results are the 3-optimal graphs presented in Chapter 2. The reductions used in obtaining 3-optimal graphs in Theorems 2.2(a) and 2.2(b) were particularly enlightening.

We begin with a result on pendant edges. From the construction in Theorem 2.2, it is clear that all pendant edges should be incident to a vertex of maximum degree. This makes for one vertex with large degree and does not affect the formation of triangles, thereby increasing $s_3(G)$. This notion is formally stated as Theorem 3.1.

<u>Theorem 3.1</u> Let G be a 3-optimal graph. Then any pendant edges in G must be incident to a vertex x which has the maximum degree in G-{pendant edges}.

Proof: Let G' = G-{pendant edges}. Assume on the contrary that G has k pendant edges incident to a vertex x with degree d_x in G' and that there is a vertex v with degree d_v in G' such that

$$d_x < d_v.$$

We perform a transformation on G. Remove the pendant edges at x and attach them at v. The number of vertices and edges in G is unchanged. The number of triangles in the graph is unchanged. The degree of x is reduced by k and the degree of v is increased by k. Since v may also have pendant edges, assume that there are $m \geq 0$ such edges incident to v. The degree of x in G is changed from d_x+k to d_x and the degree of v in G is changed from d_v+m to d_v+m+k. Using the formula (2.1), we obtain the following change in s_3:

$$\left[\binom{d_v+m+k}{2}+\binom{d_x}{2}\right]-\left[\binom{d_v+m}{2}+\binom{d_x+k}{2}\right]$$

$$= [(d_v+m+k)(d_v+m+k-1)/2 + (d_x)(d_x-1)/2]$$

$$- [(d_v+m)(d_v+m-1)/2 + (d_x+k)(d_x+k-1)/2]$$

$$= [\{d_v^2+d_v(2m+2k-1)+(m^2+k^2+2mk-m-k)\}/2 + (d_x^2- d_x)/2]$$

$$- [\{d_v^2+d_v(2m-1)+(m^2-m)\}/2 + \{d_x^2+d_x(2k-1)+(k^2-k)\}/2]$$

$$= \{(2k)(d_v-d_x)+2mk\}/2$$

$$= k(d_v-d_x)+mk > 0 \text{ since } k \geq 1,\ mk \geq 0, \text{ and } d_v > d_x.$$

Thus the transformation increases the value of s_3. Therefore G is not 3-optimal.

#

Our next result deals with cutpoints in 3-optimal graphs. It turns out that the removal of a cutpoint results in a graph with at most one non-trivial component. Otherwise, it is possible to transform the graph and obtain a better s_3.

<u>**Theorem 3.2**</u> Let G be a 3-optimal graph. Then for any vertex v in G, G-v contains at most one non-trivial component.

Proof: Let v be a cutpoint of G and assume on the contrary that two components of G-v, say C1 and C2, each contain edges. In G, there are no edges between the vertices in C1 and the vertices in C2. The vertex v is connected in G to at least one vertex of C1, say v_1. Similarly, v is connected in G to at least one vertex of C2, say v_2. Thus, in G we have the situation depicted in Figure 3.1. It is possible for v to have other neighbors in C1 and C2.

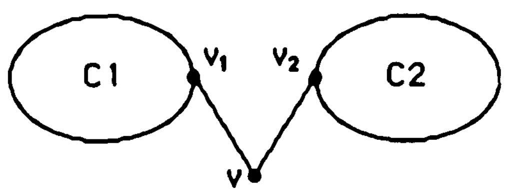


Figure 3.1. The vertex v is a cutpoint in G.

We transform G as follows. Remove the edge between v and v_2 and add a pendant edge at v. Attach C1 and C2 to each other at v_1 and v_2. Call this new vertex u. After the transformation, we are left with the situation depicted in Figure 3.2.

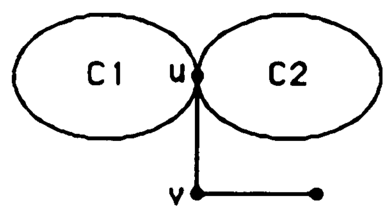


Figure 3.2. Transformed graph of Figure 3.1.

The transformation does not change the number of vertices or edges in G. The number of triangles is unchanged. The degree of v remains unchanged. Letting d_1 and d_2 be the degrees of v_1 and v_2, respectively, in G, then the vertex u has degree d_1+d_2-1. An increase in the s_3 value of G is obtained, contradicting the fact that G is 3-optimal:

$$\binom{u}{2} - \left[\binom{d_1}{2} + \binom{d_2}{2} \right]$$
$$= \binom{d_1+d_2-1}{2} - \left[\binom{d_1}{2} + \binom{d_2}{2} \right]$$
$$= [(d_1+d_2-1)(d_1+d_2-2)/2] - [(d_1)(d_1-1)/2 + (d_2)(d_2-1)/2]$$
$$= [(d_1^2+2d_1d_2-3d_1-3d_2+2)/2] - [d_1^2-d_1)/2 + (d_2^2-d_2)/2]$$
$$= (2d_1d_2-2d_1-2d_2+2)/2$$
$$= d_1d_2 - d_1 - d_2 + 1 > 0 \text{ since } d_1, d_2 \geq 2.$$

Thus the transformation increases the value of s_3. Therefore, G is not 3-optimal.

#

We now present several corollaries of Theorems 3.1 and 3.2.

Corollary 3.3 A 3-optimal graph contains at most one cutpoint. If such a vertex exists, then at least one of its neighbors has degree 1.

Proof: Let G be 3-optimal and let x be a cutpoint of G. Assume on the contrary that all of the neighbors of x have degree ≥ 2. Then the graph G-x will have are least 2 non-trivial components. By Theorem 3.2, this is impossible. So x must have neighbors of degree 1. But by Theorem 3.1, x must have the maximum degree in G-{pendant edges} and all pendant edges in G must be incident to x. So x is the only cutpoint in G and it must have neighbors of degree 1.

#

Corollary 3.4 A 3-optimal graph has a cutpoint if and only if it has a vertex of degree 1.

Proof: By the previous corollary, a cutpoint of G must have a neighbor of degree 1. Conversely, the neighbor of a vertex of degree 1 is a cutpoint in any graph $G \neq K_2$.

#

Corollary 3.5: Let G be a 3-optimal graph. If G contains more than one vertex of maximum degree, then G has no pendant edges and hence no cutpoints.

Proof: Let G 3-optimal graph with pendant edges. By Theorem 3.1, all such edges must be incident to a vertex x with maximum degree in G-{pendant edges}. Hence, if G has $k > 0$ pendant edges, the degree of x is strictly larger than that of any vertex in G.

#

From the above results, we know that G can have at most one cutpoint and that the cutpoint must have incident pendant edges. If the cutpoint is removed, then at most one non-trivial component results. Because of this, if the pendant vertices are removed from G, the resulting graph will have no cutpoints. This is the result in Corollary 3.6.

Corollary 3.6 If G is 3-optimal, then G' = G-{pendant vertices} has no cutpoints.

Proof: Let G be 3-optimal and let G' be defined as above. Assume on the contrary that G' has a cutpoint x. Then x is also a cutpoint of G. By Theorem 3.2, G-x has at most one non-trivial component. This means that G'-x must have at most one non-trivial component. But this is impossible since G' has no pendant vertices.

#

Recall that it is desirable to have a small diameter in networks. Unexpectedly, it turns out that 3-optimal graphs have a very small diameter. That this should be the case is not at all intuitive. We shall now show that the diameter of a 3-optimal graph is at most 3.

Theorem 3.7 Let G be a 3-optimal graph. Then G has diameter ≤ 3.

Proof: Let G be 3-optimal. Assume on the contrary that G has diameter ≥ 4. So there must be two vertices in G, say u and v, such that the distance between u and v is at least 4. Let the degrees of u and v be d_u and d_v, respectively.

•Case 1: Let d_u, $d_v \geq 2$ (i.e. u and v are non-pendant).

Then in G, there is a shortest path of length at least 4 between u and v and v has at least two neighbors. The situation is depicted in Figure 3.3. The marked edges will be removed when we transform the graph.

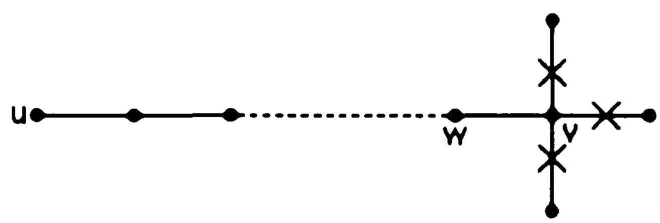


Figure 3.3 A path of length > 3 between u and v.

We now transform the graph. Observe that none of the neighbors of v are adjacent to u since otherwise d(u,v) would be 2. Let w be the neighbor of v on our path. Certainly w has degree > 1. For all other neighbors of v, remove the edge between v and its neighbor and insert an edge between u and that vertex. Figure 3.4 depicts the result of transforming Figure 3.3.

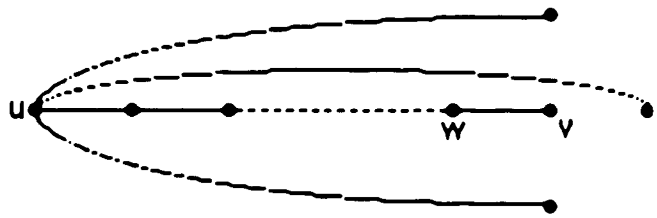


Figure 3.4. Transformed graph of Figure 3.3.

It is clear that the transformed graph is connected since any path utilizing the vertices of the path from u to v and the neighbors of v in the original graph may be transformed into a path utilizing these vertices in the transformed graph. No triangles are formed since a shortest path between u and v must contain at least 4 edges. The degree of u becomes $d_u + d_v - 1$ and the degree of v becomes 1. The value of s_3 increases, contradicting the assumption that G is 3-optimal:

$$\binom{d_u+d_v-1}{2} - [\binom{d_u}{2} + \binom{d_v}{2}]$$
$$= [(d_u+d_v-1)(d_u+d_v-2)/2] - [(d_u)(d_u-1)/2 + (d_v)(d_v-1)/2]$$
$$= [d_u^2+d_v^2+2d_ud_v-3d_u-3d_v+2)/2] - [(d_u^2-d_u)/2 + (d_v^2-d_v)/2]$$
$$= (2d_ud_v - 2d_u - 2d_v + 2)/2$$
$$= d_ud_v - d_u - d_v + 1 > 0 \text{ since } d_u, d_v \geq 2.$$

•Case 2: Note that both u and v cannot have degree 1 since then they would be adjacent to the same vertex by Theorem 3.1 and hence d(u,v) would be 2. Therefore, we are left with the case that exactly one of u, v has degree 1.

Since all vertices with degree 1 must be adjacent to the vertex which has maximum degree in G-{pendant edges}, assume that in this case u is adjacent to x and that x has maximum degree in G-{pendant edges}. Thus, for all vertices y in G, $deg(x) \geq deg(y)+1$ since x has at least one pendant edge. The situation in G is depicted in Figure 3.5.

Figure 3.5 There is a path of length > 3 between u and v.

We now transform the graph. Let w be the neighbor of v on the path between u and v. Remove the edge between v and w and insert an edge between v and x. The number of vertices and edges remain unchanged. If x had degree d_x originally, its degree now is d_x+1. The degree of w, d_w, becomes dw-1. No triangles are formed since the distance between x and v is at least 3. The transformation leads to the configuration in Figure 3.6.

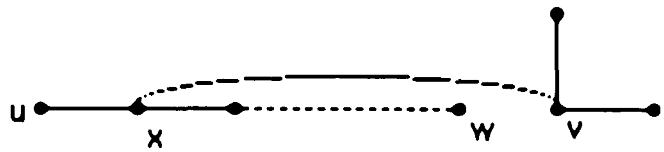


Figure 3.6. Transformed graph of Figure 3.5.

The value of s_3 increases, contradicting the assumption that G is 3-optimal:

$$\binom{d_x+1}{2} + \binom{d_w-1}{2} - [\binom{d_x}{2} + \binom{d_w}{2}]$$

$$= [(d_x+1)(d_x)/2 + (d_w-1)(d_w-2)/2]$$

$$- [(d_x)(d_x-1)/2 + (d_w)(d_w-1)/2]$$

$$= [(d_x^2+d_x)/2 + (d_w^2-3d_w+2)/2] - [(d_x^2-d_x)/2 + (d_w^2-d_w)/2]$$

$$= (2d_x - 2d_w + 2)/2$$

$$= d_x - d_w + 1 > 0 \text{ since } d_x \geq d_w + 1.$$

#

There now present several corollaries to Theorem 3.7. The first states that in 3-optimal graphs, vertices of maximum degree are at most a distance 2 away from other vertices in the graph. In networks, this corresponds to nodes with large degree being easily accessible to other vertices. This is desirable as such nodes may have particular importance commensurate with their degree.

Corollary 3.8 Let G be 3-optimal and let x be a vertex in G with maximum degree. Then for any vertex y, $d(x,y) \leq 2$.

Proof: Let G be 3-optimal and let x be a vertex in G with maximum degree. Assume on the contrary that there is a vertex v in G such that $d(x,v) \geq 3$. Then in G we have the the situation depicted in Figure 3.7.

Figure 3.7. The distance from x to v is > 2.

We transform the graph as follows. Let w be the neighbor of v on a shortest path from u to v. Remove the edge between v and w and insert an edge between v and x. The number of vertices and edges remain unchanged. If x had degree d_x originally, its degree now is d_x+1. The degree of w, d_w, becomes dw-1. No triangles are formed since the distance between x and v is at least 3. We obtain the configuration in Figure 3.8.

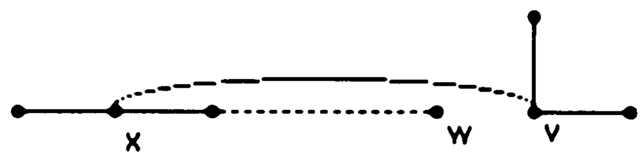


Figure 3.8. Transformed graph of Figure 3.7.

The value of s_3 increases, contradicting the assumption that G is 3-optimal:

$$\binom{d_x+1}{2} + \binom{d_w-1}{2} - [\binom{d_x}{2} + \binom{d_w}{2}]$$
$$= [(d_x+1)(d_x)/2 + (d_w-1)(d_w-2)/2]$$
$$- [(d_x)(d_x-1)/2 + (d_w)(d_w-1)/2]$$
$$= [(d_x^2+d_x)/2 + (d_w^2-3d_w+2)/2] - [(d_x^2-d_x)/2 + (d_w^2-d_w)/2]$$
$$= (2d_x - 2d_w + 2)/2$$
$$= d_x - d_w + 1 > 0 \text{ since } d_x \geq d_w + 1.$$

#

It turns out that in 3-optimal graphs, the vertices of maximum degree are in the *center* of the graph. Vertices in the center of a graph have the smallest maximum distance to all other vertices in the graph. Corollary 3.9 formalizes this notion.

<u>Corollary 3.9</u> Let G be 3-optimal and let x be a vertex with

maximum degree. Then x is in the center of G.

Proof: Let G be 3-optimal and let x be a vertex with maximum degree. By Corollary 3.8, d(x,y) = 1 or 2 for all vertices y in G. If d(x,y) = 1 for all vertices y in G, then x has degree n-1 and is clearly in the center of G. Otherwise d(x,y) = 2 for some vertex y. Thus deg(x) < n-1. In this case there can be no vertex v such that d(v,y) = 1 for all vertices y since then deg(v) = n-1 > deg(x). Therefore again x is in the center.

#

There are several properties concerning circuits in 3-optimal graphs. Li showed that every non-pendant edge in a 3-optimal graph must lie on a circuit of length 3 or a circuit of length 4. We obtained his result by private communication. The next result indicates that such a tight structure is centered about the vertices of maximum degree in 3-optimal graphs.

Theorem 3.10 Let G be a 3-optimal graph with vertex x having maximum degree in G. Then every non-pendant vertex y in G lies on a circuit of length 3 or a circuit of length 4 with x.

Proof: Let G be 3-optimal and let x be as described above. Assume on the contrary that there is a non-pendant vertex y which does not lie on a circuit of length 3 or 4 with x.

•<u>Case 1</u>: Let a shortest circuit containing both x and y have length ≥ 5.

By Corollary 3.8, d(x,y) ≤ 2. Therefore, the smallest circuit containing both x and y must have one of the configurations in Figure 3.9. We call the vertex adjacent to x on the circuit z. Note that in (b), y = z.

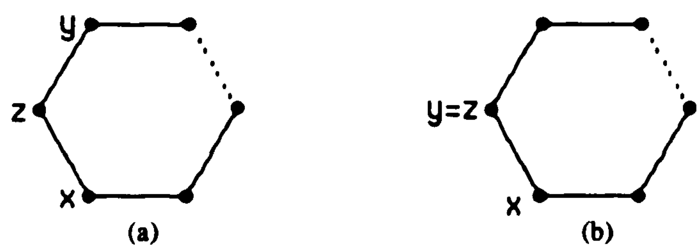


Figure 3.9. Two circuits containing vertex of maximum degree.

In each case, we can transform the graph. It is easiest to see the transformations by looking at Figure 3.10. The graphs (a) and (b) in figures 3.9 and 3.10 correspond.

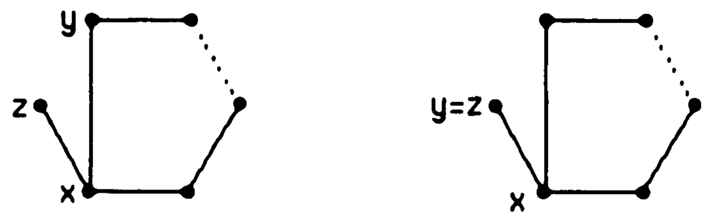


Figure 3.10. The graph in Figure 3.9 after transformation.

Note that the transformations in (a) and (b) are identical. There are no triangles formed since otherwise there would be a circuit of length 4 containing both x and y. We compute the change in the value of s_3.

Let d_x and d_z be the degrees of vertices x and z, respectively. Then the degree of x becomes d_x+1 and the degree of z becomes d_z-1.

$$\binom{d_x+1}{2}+\binom{d_z-1}{2}-[\binom{d_x}{2}+\binom{d_z}{2}]$$
$$= [(d_x+1)(d_x)/2 + (d_z-1)(d_z-2)/2]$$
$$- [(d_x)(d_x-1)/2 + (d_z)(d_z-1)/2]$$
$$= [(d_x^2+d_x)/2 + (d_z^2-3d_z+2)/2] - [(d_x^2-d_x)/2 + (d_z^2-d_z)/2]$$
$$= (2d_x - 2d_z + 2)/2$$
$$= d_x - d_z + 1 > 0 \text{ since } d_x \geq d_z.$$

•Case 2: The vertices x, y do not lie on any circuit together.

Since G is connected, there is exactly one path between x and y. So, there is a disconnecting edge in G and hence a cutpoint which is not x. This is impossible.

#

We have seen that so far, the only triangle-free graphs which are 3-optimal are bipartite. We believe that all triangle-free 3-optimal graphs are bipartite. However, we have been able to prove this result only with the additional assumption that our graph not contain an induced circuit of length 5. Nonetheless, the proof of this weakened result offers insight into the structure of 3-optimal graphs.

Theorem 3.11 Let G be a triangle-free 3-optimal graph with no induced circuits of length 5. Then G is bipartite.

Proof: Let G be a 3-optimal graph with no triangles and no induced circuits of length 5. Assume on the contrary that G is not bipartite.

Let x be a vertex of maximum degree in G. By Corollary 3.8, all other vertices in G are either a distance 1 or 2 from x. Let $V_1 = \{v \in G \,/\, d(x,v) = 1\}$ and let $V_2 = \{v \in G \,/\, d(x,v) = 2\}$.

If there are no edges among vertices in V_1 and among the vertices in

V_2, then G is bipartite. This is impossible. There can be no edges among vertices in V_1 since then G would have triangles. Therefore, there must be an edge between two vertices in V_2. But then G would have an induced circuit of length 5. This is impossible.

#

We have two additional conjectures pertaining to the structure of 3-optimal graphs. First, we believe that any 3-optimal (n,e) graph with $e \geq 2n-4$ cannot have pendant edges. Secondly, observe that in dealing with 3-optimal graphs with $e \geq n-1$, it is only reasonable to assume that such graphs are connected. However, there is no result that guarantees this. Along with the members of the SITGTG, we conjecture that this is indeed the case. Results found so far support these conjectures.

CHAPTER 4

NEW 3-OPTIMAL GRAPHS

In this chapter, we obtain all 3-optimal graphs for the cases $2n-3 \le e \le 3n-10$. Recall that the cases $n-1 \le e \le 2n-4$ were solved by Boesch and Li. Their result was given in Chapter 2 as Theorem 2.3. Also, the case for $e = 3n-9$ was solved since the complete bipartite graph $K_{3,n-3}$ is uniquely 3-optimal in that case. This was discussed in Chapter 2 as well. Combining these results, we are able to extend the known 3-optimal graphs to $e = 3n-9$.

In the first section of this chapter, we present all the 3-optimal graphs for $e = 2n-3$. The case $e = 2n-3$ is transitional in that the 3-optimal graphs are similar to both those in the range $e \le 2n-4$ and $e \ge 2n - 2$. The second section covers the cases $2n-3 < e \le 3n-10$. Finally, in the last section of this chapter, we summarize the results presented in the chapter and propose a conjecture on 3-optimal graphs for $e \le \lfloor n^2/4 \rfloor$ which generalizes the results known so far.

4.1 3-OPTIMAL GRAPHS FOR $e = 2n - 3$

Recall the graph G_A of Chapter 2. It turns out that the full case of this graph will be one of the 3-optimal graphs to be considered for $e = 2n-3$. We will call this graph G_1. Let G_2 be the graph obtained by joining two vertices of degree 2 with an edge in $K_{2,n-2}$. The graph G_2 will likewise be 3-optimal. Finally, let G_3 be the bipartite graph with the degree sequence $(n-3)^2 3^4 2^{(n-6)}$. The graph G_3 will not be 3-optimal in most cases, but it will be needed to prove some of our results. The graphs G_1, G_2, and G_3 are shown in Figure 4.1 for $n = 8$.

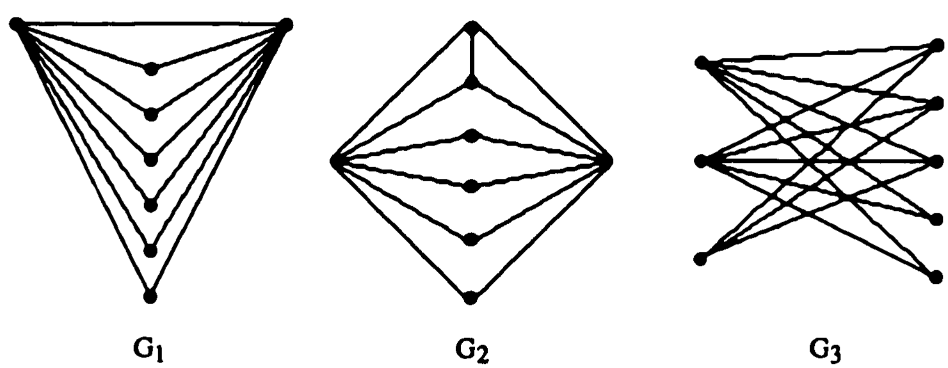


Figure 4.1. The graphs G_1, G_2, and G_3.

We will show that for $n > 7$, G_1 and G_2 are the only 3-optimal graphs. For $n \leq 7$, it will turn out that these graphs, as well as others, are 3-optimal, depending on n and e.

Observe that the graphs G_1 and G_2 both have $s_3 = (n-2)^2$. In Lemma 4.3 we show that all graphs with maximum degree n-1 have a smaller s_3 than G_1. We then show in Lemma 4.4 that all graphs with maximum degree n-2 have a smaller s_3 than G_2. Finally, in Lemma 4.5, we show that all graphs with maximum degree n-3 have a smaller s_3 than G_3. In addition to using formula (2.1) for $s_3(G)$, we will use formula (2.2):

$$s_3(G) = s_3(G-v) + IN(v) + \binom{\deg(v)}{2}$$

We begin with two results that will be used in this section and in the next. The first deals with bipartite graphs which maximize s_3. The second in a result due to Li and was obtained by us by private communication.

<u>**Lemma 4.1**</u> Let $2n-3 \le e \le 3n-9$. Among bipartite graphs having n vertices and e edges, the graph with the largest value of s_3 has the degree sequence

$$(n-3)^2(e-2n+6)3^{e-2n+6}2^{3n-9-e}.$$

Proof: Since a bipartite graph G has no triangles,

$$s_3(G) = \sum_{i=1}^{n}\binom{d_i}{2}$$

Therefore, to maximize $s_3(G)$, we need to maximize Δ and the number of vertices with degree Δ. When $2n-3 \le e \le 3n-9$, we can have at most $\Delta = n-3$ so that there are 3 vertices in one part and n-3 vertices in the other part. Furthermore, there can only be two vertices with degree Δ (unless $e = 3n-9$). The remaining $e-(2n-6)$ edges must be made incident to the remaining vertex. We obtain the degree sequence above.

#

<u>Lemma 4.2</u> Let G be a connected graph with degree sequence

$$d_1 \geq d_2 \geq d_3 \geq \ldots \geq d_n, \; d_1 < n-1.$$

Then there is a connected graph G' with $d'_1 = d_1 + 1$ such that

$$\sum_{i=1}^{n} \binom{d_i}{2} < \sum_{i=1}^{n} \binom{d'_i}{2}$$

<u>Lemma 4.3</u> Let $e = 2n-3$ and let the maximum degree be $\Delta = n-1$. Then the unique graph which maximizes s_3 under these conditions is G_1.

Proof: Let $e = 2n - 3$. Suppose that there is a graph G in the same class as G_1 that has $\Delta = n-1$ and such that $s_3(G) \geq s_3(G_1)$.

Let v be a vertex of degree n-1 in G. Then

$$s_3(G) = s_3(G\text{-}v) + IN(v) + \binom{n-1}{2}$$
$$= s_3(G\text{-}v) + \binom{n-1}{2}.$$

Let v_1 be a vertex of degree n-1 in G_1. Then

$$s_3(G_1) = s_3(G_1 - v_1) + IN(v_1) + \binom{n-1}{2}$$
$$= s_3(G_1 - v_1) + \binom{n-1}{2}$$

So,

$$s_3(G) \geq s_3(G_1) \iff$$
$$s_3(G-v) + \binom{n-1}{2} \geq s_3(G_1 - v_1) + \binom{n-1}{2} \iff$$
$$s_3(G-v) \geq s_3(G_1 - v_1).$$

Note that G-v and G_1-v_1 are in the same class. Now G_1-v_1 is a star and, by Theorem 2.3, is the unique 3-optimal graph in its class. Therefore, G-v must be that graph. But then it must be that $G = G_1$.

#

Lemma 4.4 Let e = 2n-3 and let the maximum degree be Δ = n-2. Then the unique graph which maximizes s_3 under these conditions is G_2.

Proof: Let e = 2n - 3. Assume on the contrary that there is a graph G in the same class as G_2 that has Δ = n-2 and such that $s_3(G) \geq s_3(G_2)$. Let v be a vertex of degree n-2 in G. Then

$$s_3(G) = s_3(G-v) + IN(v) + \binom{n-2}{2}$$

Let v_2 be a vertex of degree n-2 in G_2. Then

$$s_3(G_2) = s_3(G_2 - v_2) + IN(v_2) + \binom{n-2}{2}$$
$$= s_3(G_2 - v_2) + (n-2) + \binom{n-2}{2}.$$

So,

$$s_3(G) \geq s_3(G_2) \Leftrightarrow$$
$$s_3(G-v) + IN(v) + \binom{n-2}{2} \geq s_3(G_2 - v_2) + (n-2) + \binom{n-2}{2} \Leftrightarrow$$
$$s_3(G-v) + IN(v) \geq s_3(G_2 - v_2) + (n-2).$$

Note that G-v and G_2-v_2 are in the same class. Furthermore, G_2-v_2 is a star plus an edge and, by Theorem 2.3, is the unique 3-optimal graph in its class. So we have $s_3(G-v) \leq s_3(G_2-v_2)$. We consider the cases $s_3(G-v) = s_3(G_2-v_2)$ and $s_3(G-v) < s_3(G_2-v_2)$.

Suppose that $s_3(G_2-v_2) = s_3(G-v)$. Then $G-v \cong G_2-v_2$ since G_2-v_2 is the unique 3-optimal graph in this case. We need to have $IN(v) \geq n-2$. But the best we can do is $IN(v) = n-2$ since IN(v) is the degree of the vertex not adjacent to v. This can happen only if $G = G_2$.
Suppose that $s_3(G_2-v_2) < s_3(G-v)$. Then we need to have $IN(v) > n-2$. This is impossible since at most we can have $IN(v) = n-2$.

#

Lemma 4.5 Let $e = 2n-3$ and let the maximum degree be $\Delta = n-3$. Then the unique graph which maximizes s_3 under these conditions is G_3.

Proof: Let $e = 2n - 3$. Assume on the contrary that there is a graph G in the same class as G_3 that has $\Delta = n-3$ and such that $s_3(G) \geq s_3(G_3)$.

Let v be a vertex of degree $n-3$ in G. Then

$$s_3(G) = s_3(G-v) + IN(v) + \binom{n-3}{2}$$

Let v_3 be a vertex of degree $n-3$ in G_3. Then

$$\begin{aligned} s_3(G_3) &= s_3(G_3-v_3) + IN(v_3) + \binom{n-3}{2} \\ &= s_3(G_3-v_3) + n + \binom{n-3}{2} \end{aligned}$$

So,

$$\begin{aligned} &s_3(G) \geq s_3(G_3) \Leftrightarrow \\ &s_3(G-v) + IN(v) + \binom{n-3}{2} \geq s_3(G_3-v_3) + n + \binom{n-3}{2} \Leftrightarrow \\ &s_3(G-v) + IN(v) \geq s_3(G_3-v_3) + n. \end{aligned}$$

Now, $IN(v) \leq n$ since there are n edges which aren't incident to v. If $IN(v) = n$, then G is bipartite. By Lemma 4.1, G_3 has the largest s_3 value of all bipartite graphs in this class. So assume that $IN(v) < n$. In that case we must have

$$s_3(G-v) > s_3(G_3-v_3).$$

The graph G_3-v_3 = G_B is a graph in the class with n' vertices and e' edges where

$$n' = n-1$$
$$e' = e - (n-3)$$
$$= (2n-3) - (n-3)$$
$$= n' + 1.$$

By Theorem 2.3, the graph G_B is 3-optimal for $n' \leq 7$. So, for $n' \leq 7$, we have $s_3(G - v) \leq s_3(G_3 - v_3) = s_3(G_B)$. This contradicts $s_3(G\text{-}v) > s_3(G_3\text{-}v_3)$. So, we need to consider the case $n' > 7$.

Now the graph G-v must have $\Delta \leq n'\text{-}2$ since G has $\Delta = n\text{-}3$. We will show that in the class (n',n'+1), of all graphs with $\Delta \leq n'\text{-}2$, the graph G_3-v_3 = G_B has the largest s_3.

Let G-v have $\Delta = n'\text{-}2$ and v' be a vertex of degree n'-2 in G-v. Then we have

$$s_3(G\text{-}v) = s_3((G\text{-}v)\text{-}v') + IN(v') + \binom{n'-2}{2}.$$

Let v_B be a vertex of degree n'-2 in G_3-v_3 = G_B. Then

$$s_3(G_B) = s_3(G_B\text{-}v_B) + IN(v_B) + \binom{n'-2}{2}$$
$$= s_3(G_B\text{-}v_B) + 3 + \binom{n-3}{2}.$$

So,

$$s_3(G\text{-}v) > s_3(G_B) \Longleftrightarrow$$

$$s_3((G\text{-}v)\text{-}v') + IN(v') + \binom{n'-2}{2} > s_3(G_B\text{-}v_B) + 3 + \binom{n'-2}{2} \Longleftrightarrow$$

$$s_3((G\text{-}v)\text{-}v') + IN(v') > s_3(G_B\text{-}v_B) + 3.$$

But $IN(v') \leq 3$. Also, the graph $(G_B\text{-}v_B)$ is a star and so, by Theorem 2.3, is the unique 3-optimal graph in its class. Thus $s_3((G\text{-}v)\text{-}v') \leq s_3(G_B\text{-}v_B)$. So it must be that $s_3((G\text{-}v)\text{-}v') + IN(v') = s_3(G_B\text{-}v_B) + 3$. But then $(G\text{-}v)\text{-}v' = G_B\text{-}v_B$ since $G_B\text{-}v_B$ is uniquely 3-optimal and $G = G_B$.

Let G-v have $\Delta \leq n'\text{-}3$. We will construct a realizable degree sequence for a connected graph with $\Delta = n'\text{-}3$ which has the largest $\sum_{i=1}^{n'}\binom{d_i}{2}$ of all such graphs. We begin with a vertex of degree n'-3. This uses up n'-3 edges. We get

$$(n'\text{-}3)(1)^{n'-3}(0)^2.$$

We attach the remaining 4 edges to a vertex of degree 1. Two of the edges are used to connect the isolated vertices. We get

$$(n'\text{-}3)(5)(2)^2(1)^{n'-4}.$$

Let DS* denote $\sum_{i=1}^{n'}\binom{d_i}{2}$ for DS. We get

$$DS^* = \binom{n'-3}{2} + \binom{5}{2} + 2\binom{2}{2}$$

$$= ((n')^2\text{-}7n'\text{+}12)/2 + 10 + 2$$

$= ((n')^2 - 7n' + 36)/2.$

Thus, for all graphs $G'(n',e')$ with $\Delta = n'-3$, $DS^* \geq \sum_{i=1}^{n'} \binom{d_i(G')}{2} \geq s_3(G')$.

Furthermore, by Lemma 4.2, for all connected graphs G" with $\Delta < n'-3$, we have $\sum_{i=1}^{n'} \binom{d_i(G'')}{2} < DS^*$. We now compare DS^* with $s_3(G_B) = ((n')^2 - 5n' + 18)/2$:

$$((n')^2 - 5n' + 18)/2 - ((n')^2 - 7n' + 36)/2$$
$$= (2n' - 18)/2 > 0 \text{ if } n' > 9.$$

We now examine all degree sequences for n = 8 and n = 9 which have $DS^* = \sum_{i=1}^{n'} \binom{d_i}{2} > s_3(G_B)$.

For $n' = 8$, $e = 9$, $s_3(G_B) = 21$, $\Delta \leq 5$.

5 5 3 1 1 1 1 1, $DS^* = 23$ can't be 3-optimal by Corollary 3.4

5 5 2 2 1 1 1 1, $DS^* = 22$ can't be 3-optimal by Corollary 3.4

5 4 4 1 1 1 1 1, $DS^* = 22$ any realization has $\tau \geq 2$

5 4 3 2 1 1 1 1, $DS^* = 20$

Other sequences 5 x x x x x x do not have bigger DS^*.

4 4 4 2 1 1 1 1, $DS^* = 19$

Other sequences 4 x x x x x x do not have bigger DS^*.

For $n = 9$, $e = 10$, $s_3(G_B) = 27$, $\Delta \leq 6$.

6 6 2 1 1 1 1 1 1, $DS^* = 31$ can't be 3-optimal by Corollary 3.4

6 5 3 1 1 1 1 1 1, $DS^* = 28$ not realizable

6 5 2 2 1 1 1 1 1, $DS^* = 27$ any realization has $\tau \geq 2$

6 4 4 1 1 1 1 1 1, $DS^* = 27$ not realizable

6 4 3 2 1 1 1 1 1, $DS^* = 25$

Other sequences 6 x x x x x x x x do not have bigger DS^*.

5 5 4 1 1 1 1 1 1, $DS^* = 26$

Other sequences do not have bigger DS^*.

Therefore, for $n' > 7$, $s_3(G_B) > s_3(G\text{-}v)$. This contradicts $s_3(G\text{-}v) > s_3(G_3\text{-}v_3) = s_3(G_B)$.

#

Finally, we show in Lemma 4.6 that all graphs with maximum degree n-3, $n > 12$ have a smaller s_3 than $(n-2)^2$.

<u>**Lemma 4.6**</u> For $n > 12$ and $\Delta = n\text{-}3$, there is no graph which has $\sum_{i=1}^{n} \binom{d_i}{2} \geq (n-2)^2$.

Proof: We will construct degree sequences which maximize $\sum_{i=1}^{n} \binom{d_i}{2}$ and obtain upper bounds for s_3 for graphs with $e = 2n\text{-}3$, $\Delta = n\text{-}3$. A graph with $e = 2n\text{-}3$, $n > 12$, can have at most 2 vertices of degree n-3. Let u and v be those vertices. There are two cases to consider, one with u and v adjacent, and the other with u and v not adjacent.

We will not consider cases in which the distance between u and v exceeds two since it was shown in Corollary 3.8 that the s_3 could be improved in that case.

Let u and v be adjacent. In beginning the construction of such a graph, we use up 2n-7 edges. This leaves us with 4 edges. Now, u and v can have n-4, n-5, or n-6 common neighbors.

When u and v have n-4 common neighbors, the optimal degree sequence is $(n-3)^2 6^1 3^2 2^{n-7} 1^2$. We get

$$\sum_{i=1}^{n} \binom{d_i}{2} = 2\binom{n-3}{2} + \binom{6}{2} + 2\binom{3}{2} + (n-7)\binom{2}{2} + 2\binom{1}{2}$$

$$= (n^2-7n+12) + 15 + 6 + (n-7)$$

$$= n^2 - 6n + 26.$$

We have $\tau \geq n-4$ so that $s_3 \leq n^2 - 6n + 26 - 2(n-4) = n^2 - 8n + 34$.
Comparing with $(n-2)^2$, we get

$$(n^2 - 4n + 4) - (n^2 - 8n + 34) = 4n - 30 > 0 \text{ since } n > 7.$$

When u and v have n-5 common neighbors, the optimal degree sequence is $(n-3)^2 6^1 3^3 2^{n-9} 1^3$. We get

$$\sum_{i=1}^{n} \binom{d_i}{2} = 2\binom{n-3}{2} + \binom{6}{2} + 3\binom{3}{2} + (n-9)\binom{2}{2} + 3\binom{1}{2}$$

$$= (n^2-7n+12) + 15 + 9 + (n-9)$$

$$= n^2 - 6n + 27.$$

We have $\tau \geq n-5$ so that $s_3 \leq n^2 - 6n + 27 - 2(n-5) = n^2 - 8n + 37$.

Comparing with $(n-2)^2$, we get

$$(n^2 - 4n + 4) - (n^2 - 8n + 37) = 4n - 33 > 0 \text{ since } n > 9.$$

Finally, when u and v have n-6 common neighbors, the optimal degree sequence is $(n-3)^2 6^1 3^4 2^{n-11} 1^4$. We get

$$\sum_{i=1}^{n} \binom{d_i}{2} = 2\binom{n-3}{2} + \binom{6}{2} + 4\binom{3}{2} + (n-11)\binom{2}{2} + 4\binom{1}{2}$$

$$= (n^2-7n+12) + 15 + 12 + (n-11)$$

$$= n^2 - 6n + 28.$$

We have $\tau \geq n-6$ so that $s_3 \leq n^2 - 6n + 28 - 2(n-6) = n^2 - 8n + 40$.

Comparing with $(n-2)^2$, we get

$$(n^2 - 4n + 4) - (n^2 - 8n + 40) = 4n - 36 > 0 \text{ since } n > 11.$$

Let u and v be non-adjacent. In beginning the construction of such a graph, we use up 2n-6 edges. This leaves us with 3 edges. Now, u and v can have n-3 or n-4 common neighbors.

Let u and v have n-3 common neighbors and no triangles. The only degree sequence is $(n-3)^2 3^4 2^{n-6}$. We get

$$\sum_{i=1}^{n} \binom{d_i}{2} = 2\binom{n-3}{2} + 4\binom{3}{2} + (n-6)\binom{2}{2}$$

$$= (n^2-7n+12) + 12 + (n-6)$$

$$= n^2 - 6n + 18$$

$$= s_3.$$

Comparing with $(n-2)^2$, we get

$$(n^2 - 4n + 4) - (n^2 - 6n + 18) = 2n - 14 > 0 \text{ since } n > 7.$$

Otherwise, when u and v have n-3 common neighbors we have $\tau \geq 2$. The optimal degree sequence is $(n-3)^2 5^1 3^2 2^{n-6} 1^1$. We get

$$\sum_{i=1}^{n} \binom{d_i}{2} = 2\binom{n-3}{2} + \binom{5}{2} + 2\binom{3}{2} + (n-6)\binom{2}{2} + \binom{1}{2}$$

$$= (n^2-7n+12) + 10 + 6 + (n-6)$$

$$= n^2 - 6n + 22.$$

So that $s_3 \leq n^2 - 6n + 22 - 2(2) = n^2 - 6n + 18$.

Comparing with $(n-2)^2$, we get

$$(n^2 - 4n + 4) - (n^2 - 6n + 18) = 2n - 14 > 0 \text{ since } n > 7.$$

When u and v have n-4 common neighbors, the optimal degree sequence is $(n-3)^2 5^1 3^3 2^{n-8} 1^2$. We get

$$\sum_{i=1}^{n} \binom{d_i}{2} = 2\binom{n-3}{2} + \binom{5}{2} + 3\binom{3}{2} + (n-8)\binom{2}{2} + 2\binom{1}{2}$$

$$= (n^2-7n+12) + 10 + 9 + (n-8)$$

$$= n^2 - 6n + 23.$$

We have $\tau \geq 3$ so that $s_3 \leq n^2 - 6n + 23 - 2(3) = n^2 - 6n + 17$.

Comparing with $(n-2)^2$, we get

$$(n^2 - 4n + 4) - (n^2 - 6n + 17) = 2n - 13 > 0 \text{ since } n > 7.$$

In each case, the maximum possible s_3 value is smaller than $(n-2)^2$.

#

Lemma 4.7 Let $e = 2n-3$, $8 \leq n \leq 12$. Then the graphs G_1 and G_2 are the only 3-optimal graphs.

Proof: By Lemmas 4.3-4.5, we need only consider graphs with maximum degree $\leq n-4$ as possible 3-optimal graphs. The proof involves the generation of all degree sequences for such graphs for which $\sum_{i=1}^{n} \binom{d_i}{2} \geq (n-2)^2$. It turns out that almost all such sequences cannot correspond to 3-optimal graphs because they have pendant edges and more than on vertex of maximum degree (see Corollary 3.5). The remaining degree sequences turn out to be trivially non-realizable. The degree sequences and details of the proof are given in the Appendix.

#

We also obtain all the 3-optimal graphs for cases with $n \leq 7$. We give the results for these small cases of n in Lemma 4.8.

Lemma 4.8 Let $e = 2n-3$. Then for $3 \leq n < 7$, the graphs in Figure 4.2 are the only 3-optimal graphs. For $n = 7$, in addition to the graph in the figure, the graphs G_1 and G_2 are 3-optimal as well.

Proof: For n = 3 and e = 3, there is only one graph. Likewise for n = 4 and e = 5. For n = 5, 6, 7 we consider only the graphs in Lemmas 4.3, 4.4, and 4.5 since there are no graphs in these cases with maximum degree < n-3.

#

We now prove the main result of this section. Using Lemma 4.2, we show that all graphs with maximum degree < n-3 have a smaller s_3 than $(n-2)^2$.

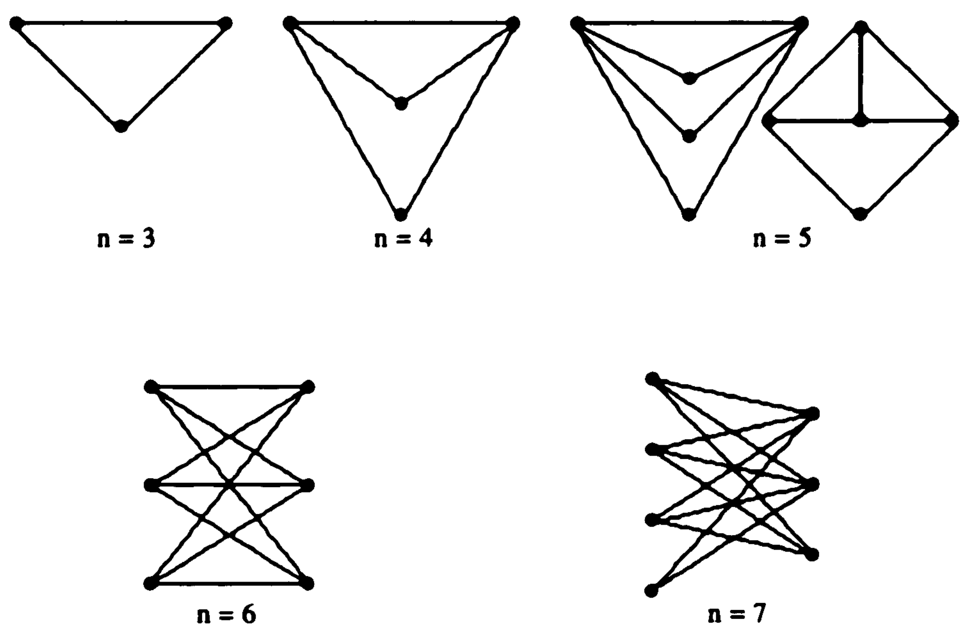


Figure 4.2. 3-optimal graphs for e = 2n-3, $3 \leq n \leq 7$.

Theorem 4.9 For $n > 7$ and $e = 2n - 3$, the unique 3-optimal graphs are G_1 and G_2. For $n = 7$, the graph in Figure 4.2 is 3-optimal in addition to G_1 and G_2. For smaller n, the 3-optimal graphs are given in Figure 4.2.

Proof: By Lemma 4.2, for any connected graph G with $\Delta(G) = n-k$, $k > 3$, there is a graph G' with $\Delta(G') = n-k+1$ such that

$$\sum_{i=1}^{n}\binom{d_i}{2} < \sum_{i=1}^{n}\binom{d'_i}{2}$$

Thus, by Lemma 4.6, all such graphs with $n > 12$ have $s_3 < (n-2)^2$. Thus, by Lemmas 4.3 and 4.4, the unique 3-optimal graphs for $n > 12$ and $e = 2n - 3$ are G_1 and G_2. Lemma 4.7 gives the result for $8 \le n \le 12$. Lemma 4.8 gives the result for $n \le 7$.

#

4.2 3-OPTIMAL GRAPHS FOR $2n-2 \le e \le 3n-10$.

We now present our result for the cases $2n-2 \le e \le 3n-10$. In general, we let $e = 2n + a$ for the range $2n-3 \le e \le 3n-9$. This corresponds to $-3 \le a \le n-9$. Though our results in this section will deal only with the cases 2n-2 $\le$ e $\le$ 3n-10, we will later use this generalization to combine these results with those obtained in the previous section.

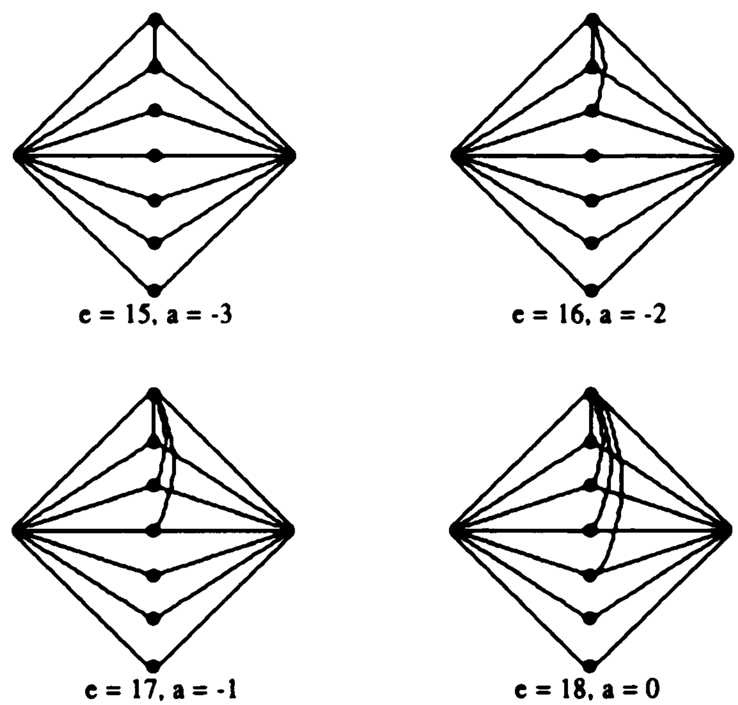


Figure 4.3 The general graph G_2 for n = 9.

The graph G_2 presented in the previous section can be generalized for 2n-3 $\le$ e $\le$ 3n-9. We begin with the complete bipartite graph $K_{2,n-2}$. This uses up 2n-4 edges. Select a vertex of degree 2 in $K_{2,n-2}$ and connect it to as many of the other vertices as possible until all the edges are used up. The number of such edges is (2n+a) - (2n-4) = a + 4. Since a + 4 $\le$ n-5, we are always able to perform this construction for our range of e. Note that the graph G_2 of Section 4.1 has a = -3. We will call this generalized graph G_2 as well. Figure 4.3 shows the graph G_2 for n = 9. Note $s_3(G_2) = (n-2)^2 + (a^2 + 7a + 12)/2$.

We need to consider a generalization of the graph G_3 as well. Begin with the complete bipartite graph $K_{3,n-3}$ This uses 3n-9 edges. We have $2n+a \leq 3n-9$ edges. Choose a vertex of degree n-3 and remove the excess edges from it. Since $e \geq 2n-3$, we are always able to perform this construction and obtain a connected graph. We will call this generalization G_3. Note that $s_3(G_3) = (n - 3)^2 + (a^2 + 5a + 54)/2$. The graph G_3 in the previous section had a = -3. Figure 4.4 shows the graph G_3 for n = 9.

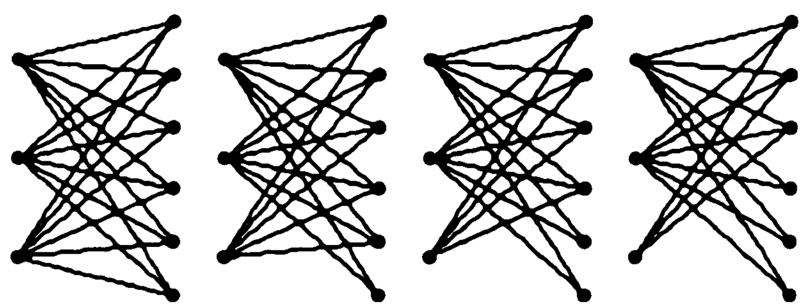


Figure 4.4. The graph G_3.

In the remainder of this section, we will show that for e = 2n+a, $2n-2 \leq e \leq 3n-10$, the only 3-optimal graphs are G_2 and G_3. Observe that $s_3(G_2) \geq s_3(G_3)$ if $n \geq 13+2a$. Otherwise, $s_3(G_2) < s_3(G_3)$. We will show that depending on these constraints on n and a, either one or both graphs will be 3-optimal. We begin with a result of Li which we state here as Lemma 4.9.

Lemma 4.10 Let G be a 3-optimal graph with a vertex x of degree n-1. Then G-x is 3-optimal in its class.

We use Lemma 4.10 to prove Lemma 4.11. The lemma eliminates graphs with maximum degree n-1 as possible 3-optimal graphs for $2n-2 \leq e \leq 3n-10$.

Lemma 4.11 For $2n-2 \leq e \leq 3n-10$, there is no 3-optimal graph with a vertex of degree n-1.

Proof: Assume on the contrary that G is a 3-optimal graph with $e = 2n + a$, $-2 \leq a \leq n-10$, and a vertex x of degree n-1. Then the graph G-x is in the class of graphs having n' vertices and e' edges such that

$$n' = n-1$$

$$\begin{aligned} e' &= e - (n-1) \\ &= 2n + a - (n-1) \\ &= n + a + 1 \end{aligned}$$

$$= (n-1) + 1 + a + 1$$
$$= (n-1) + (a + 2)$$
$$= n' + a',$$

where $a' = a + 2$.

Thus we have

$$-2 \le a \le n-10 \iff$$
$$0 \le a' \le n-8 \iff$$
$$0 \le a' \le (n-1) + 1 - 8 \iff$$
$$0 \le a' \le n' - 7.$$

By Theorem 2.3, the 3-optimal graphs with n' vertices and e' edges are G_A or G_B. Thus, by Lemma 4.10, if G is 3-optimal, then G-x is one of these graphs.

Let $G\text{-}x = G_A$. Then $s_3(G) = (n-2)^2 + (a^2+5a+6)/2$. We compare this value with $s_3(G_2) = (n-2)^2 + (a^2+7a+12)/2$:

$$[(n-2)^2 + (a^2+7a+12)/2] - [(n-2)^2 + (a^2+5a+6)/2]$$
$$= (2a+6)/2 > 0 \text{ since } a > -3.$$

So, $s_3(G) < s_3(G_2)$.

Let $G\text{-}x = G_B$. Then $s_3(G) = (n^2-5n) + (a^2+9a+34)/2$. We compare this value with $s_3(G_2) = (n-2)^2 + (a^2+7a+12)/2$:

$$[(n^2-4n+4) + (a^2+7a+12)/2] - [n^2-5n + (a^2+9a+34)/2]$$
$$= n + 4 - (2a+22)/2$$
$$= n - a - 7 > 0 \text{ if } n > a+7.$$

If $n \leq a+7$, we compare $s_3(G)$ with $s_3(G_3) = (n-3)^2 + (a^2+15a+54)/2$:

$$[(n^2-6n+9) + (a^2+15a+54)/2] - [n^2-5n + (a^2+9a+34)/2]$$
$$= -n + 9 + (6a+20)/2$$
$$= 3a + 19 - n > 0 \text{ since } n \leq a+7,\ a > -3.$$

So, $s_3(G) < s_3(G_2)$ if $n > a+7$ and $_3(G) < _3(G_3)$ if $n \leq a+7$.

#

We now prove a result similar Lemma 4.10. That is, we show that for $2n-2 \leq e \leq 3n-10$, removing a vertex of degree $\Delta = n-2$ or $\Delta = n-3$ leaves a 3-optimal graph.

<u>Lemma 4.12</u> Let G be a 3-optimal graph with $e = 2n + a$, $-2 \leq a \leq n-10$, $2n-2 \leq e \leq 3n-10$ and and let the maximum degree be $\Delta = n-2$ or $n-3$. Let x be a vertex of degree Δ. Then G-x is 3-optimal in its class.

Proof:

•<u>Case 1</u>: $\Delta = n-2$.

Assume on the contrary that there is a graph G which is 3-optimal, has a vertex x of degree $\Delta = n-2$, but that G-x is not 3-optimal. So there is a 3-optimal graph G' in the same class as G-x such that

$$s_3(G') > s_3(G\text{-}x).$$

The graphs in the class to which G-x and G' belong have n' vertices and e' edges as follows:

$$\begin{aligned} n' &= n-1 \\ e' &= e - (n-2) \\ &= (2n+a) - (n-2) \\ &= n + a + 2 \\ &= (n-1) + (a+3) \\ &= n' + a', \end{aligned}$$

where $a' = a + 3$.

Thus we have

$$\begin{aligned} &-2 \le a \le n-10 \iff \\ &1 \le a' \le n-7 \iff \\ &1 \le a' \le (n-1) + 1 - 7 \iff \\ &1 \le a' \le n' - 6. \end{aligned}$$

The 3-optimal graphs for these cases were given in Theorem 2.3.

We compute $s_3(G\text{-}x)$ using formula 2.2. Let vertex x have degree d_x. Let vertex w with degree d_w be the one vertex in G not adjacent to x. Then

$$\begin{aligned} s_3(G) &= s_3(G\text{-}x) + IN(x) + \binom{d_x}{2} \\ &= s_3(G\text{-}x) + d_w + \binom{n-2}{2} \end{aligned}$$

So,

$$s_3(G\text{-}x) = s_3(G) - d_w - \binom{n-2}{2}$$

Let G'+y denote the graph obtained by adding a vertex of degree n'-1 = n - 2 to G'. The graph G'+ y is in the same class as G. Then

$$s_3(G) \geq s_3(G'+ y).$$

We now compute $s_3(G'+y)$ using formula 2.2. Let vertex y have degree d_y = n-2. Let vertex w' with degree $d_{w'}$ be the one vertex in G' not adjacent to y. Then

$$s_3(G'+y) = s_3((G'+y)\text{-}y) + IN(y) + \binom{d_y}{2}$$

$$= s_3(G') + d_{w'} + \binom{n-2}{2}$$

So,

$$s_3(G'+y) = s_3(G') + d_{w'} + \binom{n-2}{2}$$

So the inequalities

$$s_3(G') > s_3(G\text{-}x)$$

$$s_3(G) \geq s_3(G'+ y)$$

become

$$s_3(G') > s_3(G) - \binom{n-2}{2} - d_w$$

$$s_3(G) \geq s_3(G') + \binom{n-2}{2} + d_{w'}.$$

Adding the two inequalities, we get

$$s_3(G) + s_3(G') > s_3(G) + s_3(G') - d_w + d_{w'} \iff$$

$$0 > d_{w'} - d_w \iff$$
$$d_w > d_{w'}.$$

Since any vertex in G' can be chosen as w', we must have $d_w > d_{w'}$ for all w' in G'. The 3-optimal graphs in the class of G' (i.e. $1 \le a' \le n'-4$) have maximum degree $n'-1$ or $n'-2$ where $n' = n - 1$. Thus we need $d_w > n-2$ or $d_w > n-3$.

The first case is not possible since G has maximum degree n-2. The second case is possible only if $d_w = n-2$. But then G has two non-adjacent vertices of degree n-2. The graph with the largest s_3 which has two non-adjacent vertices of degree n-2 is G_2: The construction of any graph with two non-adjacent vertices of degree n-2 begins with $K_{2,n-2}$. This leaves $(2n+a) - (2n-4) = a+4$ edges. The addition of any such edges to $K_{2,n-2}$ creates 2 triangles. Therefore, it is necessary to add the a+4 edges so as to maximize $\sum_{i=1}^{n} \binom{d_i}{2}$. We obtain the graph G_2.

Therefore $G = G_2$. Assuming that $G = G_2$ is 3-optimal, we must have $n > 13 + 2a$ since otherwise the graph G_1 has a larger s_3. In that case the graph $G\text{-}x = G_A$ is 3-optimal in the class (n',e') as stated in Theorem 2.3 since

$$n \ge 13 + 2a \iff$$
$$(n-1) \ge 13 + 2(a+3) - 1 - 6 \iff$$

$n' \geq 6 + 2a' \Rightarrow$

$n' > 5 + 2a'$.

This contradicts our assumption that G-x is not 3-optimal.

•<u>Case 2</u>: $\Delta = n-3$.

Assume on the contrary that there is a graph G which is 3-optimal, has a vertex x of degree $\Delta = n-3$, but that G-x is not 3-optimal. So there is a graph G' in the same class as G-x such that

$$s_3(G') > s_3(G-x).$$

The graphs in the class to which G-x and G' belong have n' vertices and e' edges as follows:

$$n' = n-1$$
$$\begin{aligned} e' &= e - (n-3) \\ &= (2n+a) - (n-3) \\ &= n + a + 3 \\ &= (n-1) + (a+4) \\ &= n' + a', \end{aligned}$$

where $a' = a + 4$.

Thus we have

$$-2 \leq a \leq n-10 \Leftrightarrow$$
$$2 \leq a' \leq n-6 \Leftrightarrow$$
$$2 \leq a' \leq (n-1) + 1 - 6 \Leftrightarrow$$
$$2 \leq a' \leq n' - 5.$$

The 3-optimal graphs for n' and e' are those in Theorem 2.3.

We compute $s_3(G\text{-}x)$ using formula 2.2. Let vertex x have degree d_x. Then

$$s_3(G) = s_3(G\text{-}x) + IN(x) + \binom{d_x}{2}$$
$$= s_3(G\text{-}x) + IN(x) + \binom{n-3}{2}.$$

So,

$$s_3(G\text{-}x) = s_3(G) - IN(x) - \binom{n-3}{2}.$$

Let G' + y denote the graph obtained by adding a vertex y of degree d_y = n'- 2 = n - 3 to G'. The graph G'+ y is in the same class as G. Then

$$s_3(G) \geq s_3(G' + y).$$

We thus have

$$s_3(G'+y) = s_3((G'+y)\text{-}y) + IN(y) + \binom{d_y}{2}$$
$$= s_3(G') + IN(y) + \binom{n-3}{2}.$$

where IN(y) is computed in $s_3(G'+y)$.

So, the inequalities

$$s_3(G') > s_3(G\text{-}x)$$
$$s_3(G) \geq s_3(G' + y)$$

become

$$s_3(G') > s_3(G) - IN(x) - \binom{n-3}{2}$$

$$s_3(G) \geq s_3(G') + IN(y) + \binom{n-3}{2}$$

Adding the two inequalities we get

$$s_3(G') + s_3(G) > s_3(G) - IN(x) + s_3(G') + IN(y) \iff$$

$$0 > IN(y)-IN(x) \iff$$

$$IN(x) > IN(y).$$

Now IN(y) depends upon the Adj(y) we choose, i.e., the subset of n'-2 vertices we choose in G' to be the neighbors of the added vertex y. Since there are two possible choices for G', we consider two cases.

•Case 2.1: Let $G' = G_A$ of Theorem 2.3 and not G_B.

In this case we choose Adj(y) to be the set of n'-2 vertices which are not adjacent with each other. Then

$$IN(y) = e'-1 = (e-(n-3)-1) = e-n+2.$$

So

$$IN(x) > IN(y) \Rightarrow$$

$$IN(x) > e-n+2 \iff$$

$$IN(x) \geq e-n+3.$$

Since x has degree n-3, all of the remaining e-(n-3) = e-n+3 edges must be in IN(x). This means that G is a bipartite graph with 3 vertices in one part. By Lemma 4.1, the bipartite graph with 3 vertices in one part which has the maximum s_3 is G_3 so $s_3(G_3) \geq s_3(G)$. Now, if we remove a vertex of degree n-3 from the graph G_3, we obtain the graph G_B. Since G_B is not 3-optimal in this case, we must have

$$n' > 2a' + 5 \Leftrightarrow$$
$$(n-1) > 2(a+4) + 5 \Leftrightarrow$$
$$n > 2a + 14.$$

But when $n > 2a + 14$, the graph G_2 has a better s_3 than G_3 and so $s_3(G_2) > s_3(G_3) \geq s_3(G)$. This contradicts the fact that G is 3-optimal.

•<u>Case 2.2</u>: Let $G' = G_B$ of Theorem 2.3.

In this case we choose Adj(y) to be the set of n'-2 vertices which comprise the larger part of the bipartite graph G_B. Then

$$IN(y) = e' = e-(n-3)= e-n+3.$$

So

$$IN(x) > IN(y) \Rightarrow$$
$$IN(x) > e-n+3$$

Since x has degree n-3, there remain only $e-(n-3) = e-n+3$ edges in G. Therefore it is impossible to have $IN(x) > e-n+3$.

#

We now use Lemma 4.12 to show that of all graphs with $2n-2 \leq e \leq 3n-10$ and maximum degree n-2, the graph G_2 is the only possible 3-optimal graph.

Lemma 4.13 For $2n-2 \leq e \leq 3n-10$, the only possible 3-optimal graph with a vertex of maximum degree n-2 is G_2.

Proof: Suppose that G is a 3 - optimal graph with $e = 2n + a$, $-2 \leq a \leq n-10$, and a vertex x of degree n-2. Then the graph G-x is in the class of graphs having n' vertices and e' edges such that

$$n' = n-1$$

$$\begin{aligned} e' &= e - (n-2) \\ &= 2n + a - (n-2) \\ &= n + a + 2 \\ &= (n-1) + 1 + a + 2 \\ &= (n-1) + (a + 3) \\ &= n' + a', \end{aligned}$$

where $a' = a+3$.

Thus we have

$$-2 \leq a \leq n-10 \iff$$

$$1 \leq a' \leq n-7 \iff$$

$$0 \leq a' \leq (n-1) + 1 - 7 \iff$$

$$0 \leq a' \leq n' - 6.$$

By Theorem 2.3, the 3-optimal graphs with n' vertices and e' edges are G_A or G_B. Thus, by Lemma 4.12, if G is 3-optimal, then G-x is one of these graphs.

Suppose $G\text{-}x = G_A$. Then the vertex x cannot be adjacent to the vertex of degree n'-1 in G_A sinc e then G would have maximum degree $\Delta = n-1$. So there is only one possibility. The resulting graph is $G = G_2$.

Suppose $G-x = G_B$. There are two cases to consider:

•<u>Case 1</u>:

If x is adjacent to the vertex of degree n'-2 in G_B, then G has 2 vertices of degree n-2. By Corollary 3.4, G cannot have pendant edges. Therefore either x is not adjacent to a vertex of degree 2 or x is not adjacent to the vertex of degree a+5 in G_B. If x is not adjacent to a vertex of degree 2, we obtain the graph with $\tau = n-3$ and degree sequence

$$(n-2)^2(a+6)(3)^{a+4}(2)^{n-a-7}.$$

We get $s_3(G) = (n^2-6n) + (a^2+15a+64)/2$. We compare $s_3(G)$ with $s_3(G_3) = (n-3)^2 + (a^2+15a+54)/2$:

$$[(n^2-6n+9) + (a^2+15a+54)/2] - [(n^2-6n) + (a^2+15a+64)/2]$$
$$= 9 - (10)/2$$
$$= 4 > 0.$$

If x is not adjacent to the vertex of degree a+5, we obtain the graph with $\tau = n-3$ and degree sequence

$$(n-2)^2(a+5)(3)^{a+5}(2)^{n-a-8}.$$

We get $s_3(G) = (n^2-6n) + (a^2+13a+34)/2$. We compare $s_3(G)$ with $s_3(G_3) = (n-3)^2 + (a^2+15a+54)/2$:

$$[(n^2-6n+9) + (a^2+15a+54)/2] - [(n^2-6n) + (a^2+13a+34)/2]$$
$$= 9 + (2a + 20)/2$$
$$= a + 19 > 0 \text{ since } a > -3.$$

So, $_3(G) < _3(G_3)$ in both cases.

<u>•Case 2</u>:

If x is not adjacent to the vertex of degree n'-2 in G_B, then G has τ = a+5 and degree sequence

$$(n-2)(n-3)(a+6)(3)^{a+5}(2)^{n-a-8}.$$

We get $s_3(G) = (n^2-5n) + (a^2+11a+42)/2$. We compare this value with $s_3(G_2) = (n-2)^2 + (a^2+7a+12)/2$:

$$[(n^2-4n+4) + (a^2+7a+12)/2] - [(n^2-5n) + (a^2+11a+42)/2]$$
$$= n+4 - (4a-30)/2$$
$$= n - (11 + 2a) > 0 \text{ if } n > 11+2a.$$

If $n \leq 11 + 2a$, we compare $s_3(G)$ with $s_3(G_3) = (n-3)^2 + (a^2+15a+54)/2$:

$$[(n^2-6n+9) + (a^2+15a+54)/2] - [(n^2-5n) + (a^2+11a+42)/2]$$
$$= -n + 9 + (4a+12)/2$$
$$= -n + 15 + 2a > 0 \text{ since } n \leq 11 + 2a,\ a > -3.$$

So, $_3(G) < _3(G_2)$ if $n > 11+2a$ and $_3(G) < _3(G_3)$ if $n \leq 11+2a$.

#

Similar to what was done in Lemma 4.13, we use Lemma 4.12 to show that of all graphs with $2n-2 \le e \le 3n-10$ and maximum degree n-3, the graph G_3 is the only possible 3-optimal graph.

Lemma 4.14 For $2n-2 \le e \le 3n-10$, the only possible 3-optimal graph with a vertex of maximum degree n-3 is the graph G_3.

Proof: Assume on the contrary that G is a 3-optimal graph with $e = 2n + a$, $-2 \le a \le n-10$, and a vertex x of degree n-3. Then the graph G-x is in the class of graphs having n' vertices and e' edges such that

$$\begin{aligned} n' &= n-2 \\ e' &= e - (n-3) \\ &= 2n + a - (n-3) \\ &= n + a + 3 \\ &= (n-1) + 1 + a + 3 \\ &= (n-1) + (a + 4) \\ &= n' + a'. \end{aligned}$$

Thus $a' = a + 4$ and we have

$$\begin{aligned} &-2 \le a \le n-10 \iff \\ &2 \le a' \le n-6 \iff \\ &2 \le a' \le (n-1) + 1 - 6 \iff \\ &2 \le a' \le n' - 5. \end{aligned}$$

By Theorem 2.3, the 3-optimal graphs with n' vertices and e' edges are G_A or G_B. Thus, by Lemma 4.11, if G is 3-optimal, then G-x is one of these graphs.

Let G-x = G_A. This is impossible since then G would have a vertex of degree n-2.

Let G-x = G_B. We must choose the 2 vertices in G_B to which x is not adjacent. One of these vertices must be the vertex of degree n'-2 since otherwise G would have a vertex of degree n-2. Now x must be adjacent to all the vertices of degree 1 in G_B since otherwise G would have pendant edges and more than one vertex of degree n-3. By Corollary 3.4 this is impossible. This leaves 2 possibilities. If x is not adjacent to the vertex in G_B of degree a'+2, we get G = G_3. If x is not adjacent to a vertex of degree 2 in G_B, $s_3(G) = (n^2-6n) + (a^2+13a+60)/2$. We compare this value with $s_3(G_3) = (n-3)^2 + (a^2+15a+54)/2$:

$$[(n^2-6n+9) + (a^2+15a+54)/2] - [(n^2-6n) + (a^2+13a+60)/2]$$
$$= 9 + (2a-6)/2$$
$$= 6 + a > 0 \text{ since } a > -3.$$

So, $_3(G) < {}_3(G_3)$ in this case.

#

To summarize what has been done so far, we have eliminated several possibilities for 3-optimal graphs with $2n-2 \le e \le 3n-10$. Lemma 4.11 tells us that we cannot have a maximum degree n-1. Lemmas 4.13 and 4.14 tell us that for maximum degree n-2 and n-3, the only possible 3-optimal graphs are G_2 and G_3, respectively. Thus, if we are to look for 3-optimal graphs within our range of e, we must consider only those graphs with maximum degree $\le$ n-4.

We continue to narrow our field with Lemma 4.15. The lemma eliminates graphs with minimum degree ≥ 4 as possible 3-optimal graphs for $2n-2 \le e \le 3n-10$.

<u>Lemma 4.15</u> Let G be a 3-optimal graph with $2n-2 \le e \le 3n-10$. Then G has $\delta \le 4$.

Proof:

•<u>Case 1</u>: G cannot have $\delta = 4$.

We construct a (not necessarily realizable) degree sequence for a graph with $2n-2 \le e \le 3n-10$ and $\delta = 4$ such that $\sum_{i=1}^{n} \binom{d_i}{2}$ is the maximum possible. Clearly, we will have $\sum_{i=1}^{n} \binom{d_i}{2} \ge s_3(G)$ for any G with the same n and e having $\delta = 4$. We will then show that the graphs G_2 and G_3 have $s_3 > \sum_{i=1}^{n} \binom{d_i}{2}$ for that sequence.

Let $\delta = 4$. If every degree in our sequence is at least 4, $2e \geq 4n$. We have $2e \leq 6n-20$. So $4n \leq 6n-20 \iff 0 \leq 2n-20 \iff 10 \leq n$. Thus, for $\delta = 4$, we must have $n \geq 10$.

To maximize $\sum_{i=1}^{n} \binom{d_i}{2}$, we must maximize the largest degree in the sequence. What can Δ be? Since we know all the possible 3-optimal graphs with $\Delta \geq n-3$, we consider only the cases with $\Delta \leq n-4$. We have $e = 2n + a$ and $2e = 4n + 2a$. So, after we use up 4n "degrees", we have $(4n + 2a) - 4n = 2a$ left. To construct the sequence, we begin with 4^n. We then add the remaining 2a to the first degree resulting in our first sequence:

$$DS_1 = (2a+4), 4, 4, \ldots, 4 = (2a+4)\ 4^{n-1},$$

where

$$4 \leq 2a + 4 \leq n-4.$$

It is possible for $2a + 4 > n-4$. In that case, we make the first degree the maximum possible, n-4. This uses up $(n-4) + 4(n-1) = 5n - 8$ degrees for the sequence thus far. Subtracting $(4n + 2a) - (5n - 8)$, we get $2a - n + 8$ degrees remaining. All of these are added to the second term resulting in $2a - n + 12$. It must be that $2a - n + 12 \leq n-8$ since otherwise we get $2e > 6n - 20$. This yields the second sequence under consideration:

$$DS_2 = (n-4), (2a-n+12), 4, 4, \ldots, 4 = (n-4)(2a-n+12)4^{n-2},$$

where

$$5 \le 2a - n + 12 \le n-8.$$

We show that $s_3(G_2) > \sum_{i=1}^{n} \binom{d_i}{2}$ for the degree sequence DS_1.

Let $DS_1{*}$ denote $\sum_{i=1}^{n} \binom{d_i}{2}$ for $DS_1 = (2a + 4)4^{n-1}$ with $4 \le 2a+4 \le n-4$.

We compute $DS_1{*}$:

$$\begin{aligned} DS_1{*} &= \binom{2a+4}{2} + (n-1)\binom{4}{2} \\ &= (2a+4)(2a+3)/2 + 6(n-1) \\ &= (4a^2 + 14a + 12)/2 + 6(n-1) \\ &= 6n + (4a^2 + 14a)/2. \end{aligned}$$

We compute the difference $s_3(G_2) - DS_1{*}$:

$$\begin{aligned} s_3(G_2) - DS_1{*} &= (n - 2)^2 + (a^2 + 7a + 12)/2 \\ &\quad - (6n + (4a^2 + 14a)/2) \\ &= n^2 - 10n + 4 + (-3a^2 - 7a + 12)/2 \\ &= (2n^2 - 20n - 3a^2 - 7a + 20)/2. \end{aligned}$$

We show that $s_3(G_2)-DS_1{*} > 0$ by showing that $2n^2-20-3a^2-a+20 > 0$

using $4 \le 2a + 4 \le n-4$:

$$2n^2 - 20n - 3a^2 - 7a + 20$$
$$\ge 2n^2 - 20n - 3((n-8)/2)^2 - 7(n-8)/2 + 20$$
$$= 2n^2 - 20n - 3(n^2 - 16n + 64)/4 - 7(n-8)/2 + 20$$
$$= (8n^2 - 80n - 3n^2 + 48n - 192 - 14n + 112 + 80)/4$$
$$= (5n^2 - 46n)/4 > 0 \text{ since } n \ge 10.$$

So $s_3(G_2) > DS_1^*$.

We show that $s_3(G_3) > \sum_{i=1}^{n} \binom{d_i}{2}$ for the degree sequence DS_2.

Let DS_2^* denote $\sum_{i=1}^{n} \binom{d_i}{2}$ for $DS_2 = (n-4)(2a-n+12)4^{n-2}$ with $5 \le 2a-n+12 \le n-8$. We compute DS_2^*:

$$DS_2^* = \binom{n-4}{2} + \binom{2a-n+12}{2} + (n-2)\binom{4}{2}$$
$$= (n-4)(n-5)/2 + (2a-n+12)(2a-n+11)/2 + 6(n-2)$$
$$= (n^2 - 9n + 20)/2$$
$$+ (n^2 - 23n - 4an + 4a^2 + 46a + 132)/2 + (12n-24)/2$$
$$= (2n^2 - 20n - 4an + 4a^2 + 46a + 128)/2.$$

We compute the difference $s_3(G_3) - DS_2^*$:

$$s_3(G_3) - DS_2^* = (n-3)^2 + (a^2 + 15a + 54)/2$$
$$- (2n^2 - 20n - 4an + 4a^2 + 46a + 128)/2$$

$$= (2n^2 - 12n + a^2 + 15a + 72)/2$$

$$- (2n^2 - 20n - 4an + 4a^2 + 46a + 128)/2$$

$$= (8n - 3a^2 + 4an - 31a - 56)/2.$$

We show that $s_3(G_3)-DS_2^* > 0$ by showing that $8n-3a^2+4an-31a-56 > 0$. We have

$$8n + 4an - 3a^2 - 31a - 56 = 8n - 56 + a(4n-3a-31).$$

Since $n \geq 10$, $8n-56 > 0$. Also, $2a+4 > n-4$ so $a > 0$. Hence, we need only show that $4n-3a-31 \geq 0$. Since $a \leq n-10$, we have:

$$4n-3a-31 \geq 4n-3(n-10)-31 = n-1 > 0.$$

So $s_3(G_3) > DS_2^*$.

•<u>Case 2</u>: G cannot have $\delta = 5$.

As in the case $\delta = 4$, we construct a (not necessarily realizable) degree sequence for a graph with $2n-2 \leq e \leq 3n-10$ and $\delta = 5$ such that $\sum_{i=1}^{n} \binom{d_i}{2}$ is the maximum possible. We then show that the graph G_3 has $s_3 > \sum_{i=1}^{n} \binom{d_i}{2}$ for that sequence.

Let $\delta = 5$.

Then $2e \geq 5n$. We have $2e \leq 6n-20$. So $5n \leq 6n-20 \iff 0 \leq n-20 \iff 20 \leq n$. Thus, for $\delta = 5$, we must have $n \geq 20$.

As in Case 2, we must maximize the largest degree in the sequence subject to the constraint that $\Delta \le n-4$. We have $e = 2n + a$ and $2e = 4n + 2a$. So, after we use up $5n$ "degrees", we have $(4n + 2a) - 5n = 2a - n$ left. To construct the sequence, we begin with 5^n. We then add the remaining $2a - n$ to the first term resulting in the sequence:

where 5^{n-1},

wh $5 \le 2a-n+5 \le n-15.$

The upper bound is obtained from $2e \le 6n - 20$.

The upper bound is obtained from $2e \le 6n - 20$.

We now show that $s_3(G_3) > \sum_{i=1}^{n} \binom{d_i}{2}$ for the degree sequence DS. Let DS* denote $\sum_{i=1}^{n} \binom{d_i}{2}$ for DS = $(2a-n+5)5^{n-1}$ with $5 \le 2a-n+5 \le n-15$. We compute DS*:

$$DS^* = \binom{2a-n+5}{2} + (n-1)\binom{5}{2}$$

$$= (2a-n+5)(2a-n+4)/2 + 10(n-1)$$

$$= (n^2 - 9n - 4an + 4a^2 + 18a + 20)/2 + (20n-20)/2$$

$$= (n^2 + 11n - 4an + 4a^2 + 18a)/2.$$

We compute the difference $s_3(G_3)$ - DS*:

$$s_3(G_3) - DS^* = (n - 3)^2 + (a^2 + 15a + 54)/2$$

$$- (n^2 + 11n - 4an + 4a^2 + 18a)/2$$

$$= (2n^2 - 12n + a^2 + 15a + 72)/2$$
$$- (n^2 + 11n - 4an + 4a^2 + 18a)/2$$
$$= (n^2 - 23n + 4an - 3a^2 - 3a + 72)/2.$$

We show that $s_3(G_3)$-DS* > 0 by showing that $n^2-23n+4an-3a^2-3a+72 > 0$ using $5 \le 2a-n+5 \le n-15$:

$$n^2 - 23n + 4an - 3a^2 - 3a + 72$$
$$> n^2 - 23n + 4(n/2)n - 3(n-10)^2 - 3(n-10) + 72$$
$$= n^2 - 23n + 2n^2 - 3(n-10)^2 - 3(n-10) + 72$$
$$= n^2 - 23n + 2n^2 - 3n^2 + 60n - 300 - 3n + 30 + 72$$
$$= 34n - 198 > 0 \text{ since } n \ge 20.$$

So $s_3(G_3) > DS^*$.

•<u>Case 3</u>: G cannot have $\delta \ge 6$.

Otherwise $2e = \sum_{i=\kappa}^{n} d_i \ge 6n$ so that $e \ge 3n$. But we have $e \le 3n - 10$. This is impossible.

#

We now come to one of the main results of this section. In Theorem 4.16, we prove that the graphs G_2 and G_3 are the only 3-optimal graphs for $2n-2 \le e \le 3n-11$, depending on n and e. The proof considers "adversary" graphs which may be 3-optimal. The previous lemmas in this section limit the adversaries to having maximum degree $\leq$ n-4 and minimum degree $\leq$ 3.

Theorem 4.16 Let $e = 2n + a$, with $-2 \leq a \leq n-10$ so that $2n-2 \leq e \leq 3n-10$.

If $n < 13 + 2a$, G_3 is uniquely 3-optimal.

If $n > 13 + 2a$, G_2 is uniquely 3-optimal.

If $n = 13 + 2a$, G_2 and G_3 are the only 3-optimal graphs.

Proof: We prove the result by induction on n + e.

Basis:

The smallest n and e for which we have $2n-2 \leq e \leq 3n-10$ is $n = 8$ and $e = 2(8)-2 = 14$. Thus $a = -2$ and $8 < 13+2a$. The graph G_3 is the proposed unique 3-optimal graph. G_3 has the degree sequence $5^2 4 3^4 2$, no triangles, and $s_3 = 39$.

By Lemma 4.15, any 3-optimal graph with $n = 8$ and $e = 14$ must have $\delta = 1, 2$, or 3. By Lemmas 4.11, 4.13, and 4.14, the only possible graphs which might have a larger s_3 than G_3 are those with $\Delta \leq n-4$, i.e. $\Delta \leq 4$. There are only four (not necessarily realizable) degree sequences to consider:

$$DS_1 = 4^6 3 1,\ DS_2 = 4^6 2^2,\ DS_3 = 4^5 3^2 2,\ DS_4 = 4^4 3^4.$$

By Corollary 3.4, the sequence DS_1 cannot correspond to a 3-optimal graph since there is a vertex of degree 1 and more than one vertex of maximum degree. Even if the sequences DS_2, DS_3, and DS_4 could be realized by graphs having no triangles, their values of s_3 would be too small:

$$s_3(G_{DS2}) \leq 38, \; s_3(G_{DS3}) \leq 37, \; s_3(G_{DS4}) \leq 36.$$

Induction:

Assume that the result holds for all graphs with n' vertices and e' edges such that $n' + e' < n + e$. Assume on the contrary that for n vertices and e edges there is a 3-optimal graph G, $G \neq G_2$, $G \neq G_3$, such that $s_3(G) \geq s_3(G_2)$ and $s_3(G) \geq s_3(G_3)$. . We will show that this is impossible.

By Lemma 4.15 , we need only consider the cases where $\delta = 1$, 2, and 3.

•Case 1: Let G have $\delta = 1$.

Let G_2' be the graph obtained by adding a pendant edge incident to a vertex of maximum degree in G_2. Let G_3' be the graph obtained by adding a pendant edge incident to a vertex of maximum degree in G_3. Note that G_2' and G_3' are not 3-optimal in their class. We will show that $s_3(G) < s_3(G_2')$ or $s_3(G) < s_3(G_3')$.

Let u be a vertex with degree $d_u = 1$ in G. Let x be the neighbor of u with degree d_x. Recall that by Theorem 3.1, x has the maximum degree in G. Then

$$
\begin{aligned}
s_3(G) &= s_3(G\text{-}u) + \mathbb{N}(u) + \binom{d_u}{2} \\
&= s_3(G\text{-}u) + (d_x-1) + \binom{1}{2} \\
&= s_3(G\text{-}u) + (d_x-1).
\end{aligned}
$$

The graph G-u is in the class of graphs having n' vertices and e' edges as follows:

$$
\begin{aligned}
n' &= n-1 \\
e' &= e-1 \\
&= 2n+a-1 \\
&= 2(n-1)+2+a-1 \\
&= 2(n-1)+(a+1) \\
&= 2n'+a',
\end{aligned}
$$

where $a' = a+1$.

In order to apply the Induction Hypothesis, we must have

$$
\begin{aligned}
&a' \le n' - 10 \iff \\
&a+1 \le (n-1) - 10 \iff \\
&a \le n - 12.
\end{aligned}
$$

We have two cases to consider:

$$n' \geq 13 + 2a'$$

$$n' < 13 + 2a'.$$

•<u>Case 1.1</u>: Let $n' \geq 13 + 2a'$.

We compare $s_3(G)$ with $s_3(G_2')$.

Let u_2 be the vertex of degree $du_2 = 1$ in G_2'. Then $IN(u_2)$ is simply one less than the degree of the neighbor of u_2. Recall that this vertex has degree n-2 in G_2'. We get

$$\begin{aligned} s_3(G_2') &= s_3(G_2'-u_2) + IN(u_2) + \binom{du_2}{2} \\ &= s_3(G_2(n',e')) + (n-3) + \binom{1}{2} \\ &= s_3(G_2(n',e')) + (n-3). \end{aligned}$$

By the Induction Hypothesis, $G_2(n',e')$ is 3-optimal in its class since $n' \geq 13+2a'$. Thus

$$s_3(G-u) \leq s_3(G_2(n',e')).$$

Furthermore,

$$(d_x-1) \leq (n-5).$$

Therefore

$$s_3(G-u) + (d_x-1) < s_3(G_2(n',e')) + (n-3) \iff$$
$$s_3(G) < s_3(G_2').$$

This contradicts the assumption that G is 3-optimal.

•<u>Case 1.2</u>: Let $n' < 13 + 2a'$.

We compare $s_3(G)$ with $s_3(G_3')$.

Let u_3 be the vertex of degree $du_3 = 1$ in G_3'. Its neighbor has degree n-3. We get

$$\begin{aligned} s_3(G_3') &= s_3(G_3'-u_3) + IN(u_3) + \binom{du_3}{2} \\ &= s_3(G_3(n',e')) + (n-4) + \binom{1}{2} \\ &= s_3(G_3(n',e')) + (n-4). \end{aligned}$$

By the Induction Hypothesis, $G_3(n',e')$ is uniquely 3-optimal in its class since $n' < 13+2a'$. Thus

$$s_3(G-u) < s_3(G_3(n',e')).$$

Furthermore,

$$(d_x-1) \leq (n-5).$$

Therefore

$$s_3(G-u) + (d_x-1) < s_3(G_3(n',e')) + (n-4) \iff$$

$$s_3(G) < s_3(G_3').$$

This contradicts the assumption that G is 3-optimal.

•<u>Case 1.3</u>: Let $a = n-11$.

Here the graph G-u is in the class with n' vertices and $e' = 3n'-9$

edges. We cannot use the Induction Hypothesis. However, we know that the complete bipartite graph $K_{3,n'-3}$ is uniquely 3-optimal in this case. We again consider the graph G_3' since $G_3' - u_3 = K_{3,n'-3}$.

We get

$$s_3(G_3') = s_3(G_3'-u_3) + IN(u_3) + \binom{d_{u_3}}{2}$$

$$= s_3(K_{3,n'-3}) + (n-4) + \binom{1}{2}$$

$$= s_3(K_{3,n'-3}) + (n-4).$$

Since $K_{3,n'-3}$ is uniquely 3-optimal in its class,

Sin

$$s_3(G-u) < s_3(K_{3,n'-3}).$$

Furthermore,

Furthermore,

$$(d_x-1) \leq (n-5).$$

$$(d_x-1) \leq (n-5).$$

Therefore

$$s_3(G-u) + (d_x-1) < s_3(K_{3,n'-3}) + (n-4) \iff$$

$$s_3(G) < s_3(G_3').$$

This contradicts the assumption that G is 3-optimal.

•<u>Case 1.4</u>: Let $a = n-10$.

We compare $s_3(G)$ with $s_3(G_3)$.

Observe that $s_3(G-u) = s_3((G-u) \cup u)$. Thus

$$s_3(G) = s_3((G\text{-}u) \cup u) + (d_x\text{-}1).$$

Now the graph $(G\text{-}u) \cup u$ is in the class of graphs with $n' = n$ vertices and $e' = 3n'\text{-}11$ edges. By the Induction Hypothesis, $G_3(n',e')$ is 3-optimal since

$$n \le 13 + 2(n\text{-}11) \iff$$
$$n \le 13 + 2n\text{-}22 \iff$$
$$n \ge 9.$$

We compare $s_3(G)$ with $s_3(G_3(n,3n\text{-}10))$. If we add an edge to $G_3(n,3n\text{-}11)$ between the vertex of degree n-5 and a vertex of degree 2, we obtain $G_3(n,3n\text{-}10)$ and an increase in s_3 of

$$(n\text{-}2)^2 + ((n\text{-}10)^2 + 15(n\text{-}10) + 54)/2$$
$$- [(n\text{-}2)^2 + ((n\text{-}11)^2 + 15(n\text{-}11) + 54)/2]$$
$$= ((n\text{-}10)^2 - (n\text{-}11)^2 + 15)/2$$
$$= ((n^2 - 20n + 100) - (n^2 - 22n + 121) + 15)/2$$
$$= (2n - 6)/2$$
$$= n - 3.$$

Therefore we have

$$s_3(G_3(n,3n\text{-}10)) = s_3(G_3(n,3n\text{-}11)) + (n\text{-}3).$$

Since $G_3(n,3n\text{-}11)$ is 3-optimal, we have

$$s_3((G\text{-}u) \cup u) \le s_3(G_3(n,3n\text{-}11)).$$

Furthermore

$$(d_x-1) < (n-5).$$

Therefore

$$s_3((G-u) \cup u) + (d_x-1) < s_3(G_3(n,3n-11)) + (n-3) \Leftrightarrow$$
$$s_3(G) < s_3(G_3(n,3n-10)).$$

This contradicts the assumption that G is 3-optimal.

This completes the proof of Case 1. #

•<u>Case 2</u>: Let G have $\delta = 2$.

Let u be a vertex with degree $d_u = 2$ in G. Then

$$s_3(G) = s_3(G-u) + IN(u) + \binom{d_u}{2}.$$

We consider two cases:

$$n \geq 13 + 2a$$
$$n < 13 + 2a.$$

•<u>Case 2.1</u>: Let $n \geq 13 + 2a$.

Then the proposed 3-optimal graph is G_2. Let u_2 be a vertex of degree 2 in G_2. Thus

$$s_3(G_2) = s_3(G_2-u_2) + IN(u_2) + \binom{2}{2}.$$

where $IN(u_2) = 2(n-3)$.

So we have

$$s_3(G) \geq s_3(G_2) \iff$$
$$s_3(G-u) + IN(u) + \binom{2}{2} \geq s_3(G_2-u_2) + IN(u_2) + \binom{2}{2}$$

Now G_2-u_2 and G-u are in the same class since we are removing one vertex and two edges from each. The number of vertices and edges in the class are n' and e', respectively:

$$n' = n-1$$
$$\begin{aligned} e' &= e-2 \\ &= (2n+a) - 2 \\ &= 2(n-1)+2+a-2 \\ &= 2(n-1)+a \\ &= 2n' + a', \end{aligned}$$

where $a' = a$.

By the Induction Hypothesis, either G_2 or G_3 or both are uniquely 3-optimal in this class (with n' vertices and e' edges). Note that $G_2(n',e') = G_2(n,e) - u_2$. There are two possibilities to consider:

$$n' \geq 13 + 2a'$$
$$n' < 13 + 2a'.$$

•Case 2.1.1: Let $n' \geq 13 + 2a'$.

By the Induction Hypothesis, $G_2(n,e)-u_2 = G_2(n',e')$ is 3-optimal. Hence

$$s_3(G\text{-}u) \leq s_3(G_2\text{-}u_2).$$

Furthermore, $IN(u) < 2(n-3)$. Otherwise, one of the two neighbors of u would have at least n-3 incident edges from IN(u). In addition there is the edge between u and that vertex giving it degree $\geq$ n-2. This is impossible since the maximum degree in G is $\leq$ n-4.

Therefore

$$s_3(G\text{-}u) + IN(u) + \binom{2}{2} < s_3(G_2\text{-}u_2) + 2(n-3) + \binom{2}{2} \Leftrightarrow$$

$$s_3(G) < s_3(G_2).$$

This contradicts the assumption that G is 3-optimal.

•Case 2.1.2: Let $n' < 13 + 2a'$.

Recall that $n' = n-1$ and $a' = a$. So

$$n' < 13 + 2a' \Leftrightarrow (n-1) < 13 + 2a \Leftrightarrow n < 14 + 2a.$$

Since we have $n \geq 13 + 2a$, it must be that $n = 13 + 2a$. So

$$n' = n-1 = 13+2a-1 = 12+2a = 12+2a'.$$

In this case, the graph $G_2(n,e) - u_2 = G_2(n',e')$ is not 3-optimal. By the

Induction Hypothesis, the graph $G_3(n',e')$ is uniquely 3-optimal. We now calculate the difference $s_3(G_3(n',e')) - s_3(G_2(n',e'))$:

$$s_3(G_3(n',e')) = (n'-3)^2 + (a'^2 + 15a' + 54)/2$$

$$s_3(G_2(n',e')) = (n'-2)^2 + (a'^2 + 7a' + 15)/2$$

$$\begin{aligned} s_3(G_3(n',e')) - s_3(G_2(n',e')) & \\ &= n'^2 - 6n' + 9 + (a'^2 + 15a' + 54)/2 \\ &\quad - (n'^2 - 4n' + 4 + (a' + 7a' + 12)/2) \\ &= -2n' + 4a' + 26 \\ &= -2(12+2a') + 4a' + 26 \\ &= 2 \end{aligned}$$

Thus, $s_3(G_2(n,e) - u_2) = s_3(G_3(n',e')) - 2$.

So,

$$s_3(G\text{-}u) + IN(u) + \binom{2}{2} \geq s_3(G_2(n,e)\text{-}u_2) + 2(n-3) + \binom{2}{2} \Leftrightarrow$$

$$s_3(G\text{-}u) + IN(u) + \binom{2}{2} \geq s_3(G_3(n,e)\text{-}u_2) - 2 + 2(n-3) + \binom{2}{2}.$$

Now $s_3(G_3(n',e')) \geq s_3(G\text{-}u)$. Furthermore $2(n-3) - 2 > IN(u)$. Otherwise, one of the two neighbors of u would have at least n-4 incident edges from IN(u). In addition there is the edge between u and that vertex giving it a degree $\geq$ n-3. This is impossible since the maximum degree in G is $\leq$ n-4.

Therefore, it is impossible to have

$$s_3(G\text{-}u) + 2 + IN(u) + \binom{2}{2} \geq s_3(G_3(n',e')) + 2(n-3) + \binom{2}{2} \Leftrightarrow$$

$$s_3(G) \geq s_3(G_3).$$

•<u>Case 2.2</u>: Let $n < 13 + 2a$.

Then the proposed unique 3-optimal graph is G_3 and G_3 has a vertex of degree 2. Call that vertex u_3. Thus we may write

$$s_3(G_3) = s_3(G_3\text{-}u_3) + IN(u_3) + \binom{2}{2}$$

where $IN(u_3) = 2(n\text{-}3)$.

So we have

$$s_3(G_3) \leq s_3(G) <=>$$

$$s_3(G_3\text{-}u_3) + IN(u_3) + \binom{2}{2} \leq s_3(G\text{-}u) + IN(u) + \binom{2}{2}$$

Now $G_3\text{-}u_3$ and $G\text{-}u$ are in the same class since we are removing one vertex and two edges from each. The number of vertices and edges in the class are n' and e', respectively:

$$n' = n\text{-}1$$

$$\begin{aligned} e' &= e\text{-}2 \\ &= (2n+a) - 2 \\ &= 2(n\text{-}1)+2+a\text{-}2 \\ &= 2(n\text{-}1)+a \\ &= 2n' + a', \end{aligned}$$

where $a' = a$.

By the Induction Hypothesis, either G_2 or G_3 or both graphs are uniquely 3-optimal in this class (with n' vertices and e' edges). Note that $G_3(n',e') = G_3(n,e) - u_3$. There are two possibilities to consider:

$$n' \leq 13 + 2a'$$

$$n' > 13 + 2a'.$$

•<u>Case 2.2.1</u>: Let $n' \leq 13 + 2a'$.

By the Induction Hypothesis, $G_3(n,e)-u_3 = G_3(n',e')$ is 3-optimal. Hence

$$s_3(G-u) \leq s_3(G_3-u_3).$$

Furthermore, $IN(u) < 2(n-3)$. Otherwise, one of the two neighbors of u would have at least n-3 incident edges from IN(u). In addition there is the edge between u and that vertex giving it degree $\geq$ n-2. This is impossible since the maximum degree in G is $\leq$ n-4.

Therefore

$$s_3(G-u) + IN(u) + \binom{2}{2} < s_3(G_3-u_3) + 2(n-3) + \binom{2}{2} \Leftrightarrow$$

$$s_3(G) < s_3(G_3).$$

This contradicts the assumption that G is 3-optimal.

•<u>Case 2.2.2</u>: Let $n' > 13 + 2a'$.

But we have $n < 13 + 2a$ where $n = n'+1$ and $a = a'$. This is impossible.

This completes the proof of Case 2. ∞

•<u>Case 3</u>: Let G have $\delta = 3$.

Let u be a vertex with degree $d_u = 3$ in G. Then

$$s_3(G) = s_3(G\text{-}u) + IN(u) + \binom{d_u}{2}$$

We have two cases to consider:

$$n \leq 13 + 2a$$

$$n > 13 + 2a$$

•<u>Case 3.1</u>: Let $n \leq 13 + 2a$.

Then the proposed 3-optimal graph is G_3 and G_3 has a vertex of degree 3. Call that vertex u_3. Thus we may write

$$s_3(G_3) = s_3(G_3\text{-}u_3) + IN(u_3) + \binom{3}{2}$$

where $IN(u_3) = e\text{-}3$.

So we have

$$s_3(G_3) \leq s_3(G) \iff$$

$$s_3(G_3\text{-}u_3) + IN(u_3) + \binom{3}{2} \le s_3(G\text{-}u) + IN(u) + \binom{3}{2}$$

Now G_3-u_3 and G-u are in the same class since we are removing one vertex and three edges from each. The number of vertices and edges in the class are n' and e', respectively:

$$n' = n-1$$
$$e' = e-3$$
$$= (2n+a) - 3$$
$$= 2(n-1)+2+a-3$$
$$= 2(n-1) + (a-1)$$
$$= 2n' + a',$$

where $a' = a - 1$.

If $a \geq -1$, then $a' \geq -2$ and by the Induction Hypothesis, either G_2 or G_3 or both graphs are the unique 3-optimal graphs in the class (with n' vertices and e' edges). When $a = -2$, however, $a' = -3$ and we cannot use the Induction Hypothesis. However, it was shown in Theorem 4.9 that for $e = 2n - 3$, the only graphs which are 3-optimal are G_2, G_3, or both, plus G_1. It is impossible for G_1 = G-u since then G would have vertices of degree $\geq n-2$. So we need not give any special consideration to the case $a' = -3$. There are two possibilities:

$$n' \leq 13 + 2a'$$
$$n' > 13 + 2a'.$$

•<u>Case 3.1.1</u>: Let $n' \leq 13 + 2a'$.

By the Induction Hypothesis, $G_3(n,e)-u_3 = G_3(n',e')$ is 3-optimal. Hence

$$s_3(G_3-u_3) \geq s_3(G-u).$$

But we have

$$s_3(G_3-u_3) + (e-3) + \binom{3}{2} \leq s_3(G-u) + IN(u) + \binom{3}{2}.$$

So, $IN(u) \geq e-3$. $IN(u) > e-3$ is impossible since u has degree 3 and we would need to have more than e edges in G to have $IN(u) > e-3$. So the best we can do is $IN(u) = e-3$. In that case, $s_3(G_3-u_3) = s_3(G-u)$, $G_3-u_3 = G-u$, and so $G_3 = G$.

•<u>Case 3.1.2</u>: Let $n' > 13 + 2a'$.

Recall that $n' = n-1$ and $a' = a-1$. So

$$n' > 13 + 2a' \iff$$
$$(n-1) > 13 + 2(a-1)a \iff$$
$$n > 12 + 2a.$$

Since we have $n \leq 13 + 2a$, it must be that $n = 13 + 2a$. So

$$n' = n-1 = 13+2a-1 = 13+2(a-1) + 1 = 14+2a'.$$

In this case, the graph $G_3(n,e) - u_3 = G_3(n',e')$ is not 3-optimal. By the Induction Hypothesis, the graph $G_3(n',e')$ is uniquely 3-optimal. We now calculate the difference $s_3(G_2(n',e')) - s_3(G_3(n',e'))$:

$$s_3(G_2(n',e')) = (n'-2)^2 + (a'^2 + 7a' + 15)/2$$

$$s_3(G_3(n',e')) = (n'-3)^2 + (a'^2 + 15a' + 54)/2$$

$$\begin{aligned} s_3(G_2(n',e')) - s_3(G_3(n',e')) \\ &= n'^2 - 4n' + 4 + (a'^2 + 7a' + 12)/2 \\ &\quad - (n'^2 - 6n' + 9 + (a'^2 + 15a' + 54)/2) \\ &= 2n - 4a' - 26 \\ &= 2(14+2a') - 4a' - 26 = 2. \end{aligned}$$

Thus,

$$s_3(G_3(n,e) - u_3) = s_3(G_2(n',e')) - 2.$$

So,

$$s_3(G\text{-}u) + IN(u) + \binom{3}{2} \geq s_3(G_3(n,e)\text{-}u_3) + (e-3) + \binom{3}{2} \iff$$

$$s_3(G\text{-}u) + IN(u) + \binom{3}{2} \geq s_3(G_2(n',e')) - 2 + (e-3) + \binom{3}{2}$$

Since $s_3(G_2(n',e')) > s_3(G\text{-}u)$, $(e-3) - 2 < IN(u)$, i.e. $IN(u) \geq e-4$.

Let v, w, and x be the neighbors of u. Let $v_1, v_2, \ldots v_m$ be the neighbors of v, w, x, with $v_i \neq u$. Then $\{v_1, v_2, \ldots v_m\} = V(G) - \{u,v,w,x\}$:

Since there is at most one edge left in G which is not in Adj(u) and is not counted in IN(u), that edge would have to be used to attach any vertices not in $\{v_1, v_2, \ldots v_m\}$. But that would result in a vertex of degree 1 which is impossible since $\delta = 3$. So, $m = n-4$.

Now 3 edges are used for the three neighbors of u. This leaves n-3 edges for the rest of the graph. We have two possibilities: $IN(u) = e-4$ and there is one edge not counted in $IN(u)$, or $IN(u) = e-3$. Since $\delta = 3$, each of $v_1, v_2, ...v_m$ must have degree ≥ 3.

Case 1: None of $v_1, v_2, ...v_m$ are adjacent.

Then at least another $3(n-4) = 3n - 12$ edges are needed in G in order to make $deg(v_i) \geq 3$ for all i. But then we would have $3n - 12 + 3 = 3n - 9 > 3n - 10$ edges. This is impossible.

Case 2: Exactly two vertices of $v_1, v_2, ...v_m$ are adjacent.

Then at least another $3(n-4) - 2 = 3n - 14$ edges are needed in G. Thus G must have at lease $(3n-14) + 3 + 1 = 3n - 10$ edges. In fact, this is the maximum value e can take on. We then have $a = n-10$ and since $n = 13 + 2a$, we get

$$n = 13 + 2(n-10) \iff n = 7.$$

But we have $n \geq 8$ so this is impossible.

•Case 3.2: Let $n > 13 + 2a$.

Then the proposed unique 3-optimal graph is G_2 and G_2 has a vertex of degree 3. Call that vertex u_2. Thus we may write

$$s_3(G_2) = s_3(G_2-u_2) + IN(u_2) + \binom{3}{2}$$

where $IN(u_2) = e-3$.

So we have

$$s_3(G_2) \leq s_3(G) \iff$$
$$s_3(G_2\text{-}u_2) + IN(u_2) + \binom{3}{2} \leq s_3(G\text{-}u) + IN(u) + \binom{3}{2}$$

Now G_2-u_2 and G-u are in the same class since we are removing one vertex and three edges from each. The number of vertices and edges in the class are n' and e', respectively:

$$\begin{aligned} n' &= n-1 \\ e' &= e-3 \\ &= (2n+a) - 3 \\ &= 2(n-1)+2+a-3 \\ &= 2(n-1) + (a-1) \\ &= 2n' + a', \end{aligned}$$

where a' = a - 1.

As in Case 3.1, G_2 or G_3 or both graphs are the only 3-optimal graphs in the class (with n' vertices and e' edges). This is the case either by the Induction Hypothesis if a' > -3, or by Theorem 4.9 if a' = 3. We have two possibilities:

$$n' \geq 13 + 2a'$$
$$n' < 13 + 2a'.$$

•<u>Case 3.2.1</u>: Let $n' \geq 13 + 2a'$.

By the Induction Hypothesis, $G_2(n,e)$-u_2 = $G_2(n',e')$ is 3-optimal.

Hence

$$s_3(G_2\text{-}u_2) \geq s_3(G\text{-}u).$$

But we have

$$s_3(G_2\text{-}u_2) + (e\text{-}3) + \binom{3}{2} \leq s_3(G\text{-}u) + IN(u) + \binom{3}{2}.$$

So, $IN(u) \geq e\text{-}3$. $IN(u) > e\text{-}3$ is impossible since u has degree 3 and we would need to have more than e edges in G to have $IN(u) > e\text{-}3$. So the best we can do is $IN(u) = e\text{-}3$. In that case, $s_3(G_2\text{-}u_2) = s_3(G\text{-}u)$, $G_2\text{-}u_2 = G\text{-}u$, and so $G_2 = G$.

•Case 3.2.2: Let $n' < 13 + 2a'$.

Recall that $n' = n\text{-}1$ and $a' = a\text{-}1$. So

$$n' < 13+2a' \iff n\text{-}1 < 13+2(a\text{-}1) \iff n < 12+ 2a.$$

But we have $n \geq 13 + 2a$, so this is impossible.

This completes the proof of Case 3. #

We can now conclude that there is no graph G in the same class as G_2 and G_3 which has $s_3(G) \geq s_3(G_2)$ and $s_3(G) \geq s_3(G_3)$. Hence G_2 and G_3 are the unique 3-optimal graphs as per the constraints on n and a.

#

We now combine Theorems 4.9 and 4.16 with the result on complete bipartite graphs in Chapter 2 into a single result covering all cases $2n - 3 \le e \le 3n - 9$. Note that we need not restrict ourselves to $n > 7$. The graphs with $n = 6$ and $n = 7$ of Lemma 4.6 fall within the pattern of 3-optimal graphs within our range. Graphs with smaller n fall within the pattern also but do not satisfy $2n - 3 \le e \le 3n - 9$.

Theorem 4.17 Let $e = 2n + a$ with $2n-3 \le e \le 3n-9$ and $-3 \le a \le n-9$. Then the following are the only 3-optimal graphs:

If $n \ge 13 + 2a$, G_2 is 3-optimal.

If $n \le 13 + 2a$, G_3 is 3-optimal.

In addition, for $a = -3$, $a \ne n-9$, G_1 is 3-optimal.

Proof:

In Theorem 4.9 we showed that the result is true for $e = 2n - 3$. In Theorem 4.16, we showed the result for $2n-2 \le e \le 3n-10$. From our discussion in Chapter 2, $K_{3,n-3}$ is uniquely 3-optimal for $e = 3n-9$.

#

We conclude this section by addressing the issue of uniformly vertex reliable graphs. Recall that such graphs minimize the unreliability polynomial for all probabilities of node failure q. Such graphs have to be both κ-optimal and 3-optimal. Recall that κ-optimal graphs must be max-κ. That is, they must have $\kappa = \lfloor 2e/n \rfloor$. Unfortunately, with the exception of the star, K_n minus the edges in a matching, and regular complete bipartite graphs, none of the 3-optimal graphs found so far are max-κ. In particular, this is the case for the range $2n - 3 \leq e \leq 3n - 9$: except for the cases noted above, there are no uniformly optimally reliable graphs for this range of e. We note here that Stivaros and Suffel have shown that the star and K_n minus the edges in a matching are uniformly vertex reliable. We have obtained their results by private communication.

4.3 3-OPTIMAL GRAPHS FOR $e \leq \lfloor n^2/4 \rfloor$

In the final section of this paper, we present a conjecture which generalizes the results of Theorems 2.3 and 4.17.

Recall that in Theorem 2.3, the 3-optimal graphs were G_A and G_B. G_A can be viewed as the complete bipartite graph $K_{1,n-1}$ with edges added and G_B can be viewed as the complete bipartite graph $K_{2,n-2}$ with edges removed. This covered the range of edges $n-1 \leq e \leq 2n-4$.

In Theorem 4.17, a similar situation existed. There the range of edge values was $2n-3 \leq e \leq 3n-9$. The graphs G_2 and G_3 were 3-optimal. G_2 can be viewed as the complete bipartite graph $K_{2,n-2}$

with edges added. G_3 can be viewed as the complete bipartite graph $K_{3,n-3}$ with edges removed.

In our conjecture, we will use complete bipartite graphs as the basis for constructing 3-optimal graphs. After finding the appropriate range into which e fits, we will either add edges to one complete bipartite graph or remove edges from another complete bipartite graph. Which procedure is to be followed is determined by constraints on n and e.

Note that the graph G_1 was 3-optimal as well as G_2 and G_3 when e = 2n-3. We do not as yet have a conjecture regarding a generalization of this case. However, we strongly suspect that other graphs will be 3-optimal in certain cases besides those proposed here.

We let n be the number of vertices. The number of edges will be expressed in terms of two integers, k and a. The values of n, e, k, and a must satisfy the following:

$$e = kn + a.$$

$$1 \leq k \leq n-k$$

$$-(k^2 - 1) \leq a \leq n - (k + 1)^2.$$

Note that in Theorem 2.3, we had k = 1 in that e = n+a. The case for e = n-1, although covered in Theorem 2.3, is outside the range $-(k^2 - 1) \leq a \leq n - (k + 1)^2$. The exception is due to that fact that the 3-optimal graph in that case is the complete bipartite graph $K_{1,n-1}$. The range for k = 1 is $0 \leq a \leq n - 4$ or $n \leq e \leq 2n - 4$. In Theorem 4.16, we had k = 2 and e = 2n+a. The ranges for a and e were $-3 \leq a \leq n - 9$ and $2n-3 \leq e \leq 3n - 9$. In general, we have the following range for e:

$$kn-k^2 + 1 \leq e \leq (k+1)n - (k+1)^2.$$

Now, consider the complete bipartite graphs $K_{k,n-k}$ and $K_{k+1,n-(k+1)}$. $K_{k,n-k}$ has n vertices and $e_1 = kn - k^2$ edges. $K_{k+1,n-(k+1)}$ has n vertices and $e_2 = (k+1)n - (k+1)^2$ edges. So, we have

$$kn-k^2 + 1 \leq e \leq (k+1)n - (k+1)^2 \iff$$

$$e_1 + 1 \leq e \leq e_2.$$

It is the graphs $K_{k,n-k}$ and $K_{k+1,n-(k+1)}$ which will serve as the basis for constructing our proposed 3-optimal graphs. We will add edges to graph $K_{k,n-k}$ or remove edges from the graph $K_{k+1,n-(k+1)}$. As in Theorems 2.3 and 4.17, there are three cases to consider, depending on constraints. In Theorem 4.15, we compared n with $2a + 13$. That was because when $n = 2a+ 3$, $s_3(G_2) = s_3(G_3)$. Similarly, $n > 2a+13$ corresponded to $s_3(G_2) > s_3(G_3)$, and $n < 2a+13$ corresponded to $s_3(G_2) < s_3(G_3)$. We will call the number used in the constraints C_k in general. The computation of C_k will be given after the construction of the proposed 3-optimal graphs is presented.

We propose that the following graphs are 3-optimal, given n, e, k, and a as defined above:

•Case 1 Let $n \geq 2a + C_k$.

Begin with the graph $K_{k,n-k}$. Add $(kn+a) - (kn-k^2) = a + k^2$ edges. All of the added edges will have as one endpoint a vertex originally of degree k. For each edge, the other endpoint will be one of the other vertices of degree k. In addition, if $a + k^2 - 1 \leq k$, all of the added edges may be placed between vertices originally of degree n-k in the same fashion.

•<u>Case 2</u> Let $n \leq 2a + C_k$.

Begin with the graph $K_{k+1,n-(k+1)}$. Remove $(k+1)(n-k-1) - (kn+a) = n-(a+(k+1)^2)$ edges with all of the removed edges incident to a vertex originally of degree $n-(k+1)$.

We now compute the value of C_k. We believe that the significance of C_k is purely number theoretic. Because of this, we have no intuitive explanation for its value. Suffice it to say that the number is related to the comparison of the s_3 values of the two proposed 3-optimal graphs. Compute C_k recursively as follows:

$$C_1 = 5,$$

$$C_k = C_{k-1} + 4k \text{ for } k > 1.$$

More simply, we have

$$C_k = 5 + \sum_{i=2}^{k} i.$$

APPENDIX

We present the proofs of Theorems 2.21 and 2.2b, and Lemma 4.5.

Theorem 2.2a For n vertices and e = n+1 edges, n > 7, the unique 3-optimal graph is $G_A(n,n+1)$. For smaller n, the 3-optimal graphs are shown in Figure A1.

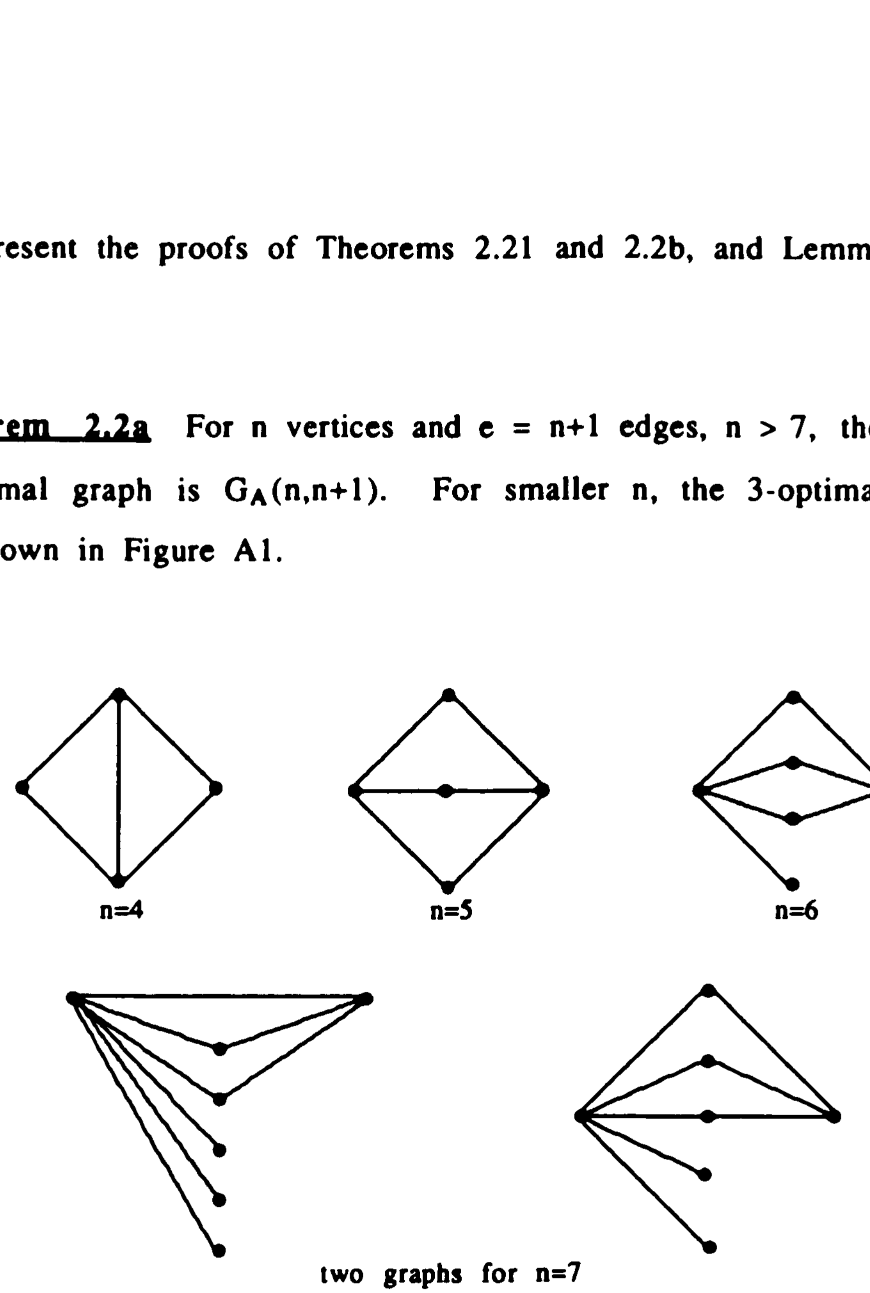
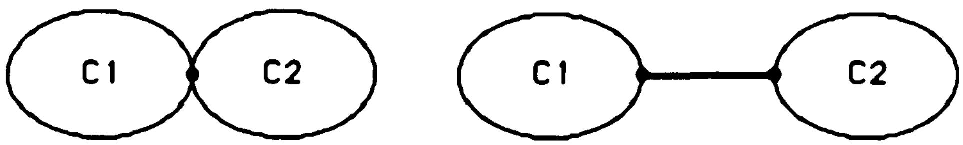


Figure A1. The 3-optimal graphs for e = n + 1, n ≤ 7.

Proof: Observe that any graph G with n vertices and e = n+1 edges is planar and contains two circuits, C_1 and C_2. These circuits may have no edges in common or they may have an edge in common. In the latter case, any common edges will constitute a single path. The possibilities are shown in Figure A2. In addition, G may have trees attached at any vertex. See Figure A3(a).



(a) C_1 and C_2 have no common edges.

(b) C_1 and C_2 have at least one edge in common

Figure A2. G has n vertices and e = n+1 edges.

We transform G by performing the steps below.

•<u>Step 1</u>: Convert all trees to stars.

Let v be a vertex which lies on a circuit or on a path between circuits so that v also lies on a tree. Thus v has degree d ≥ 3. Let v_1 be a vertex on the tree which is adjacent to v and has degree $d_1 \geq 2$. Contract the edge between v and v_1 and add a pendant edge at v. See Figure A3 for an example.

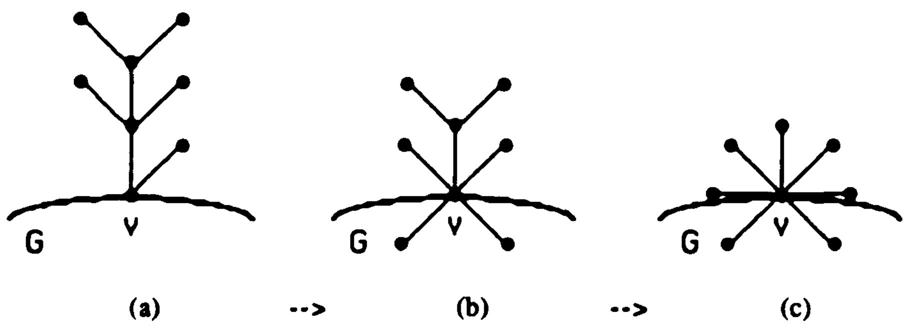


Figure A3. Contract trees to stars.

Since the number of triangles in G is not affected, in order to determine the difference in s_3 values between the two graphs, we need only examine the difference in the value of $\sum_{i=1}^{n} \binom{d_i}{2}$. This is equivalent to examining the difference in $\sum_{i=1}^{n} d_i^2$ between the transformed graph and the original graph. Only the degrees of v, v_1, and the new vertex adjacent to v are affected. We get

$$((d + d_1 - 1)^2 + 1) - (d^2 + d_1^2) = 2(dd_1 - d - d_1 + 1) > 0$$

$$\text{since } d \geq 3,\ d_1 \geq 2.$$

Step 1 is repeated until all trees are transformed into stars.

<u>•Step 2</u>: Contract non-pendant edges which do not lie on circuits.

Here such edges lie on the path between the two circuits (Figure A2(a)). Let v be a vertex which lies on a circuit and has a non-pendant incident edge which does not lie on a circuit. Let v_1 be the other endpoint of that edge. Thus v has degree $d \geq 3$ and v_1 has degree $d_1 \geq 2$. Contract the edge between v and v_1 and add a pendant edge at v. See Figure A4 for an example. As in Step 1, triangles are not affected and we have

$$((d+d_1-1)^2+1) - (d^2+d_1^2) > 0 \text{ since } d \geq 3,\ d_1 \geq 2.$$

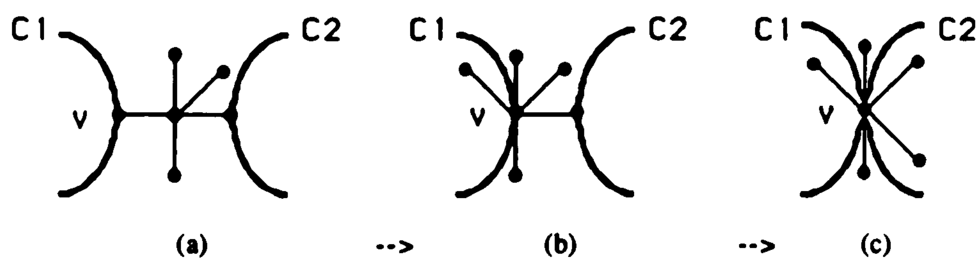


Figure A4. Contract the path between C_1 and C_2 to a vertex.

Step 2 is repeated until all non-pendant edges on the path are contracted.

<u>•Step 3</u>: Combine all attached stars into a single star.

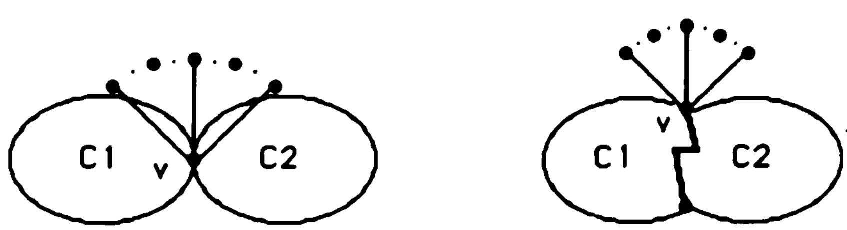
Let E_p be the set of pendant edges in G. Let V_m be the set of vertices in G which have the maximum degree in G-E_p. Choose $v \in V_m$ to be the vertex whose degree in G is maximal compared to all other vertices in V_m. Thus v has degree $d \geq 3$. Let v_1 be the center of a star, $v \neq v_1$. Thus v_1 has degree $d_1 \geq 3$. Let k denote the degree of v_1 in G-E_p. Then k = 2 or k = 3, and $d_1 > k$. Move the star at v_1 to v. As before, triangles are not affected by moving these d_1-k edges and only the degrees of v and v_1 are changed. We get

$$((d + d_1 - k)^2 + k^2) - (d^2 + d_1^2) = 2(dd_1 - kd - kd_1 + k^2).$$

We examine this expression for all possible values of k.

Case k=2: $d \geq 3$, $d_1 \geq 3$ and $2(dd_1 - 2d - 2d_1 + 2^2) > 0$.
Case k=3: $d \geq 3$, $d_1 \geq 4$ and $2(dd_1 - 3d - 3d_1 + 3^2) > 0$ unless d=3. This is impossible since then v_1 would have been selected instead of v.

Step 3 is repeated until there is only one star centered at v. In the end, we are left with one of the two configurations in Figure A5.



(a) One common vertex. (b) One common path.

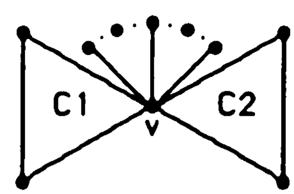
Figure A5. The graph G after Step 3.

•<u>Step 4</u>: Contract the circuits C_1 and C_2 into triangles.

The cases correspond to Figure A5.

Case (a): C_1 and C_2 have exactly one vertex in common.
Let v_1 be a vertex adjacent to v such that v_1 lies on a circuit which is not a triangle. The degree of v is $d \geq 4$ and the degree of v_1 is $d_1 = 2$. Contract the edge between v and v_1 and add a pendant edge at v. See Figure A6(a).

(a) Contract the edge between v and v_1 and add a pendant edge at v.



(b) Continue contractions until circuits are triangles.

Figure A6. Edges on circuits are contracted.

If no triangles are formed by this contraction, the difference in $\sum_{i=1}^{n} d_i^2$ between the two graphs needs to be examined. Only the degrees of v and v_1 are affected. We get:

$$((d + 1)^2 + 1) - (d^2 + 2^2) = 2d - 2 > 0 \text{ since } d \geq 4.$$

If a single triangle is formed by this contraction, the difference in $\sum_{i=1}^{n}\binom{d_i}{2} - 2\tau(G)$ between the two graphs needs to be examined:

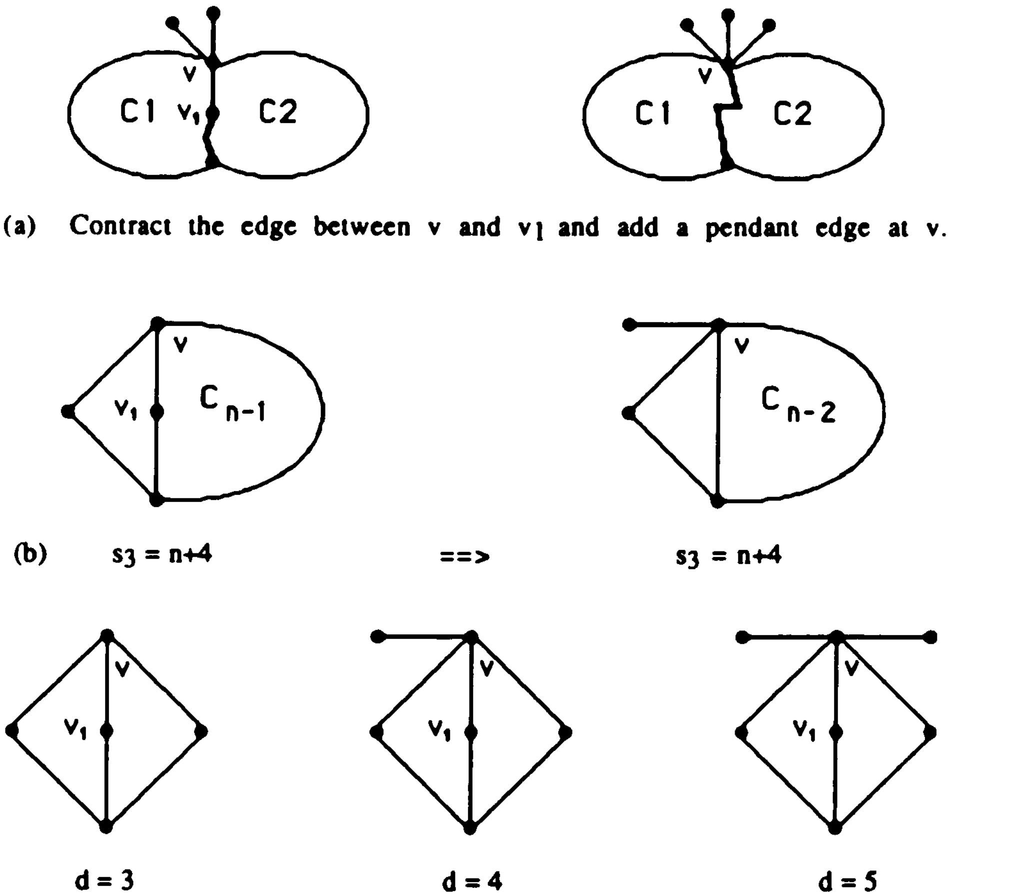
$$\left[\binom{d+1}{2}+\binom{1}{2} - 2(1)\right] - \left[\binom{d}{2}+\binom{2}{2}\right] = d - 3 > 0 \text{ since } d \geq 4.$$

After performing all such contractions, we arrive at the graph in Figure A6(b). The s_3 value for this graph is $\binom{n-1}{2}$. The value of s_3 for $G_A(n,n+1)$ is $\binom{n-1}{2} + 1 > \binom{n-1}{2}$.

<u>Case (b)</u>: C_1 and C_2 have exactly one path in common.

Without loss of generality, choose C_1 and C_2 so that the path they share is as short as possible. Here v has degree $d \geq 3$. We begin by contracting the path common to both circuits to a single edge. Let v_1 be a vertex adjacent to v such that v_1 lies on both circuits and has degree 2. Contract the edge between v and v_1 and add a pendant edge at v. See Figure A7(a).

If no triangles are formed, we need to check 2d-2 as was done in Case(a) above. Here $2d-2 > 0$ because $d \geq 3$. Similarly, if one triangle is formed, the difference in s_3 values is d-3. For $d > 3$, $d-3 > 0$.



(a) Contract the edge between v and v_1 and add a pendant edge at v.

(b) $s_3 = n+4$ ==> $s_3 = n+4$

(c) d = 3 d = 4 d = 5

Figure A7. Edges on circuits are contracted.

For d = 3, we have a graph of the form shown in Figure A7(b). Unless the construction terminates at this step, further contractions of edges which do no lie on triangles will increase the s_3 value. Since n > 7, further contractions will take place. If two triangles are formed, we need to examine the difference in s_3 values :

$$\left[\binom{d+1}{2} + \binom{1}{2} - 2(2) \right] - \left[\binom{d}{2} + \binom{2}{2} \right] = d - 5 > 0 \text{ for } d > 5.$$

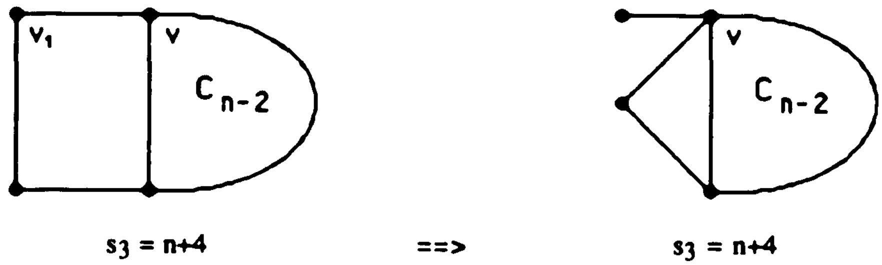


Figure A8. Edges on circuits are contracted.

For $3 \leq d \leq 5$, we have the graphs in Figure A7(c). In all cases, $n \leq 7$.

After all such contractions are performed, we are left with exactly one edge common to C_1 and C_2. We now contract the circuits to triangles. As before, contract the edge between v and an adjacent vertex v_1 which does not lie on a triangle and has degree $d_1 = 2$, and add a pendant edge at v. If no triangles are formed, the s_3 value increases since $2d - 2 > 0$ for $d \geq 3$. If one triangle is formed, the difference in s_3 values is $d - 3 > 0$ for $d > 3$. For $d = 3$, we have a graph of the form in Figure A8. Unless $n = 5$, subsequent contractions of edges will cause an increase in the value of s_3. We have $n > 7$.

When all such contractions have been performed, we are left with the desired graph.

#

Theorem 2.2b For n vertices and e = n+2 edges, n > 9, the unique 3-optimal graph is $G_A(n,n+2)$. The 3-optimal graphs for smaller n are shown in Figure A9.

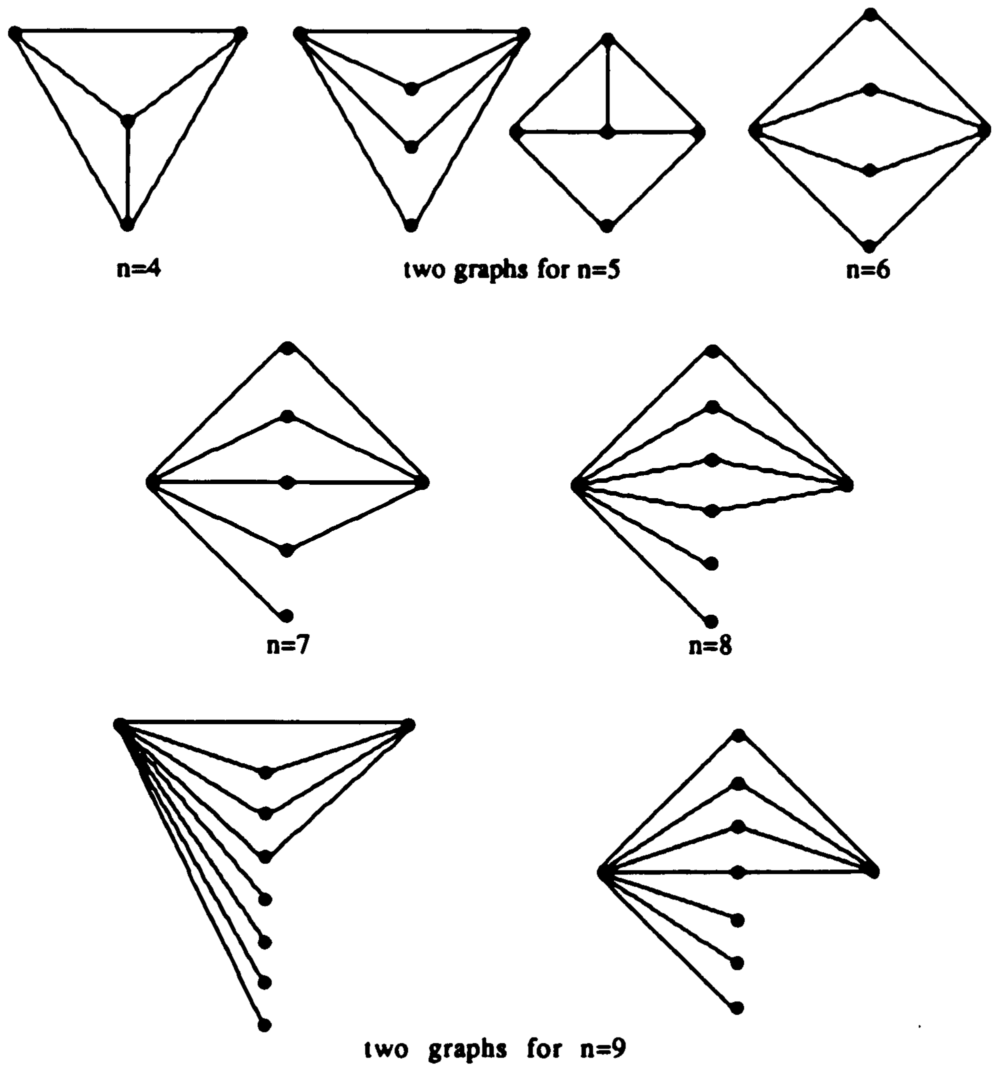


Figure A9. The 3-optimal graphs for e = n+2, n ≤ 9.

Proof: Observe that any graph G with n vertices and e = n+2 edges is planar and and contains three circuits, C_1, C_2, and C_3. The interactions
of these circuits in G gives rise to four types of graphs, as illustrated in Figures A10(a) - (d).

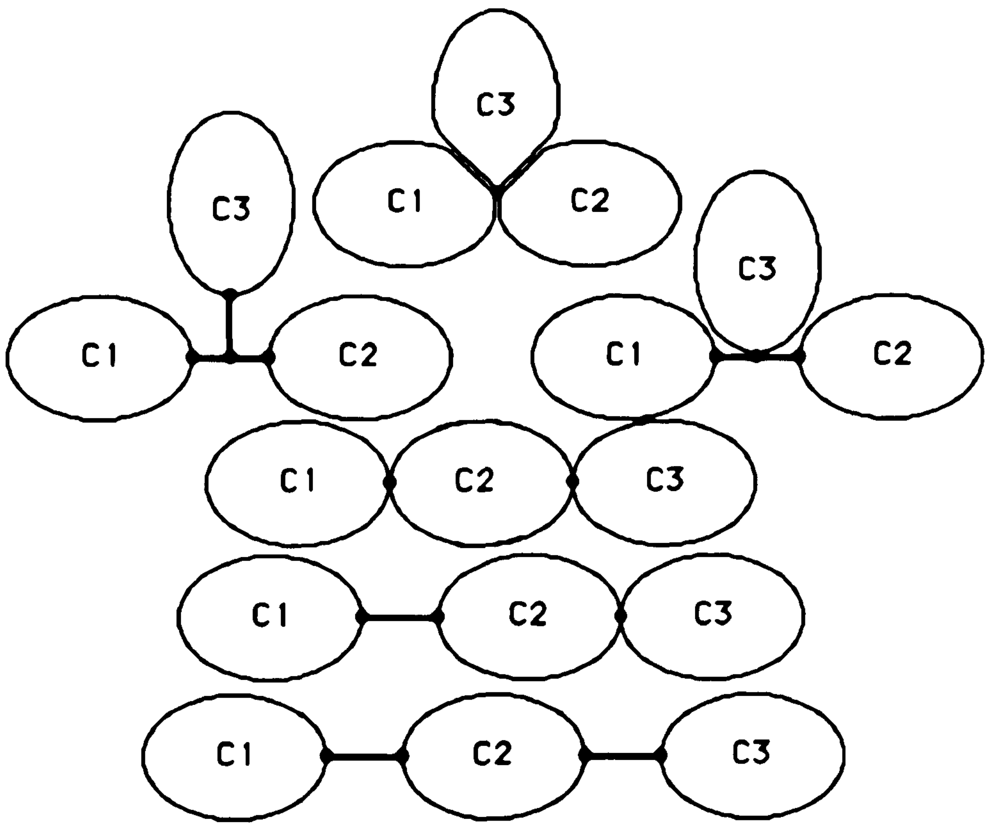


Figure A10(a). Case 1: G contains exactly 3 distinct circuits.

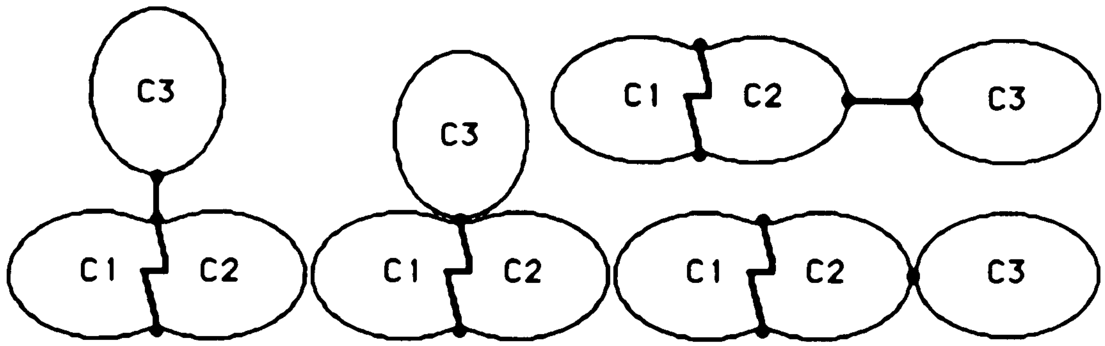


Figure A10(b). Case 2: G contains exactly 4 distinct circuits.

In Case 1, the three circuits have no common edges but may have common vertices. The total number of distinct circuits in such graphs is 3. In Case 2, two of the circuits have an edge in common. Any common edges, say between C_1 and C_2, form a path. The graphs in this case are those which have exactly 4 distinct circuits. Case 3 consists of graphs which have 6 distinct circuits. Similarly, Case 4 consists of those graphs which contain 7 distinct circuits. In addition, G may have trees attached at any vertex.

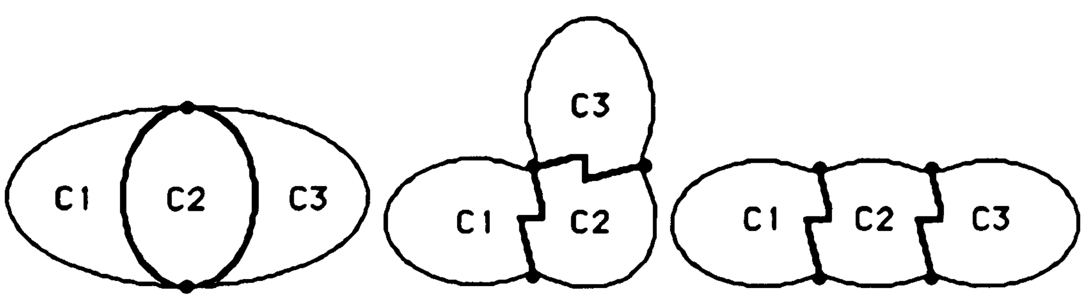


Figure A10(c). Case 3: G contains exactly 6 distinct circuits.

•Case 1: G has exactly 3 distinct circuits.

Step 1.1: Convert all trees to stars as was done in the proof of Theorem 2.2a.

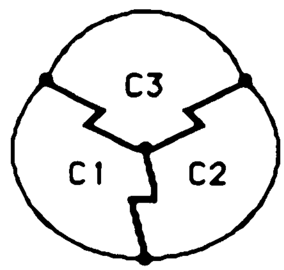


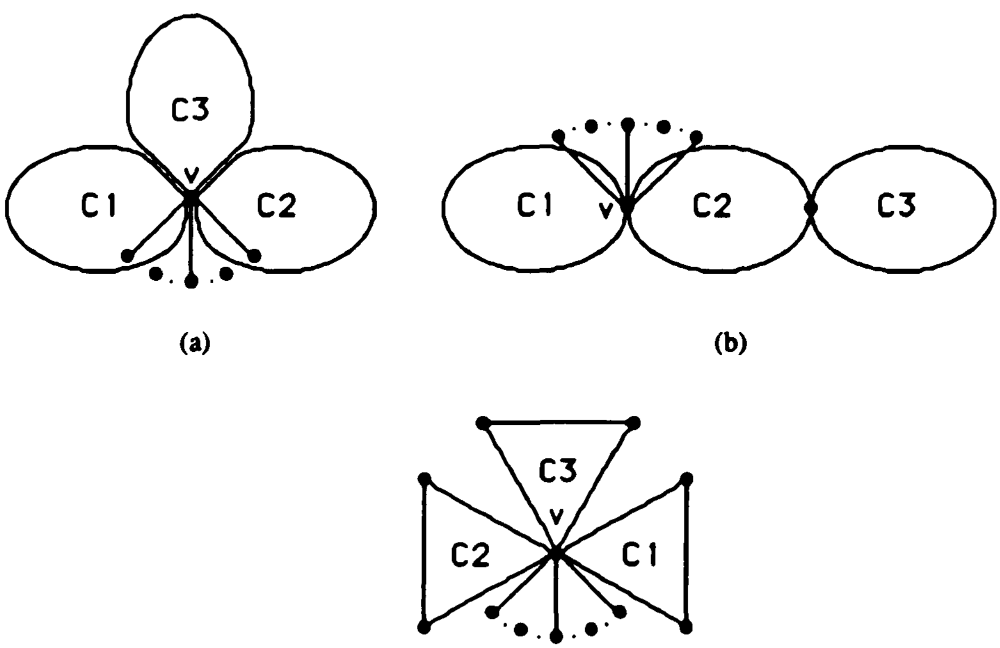
Figure A10(d). Case 4: G contains exactly 7 distinct circuits.

Step 1.2: Contract any non-pendant edges which do not lie on circuits as was done in the proof of Theorem 2.2a.

Step 1.3: Combine all attached stars into a single star.
Choose v as was done in Step 3 of the proof of Theorem 2.2a. That is, let E_p be the set of pendant edges in G. Let V_m be the set of vertices in G which have the maximum degree in G-E_p. Choose $v \in V_m$ to be the vertex whose degree in G is maximal compared to all other vertices in V_m. Here v has degree $d \geq 4$. Let v_1 be the center of a star, $v \neq v_1$. Thus v_1 has degree $d_1 \geq 3$. Let k denote the degree of v_1 in G-E_p. Then k = 2, 3, or 4 and $d_1 > k$. Move the edges pendant at v_1

to v . As in Theorem 2.2a, no triangles are formed and we need consider $((d + d_1 - k)^2 + k^2) - (d^2 + d_1^2) = 2(dd_1 - kd - kd_1 + k^2)$ for the different k:

Case k=2: $d \geq 4$, $d_1 \geq 3$ and $2(dd_1 - 2d - 2d_1 + 2^2) > 0$.
Case k=3: $d \geq 4$, $d_1 \geq 4$ and $2(dd_1 - 3d - 3d_1 + 3^2) > 0$.
Case k=4: $d \geq 4$, $d_1 \geq 5$ and $2(dd_1 - 4d - 4d_1 + 4^2) > 0$ unless d=4. This is impossible since then v_1 would have been selected instead of v.



(c) Contract circuits into triangles (Step 4).

Figure A11. Case 1 graphs at Steps 3 and 4.

After all stars have been moved to v, we are left with either the configuration in Figure A11(a) or the configuration in Figure A11(b). Without loss of generality, we let v be as in the figure.

We now transform the graph in Figure A11(b) into the graph in Figure A11(a). Let v be as in Figure A11(b). Let v_1 be the vertex by which C_3 is attached to the rest of the graph. Remove C_3 and reattach the circuit at v. No triangles are formed. The degree of v_1 becomes 2 and the degree v is increased by 2. The difference in s_3 values is $[\binom{d+2}{2} + \binom{2}{2}] - [\binom{d}{2} + \binom{4}{2}] = 2d-4 > 0$ since $d \geq 4$. We are left with a graph of the form in Figure A11(a) and so $d \geq 6$.

<u>Step 1.4</u>: Contract the circuits into triangles.

Let v_1 be a vertex adjacent to v such that v_1 lies on a circuit which is not a triangle. Thus the degree of v_1 is $d_1 = 2$. Contract the edge between v and v_1 and add a pendant edge at v. Essentially the same construction was illustrated in Figure A6(a).

If no triangles are formed, we have $((d + 1)^2 + 1) - (d^2 + 2^2) = 2d-2 > 0$ since $d \geq 4$. If one triangle is formed, we have

$$[\binom{d+1}{2} + \binom{1}{2} - 2(1)] - [\binom{d}{2} + \binom{2}{2}] = d - 3 > 0 \text{ since } d \geq 6.$$

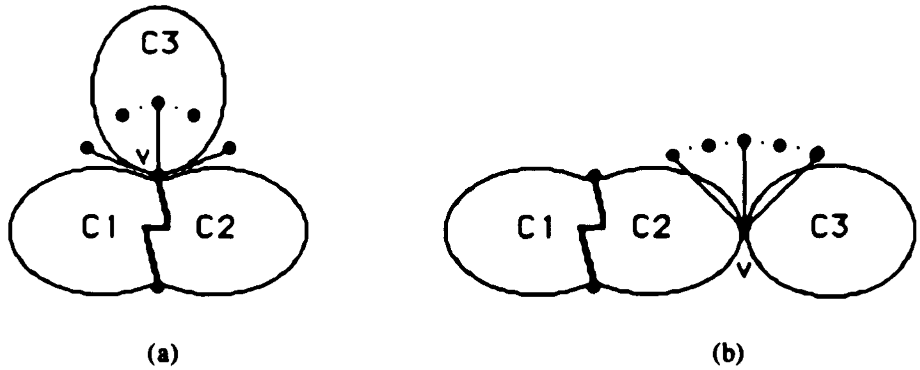


Figure A12. Case 2 graphs after Step 3.

When all edges have been contracted, we are left with the graph in Figure A11(c) which has $s_3 = \binom{n-1}{2}$. C(n,n+2) has $s_3 = \binom{n-1}{2} + 3$.

•Case 2: G has exactly 4 distinct circuits.

Without loss of generality, assume C_1 and C_2 have a common edge as in Figure A10(b).

Step 2.1: Convert all trees to stars.

Step 2.2: Contract any non-pendant edges which do not lie on circuits.

Step 2.3: Combine all attached stars into a single star as in Step 3, Case 1.

Here the vertex v has degree $d \geq 4$. Any vertex v_1 which is the center of a star, $v \neq v_1$ has degree $d_1 \geq 3$. The degree of v_1 in $G\text{-}E_p$ is $k = 2$ or 3 and $d_1 > k$. The cases are as above.

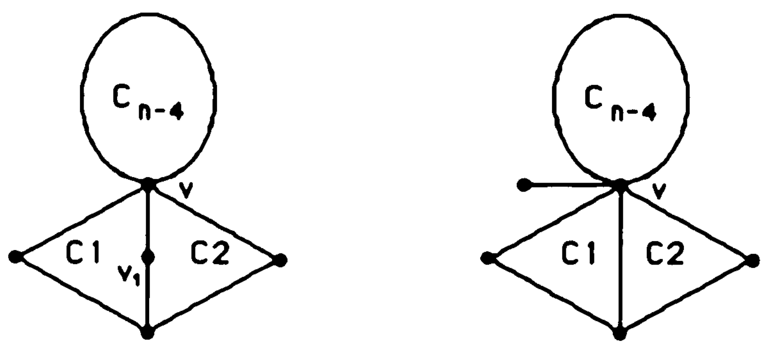
When all stars have been moved to v, we are left with one of the configurations in Figure A12. Without loss of generality, we let the vertex be as in the figure.

We now transform the graph in Figure A12(b) into the graph in Figure A12(a). Let v be as in Figure A12(b). Let v_1 be a vertex of degree 3 which C_1 and C_2 have in common. Remove the pendant edges of the star at v and reattach them at v_1. Remove C_3 and reattach the circuit at v_1 as well. No triangles are formed. The degree of v is reduced by d-2 to 2 and the degree v_1 is increased to d+1. The difference in s_3 values is $[\binom{d+1}{2} + \binom{2}{2}] - [\binom{d}{2} + \binom{3}{2}] = d-2 > 0$ since $d \geq 4$. Let the vertex v_1 become the new vertex v. We are left with a graph of the form in Figure A12(a) and so $d \geq 5$.

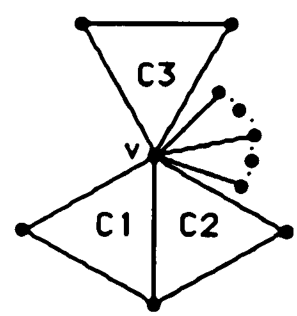
<u>Step 2.4</u>: Contract circuits into triangles.

First we contract the path that C_1 and C_2 have in common into a single edge. Without loss of generality, choose C_1 and C_2 so that the path they share is as short as possible. Let v_1 be a vertex adjacent to v so that v_1 lies on both circuits and has degree 2. Contract the edge between v and v_1 and add a pendant edge at v.

If no triangles are formed, we have 2d- 2 > 0 and if one triangle is formed, we have d-3 > 0 because d ≥ 5. If two triangles are formed, the difference in s_3 values is $[\binom{d+1}{2}+\binom{1}{2}-2(2)] - [\binom{d}{2}+\binom{2}{2}] = d-5$ > 0 for d > 5. For d = 5, we have the graph in Figure A13(a). Since we have n > 9, subsequent contractions will increase the value of s_3



(a) s_3 = n+11 ==> s_3 = n+11



(b) Contract circuits into triangles (Step(4)).

Figure A13. Case 2 graphs.

After contracting all but one of the edges common to C_1 and C_2, we contract the remaining edges on the circuits until they are triangles. Let v_1 be a vertex adjacent to v such that v_1 lies on a circuit which is not a triangle. Thus the degree of v_1 is 2. Contract the edge between v and v_1 and add a pendant edge at v. If no triangles are formed, we have $2d-2 > 0$ and if one triangle is formed, we have $d-3 > 0$ because $d \geq 5$. After performing all such contractions, we are left with the graph in Figure A13(b) which has $s_3 = \binom{n-1}{2} + 1$. C(n,n+2) has $s_3 = \binom{n-1}{2} + 3$.

•Case 3: G has exactly 6 distinct circuits.

Without loss of generality, we assume that C_1, C_2, and C_3 are as in Figure A10(c).

Step 3.1: Convert all trees to stars.

Step 3.2: Combine all attached stars into a single star.

When all stars have been moved to v, we are left with one of the configurations in Figure A14. Without loss of generality, we let the vertex v be as in the figure.

We now transform the graph in Figure A14(c) to a graph of the form in Figure A14(b). The vertex v chosen in Step 2 has degree $d \geq 3$. We contract the sequence of edges which lie solely on C_2 beginning at v. Let v_1 be adjacent to v so that v_1 lies only on C_2 and has degree 2. If the edge between v and v_1 is contracted and a pendant edge is added at v, no triangles are formed and we have 2d-

$2 > 0$ since $d \geq 3$. Eventually we are left with one edge incident to v which lies only on C_2. The other endpoint of that edge has degree 3. Contract that edge and add a pendant edge at v. If no triangles are formed, we have $((d + 2)^2 + 1) - (d^2 + 3^2) = 4d - 4 > 0$ since $d \geq 3$. If one triangle is formed, we have

$$[\binom{d+2}{2} + \binom{1}{2} - 2(1)] - [\binom{d}{2} + \binom{2}{2}] = 2d - 2 > 0 \text{ since } d \geq 3.$$

After all such contractions are performed, we are left with the configuration in Figure A14(b).

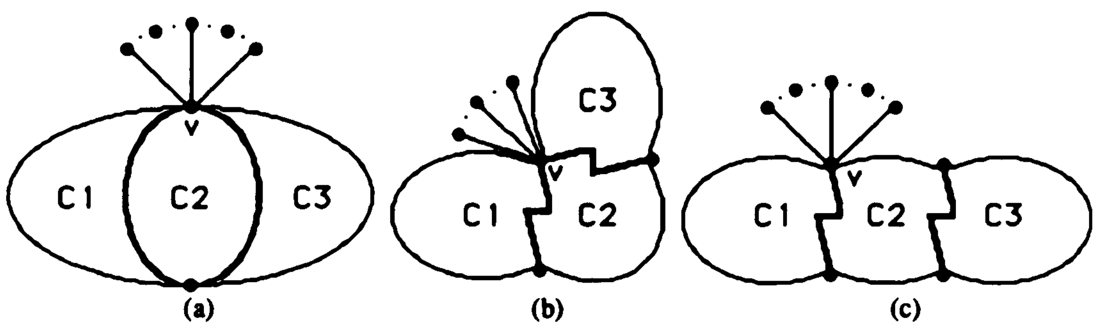


Figure A14. Case 3 graphs after Step 2.

We now proceed to convert a graph of the form in Figure A14(b) to one of the form in Figure A14(a). Let the vertex v be as in Figure A14(b). We contract the edges which lie only on C_2. Let v_1 be a vertex on C_2, with degree 3 and let v_2 be adjacent to v_1 such that v_2 lies only on C_2 and has degree 2. Contract the edge between v_1 and v_2 and insert a new edge at v_1 which lies on C_2. Clearly no triangles are formed and the number of vertices of a given degree remains unchanged so that the s_3 value is likewise unchanged. Finally we are left with one edge incident at v_1 which lies only on C_2. The other endpoint of that edge has degree 3. Contract that edge and insert a new edge at v_1 which lies on C_2. Again no triangles are formed. However, the degree of v_1 becomes 4 and a vertex of degree 3 is replaced by a vertex of degree 2. As a result of this, the s_3 value is increased: $\left(\binom{4}{2} + \binom{2}{2} \right) - 2\binom{3}{2} = 1$. When all possible edges have been moved, we are left with the configuration in Figure A14(a).

Here v has degree $d \geq 4$. Without loss of generality, choose C_1, C_2, and C_3 so that the number of edges common to C_1 and C_2 is minimized and the number of edges common to C_1 and C_3 is minimized.

<u>Step 3.3</u>: Contract C_2 into a triangle.

Let v_1 be a vertex adjacent to v such that v_1 lies on C_2, does not lie on a triangle, and has degree 2. Contract the edge between v and v_1 and add a pendant edge at v.

If no triangles are formed, we have $2d-2 > 0$ and if one triangle is formed, we have $d-3 > 0$ because $d \geq 4$. If two triangles are formed, say C_1 and C_2, we have $d-5 > 0$ for $d > 5$. If $d = 4$, we have a graph of the form in Figure A15(a) and subsequent contractions of C_3 will cause an increase in s_3. This will occur since we have $n > 9$. If $d = 5$, we have a graph of the form in Figure A15(b) and subsequent contractions will cause an increase in s_3 since we have $n > 9$. If three triangles are formed, we have reached $G_A(n,n+2)$. The difference in the s_3 value is

$$[\binom{d+1}{2} + \binom{1}{2} - 2(3)] - [\binom{d}{2} + \binom{2}{2}] = d - 7 > 0 \text{ since } d > 7,\ n > 9.$$

After all such contractions are performed, C_2 is a triangle.

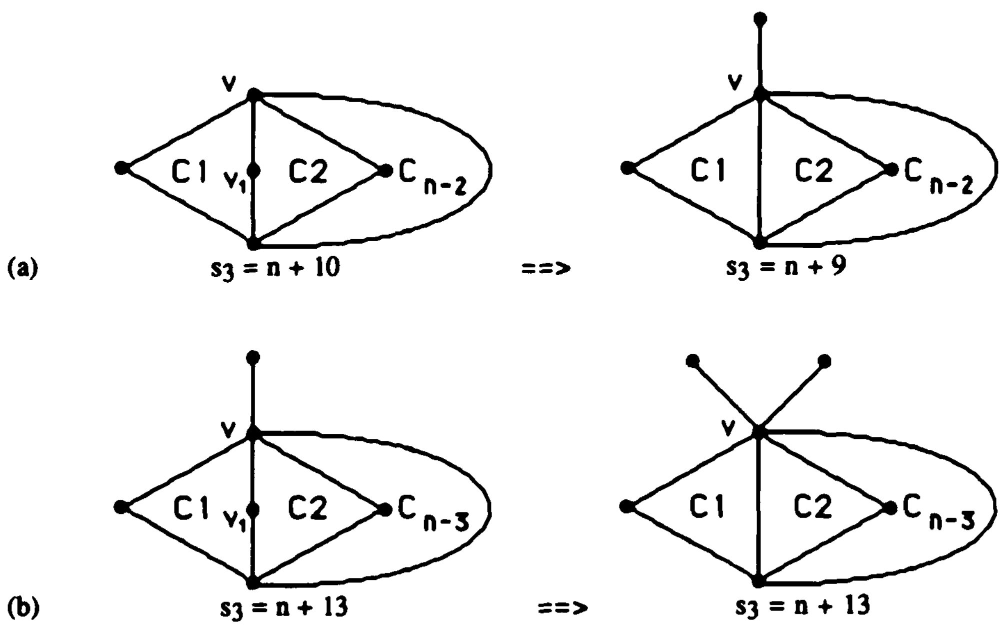
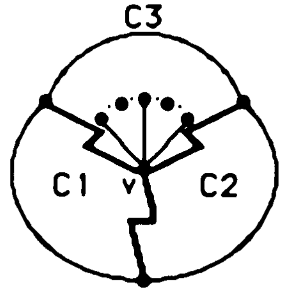


Figure A15. Case 3 graphs during Step 3.



(a) Case 4 graphs after Step 2.

(b) Contract the edge between v_1 and v_2 and append an edge at v.

(c) ==>

Figure A16. Case 4 graphs during Steps 2 and 3.

<u>Step 3.4</u>: Contract C_1 and C_3 into triangles.

Let v_1 be a vertex adjacent to v such that v_1 does not lie on a triangle. Thus v_1 has degree 2. Contract the edge between v and v_1

and add a pendant edge at v. If no triangles are formed, we have $2d-2 > 0$ because $d \geq 4$. If one triangle is formed, we have $d-3 > 0$ because $d \geq 4$. When all such edges have been contracted, we are left with $G_A(n,n+2)$.

<u>•Case 4: G has exactly 7 distinct circuits.</u>

<u>Step 4.1</u>: Convert all trees to stars.

<u>Step 4.2</u>: Combine all attached stars into a single star.

Once a single star has been formed, move that star to the vertex which lies on all three circuits. This vertex has degree $d \geq 3$. Call this vertex v. We are left with the graph in Figure A16(a).

<u>Step 4.3</u>: Contract exterior edges.

Let v_1 be a vertex of degree 3, $v \neq v_1$. Let v_2 be a vertex adjacent to v_1 so that v_2 has degree 2. Contract the edge between v_1 and v_2 and add a pendant edge at v. The degree of v_1 is not affected. If no triangles are formed, we have $2d-2 > 0$ because $d \geq 3$. If one triangle is formed, we have $d - 3 > 0$ for $d > 3$. If $d = 3$, we have a graph of the form in Figure A16(b) and subsequent contractions will cause an increase in s_3 since we have $n > 9$. If two triangles are formed, we have the graph in Figure A16(c). Before the contraction, the graph has $s_3 = \binom{n-2}{2} + 6$. After the contraction $s_3 = \binom{n-1}{2} + 1$. For $n > 7$ the second graph has a greater s_3.

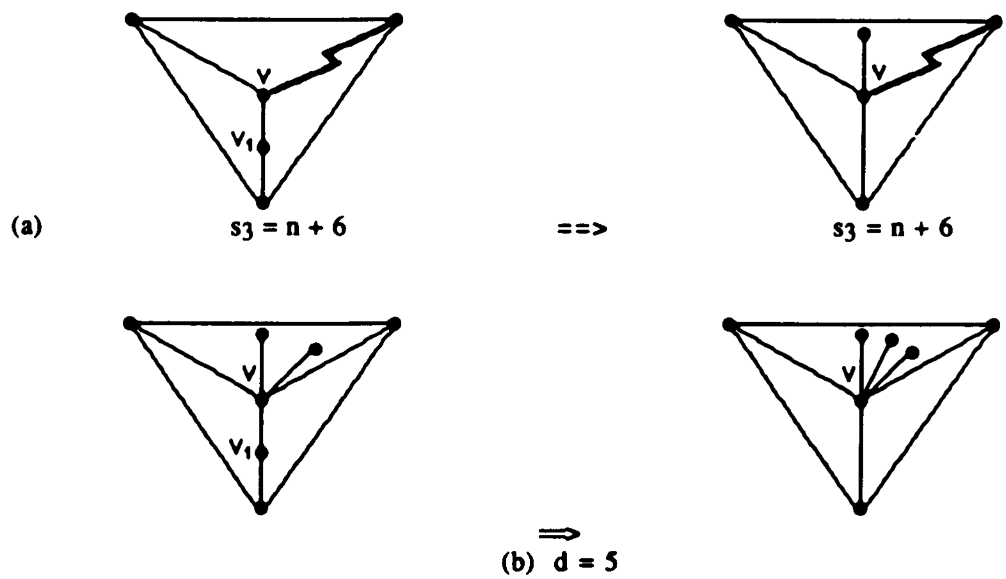


Figure A17. Case 4 graphs during Step 4.

<u>Step 4.4</u>: Contract the edges incident to v.

Let v_1 be a vertex adjacent to v so that v_1 has degree 2. Contract the edge between v and v_1 and add a pendant edge at v. If no triangles are formed, we have $2d - 2 > 0$ because $d \geq 3$. If one triangle is formed, we have $d - 3 > 0$ for $d > 3$. If $d = 3$, we have a graph of the form in Figure A17(a) and two additional contractions are needed to increase s_3. This will occur for $n \geq 7$. If two triangles are formed, we have $d-5 > 0$ for $d > 5$. In this case, the construction terminates and we obtain the second graph in Figure A17(b) with $n = 7$. We have $n > 9$.

When all such contractions have been performed, the construction terminates with the second graph in Figure A16(c). This graph has $s_3 = \binom{n-1}{2} + 1$ while $G_A(n,n+2)$ has $s_3 = \binom{n-1}{2} + 3$.

#

Lemma 4.5 Let $e = 2n-3$, $8 \le n \le 12$. Then the graphs G_1 and G_2 are the only 3-optimal graphs.

Proof: We will examine all (not necessarily realizable) degree sequences for which $\sum_{i=1}^{n} \binom{d_i}{2} \ge (n-2)^2$. By Lemmas 4.1-4.3, we need to consider only the cases with maximum degree $\Delta \le n-4$. By Corollary 3.5, degree sequences which have vertices of degree 1 and more than one vertex of maximum degree cannot correspond to 3-optimal graphs. None of the remaining sequences are realizable because of the number of vertices of degree 1. For convenience, we will refer to $\sum_{i=1}^{n} \binom{d_i}{2}$ as DS*.

•Case 1: For $n = 8$, $e = 2n-3 = 13$, $(n-2)^2 = 36$, $\Delta \le n-4 = 4$.

4 4 4 4 4 4 1 1, DS* = 36 can't be 3-optimal

4 4 4 4 4 3 2 1, DS* = 34

Other sequences 4 4 x x x x x do not have bigger DS*.

•Case 2: For $n = 9$, $e = 2n-3 = 15$, $(n-2)^2 = 49$, $\Delta \le n-4 = 5$.

5 5 5 5 5 2 1 1 1, DS* = 51 can't be 3-optimal

5 5 5 5 4 3 1 1 1, DS* = 49 can't be 3-optimal

5 5 5 5 4 2 2 1 1, DS* = 48

Other sequences 5 5 5 5 x x x x x do not have bigger DS*.

5 5 5 4 4 4 1 1 1, DS* = 48

Other 5 x x x x x x x x do not have bigger DS*.

4 4 4 4 4 4 4 1 1, DS* = 42

Other sequences 4 x x x x x x x x do not have bigger DS*.

•<u>Case 3</u>: For n = 10, e = 2n-3 = 17, $(n-2)^2 = 64$, $\Delta \le n-4 = 6$.

6 6 6 6 5 1 1 1 1 1, DS* = 70 can't be 3-optimal

6 6 6 6 4 2 1 1 1 1, DS* = 67 can't be 3-optimal

6 6 6 6 3 3 1 1 1 1, DS* = 66 can't be 3-optimal

6 6 6 6 3 2 2 1 1 1, DS* = 65 can't be 3-optimal

6 6 6 6 2 2 2 2 1 1, DS* = 64 can't be 3-optimal

6 6 6 5 5 2 1 1 1 1, DS* = 66 can't be 3-optimal

6 6 6 5 4 3 1 1 1 1, DS* = 64 can't be 3-optimal

6 6 6 5 3 3 2 1 1 1, DS* = 62

Other sequences 6 6 6 x x x x x x x do not have bigger DS*.

6 6 5 5 5 3 1 1 1 1, DS* = 63

Other sequences 6 x x x x x x x x x do not have bigger DS*.

5 5 5 5 5 5 1 1 1 1, DS* = 60

Other sequences 5 x x x x x x x x x do not have bigger DS*.

4 4 4 4 4 4 4 4 1 1, DS* = 48

Other sequences 4 x x x x x x x x x do not have bigger DS*.

•<u>Case 4</u>: For n = 11, e = 2n-3 = 19, $(n-2)^2 = 81$, $\Delta \le n-4 = 7$.

7 7 7 7 4 1 1 1 1 1 1, DS* = 90 can't be 3-optimal

7 7 7 7 3 2 1 1 1 1 1, DS* = 88 can't be 3-optimal

7 7 7 7 2 2 2 1 1 1 1, DS* = 87 can't be 3-optimal

7 7 7 6 5 1 1 1 1 1 1, DS* = 88 can't be 3-optimal

7 7 7 6 4 2 1 1 1 1 1, DS* = 85 can't be 3-optimal

7 7 7 6 3 3 1 1 1 1 1, DS* = 84 can't be 3-optimal

7 7 7 6 3 2 2 1 1 1 1, DS* = 83 can't be 3-optimal

7 7 7 6 2 2 2 2 1 1 1, DS* = 82 can't be 3-optimal

7 7 7 5 5 2 1 1 1 1 1, DS* = 84 can't be 3-optimal

7 7 7 5 4 3 1 1 1 1 1, DS* = 82 can't be 3-optimal

7 7 7 5 4 2 2 1 1 1 1, DS* = 81 can't be 3-optimal

7 7 7 5 3 3 2 1 1 1 1, DS* = 80

Other sequences 7 7 7 x x x x x x x x do not have bigger DS*.

7 7 6 6 6 1 1 1 1 1 1, DS* = 87 can't be 3-optimal

7 7 6 6 5 2 1 1 1 1 1, DS* = 83 can't be 3-optimal

7 7 6 6 4 3 1 1 1 1 1, DS* = 81 can't be 3-optimal

7 7 6 6 4 2 2 1 1 1 1, DS* = 80

7 7 6 6 3 3 2 1 1 1 1, DS* = 79

7 7 6 5 5 3 1 1 1 1 1, DS* = 80

Other sequences 7 7 x x x x x x x x x do not have bigger DS*.

7 6 6 6 6 2 1 1 1 1 1, DS* = 82 not realizable

7 6 6 6 5 3 1 1 1 1 1 , DS* = 79

Other sequences 7 x x x x x x x x x x do not have bigger DS*.

6 6 6 6 6 3 1 1 1 1 1, DS* = 78

Other sequences 6 x x x x x x x x x x do not have bigger DS*.

5 5 5 5 5 5 4 1 1 1 1, DS* = 66

Other sequences 5 x x x x x x x x x x do not have bigger DS*.

•Case 5: For $n = 12$, $e = 2n-3 = 21$, $(n-2)^2 = 100$, $\Delta \leq n-4 = 8$.

8 8 8 8 3 1 1 1 1 1 1 1, DS* = 115 can't be 3-optimal

8 8 8 8 2 2 1 1 1 1 1 1, DS* = 114 can't be 3-optimal

8 8 8 7 4 1 1 1 1 1 1 1, DS* = 111 can't be 3-optimal

8 8 8 7 3 2 1 1 1 1 1 1, DS* = 109 can't be 3-optimal

8 8 8 7 2 2 2 1 1 1 1 1, DS* = 108 can't be 3-optimal

8 8 8 6 5 1 1 1 1 1 1 1, DS* = 109 can't be 3-optimal

8 8 8 6 4 2 1 1 1 1 1 1, DS* = 106 can't be 3-optimal

8 8 8 6 3 3 1 1 1 1 1 1, DS* = 105 can't be 3-optimal

8 8 8 6 3 2 2 1 1 1 1 1, DS* = 104 can't be 3-optimal

8 8 8 6 2 2 2 2 1 1 1 1, DS* = 103 can't be 3-optimal

8 8 8 5 5 2 1 1 1 1 1 1, DS* = 105 can't be 3-optimal

8 8 8 5 4 3 1 1 1 1 1 1, DS* = 103 can't be 3-optimal

8 8 8 5 4 2 2 1 1 1 1 1, DS* = 102 can't be 3-optimal

8 8 8 5 3 3 2 1 1 1 1 1, DS* = 101 can't be 3-optimal

8 8 8 5 3 2 2 2 1 1 1 1, DS* = 100 can't be 3-optimal

8 8 8 5 2 2 2 2 2 1 1 1, DS* = 100 can't be 3-optimal

8 8 8 4 4 4 1 1 1 1 1 1, DS* = 102 can't be 3-optimal

8 8 8 4 4 3 2 1 1 1 1 1, DS* = 100 can't be 3-optimal

8 8 8 4 4 2 2 2 1 1 1 1, DS* = 99

Other sequences 8 8 8 x x x x x x x x x do not have bigger DS*.

8 8 7 7 5 1 1 1 1 1 1 1, DS* = 108 can't be 3-optimal

8 8 7 7 4 2 1 1 1 1 1 1, DS* = 105 can't be 3-optimal

8 8 7 7 3 3 1 1 1 1 1 1, DS* = 104 can't be 3-optimal

8 8 7 7 3 2 2 1 1 1 1 1, DS* = 103 can't be 3-optimal

8 8 7 7 2 2 2 2 1 1 1 1, DS* = 102 can't be 3-optimal

8 8 7 6 6 1 1 1 1 1 1 1, DS* = 107 can't be 3-optimal

8 8 7 6 5 2 1 1 1 1 1 1, DS* = 103 can't be 3-optimal

8 8 7 6 4 3 1 1 1 1 1 1, DS* = 101 can't be 3-optimal

8 8 7 6 4 2 2 1 1 1 1 1, DS* = 100 can't be 3-optimal

8 8 7 6 3 3 2 1 1 1 1 1, DS* = 99

Other sequences 8 8 7 6 x x x x x x x x do not have bigger DS*.

8 8 7 5 5 3 1 1 1 1 1 1, DS* = 100 can't be 3-optimal

8 8 7 5 5 2 2 1 1 1 1 1, DS* = 99

Other sequences 8 8 7 5 x x x x x x x x do not have bigger DS*.

8 8 7 4 4 4 2 1 1 1 1 1, DS* = 96

Other sequences 8 8 7 x x x x x x x x x do not have bigger DS*.

8 8 6 6 6 2 1 1 1 1 1 1, DS* = 102 can't be 3-optimal

8 8 6 6 5 3 1 1 1 1 1 1, DS* = 99

Other sequences 8 8 6 6 x x x x x x x x do not have bigger DS*.

8 8 6 5 5 4 1 1 1 1 1 1, DS"* = 94

Other sequences 8 8 x x x x x x x x x x do not have bigger DS*.

8 7 7 7 6 1 1 1 1 1 1 1, DS* = 106 not realizable

8 7 7 7 5 2 1 1 1 1 1 1, DS* = 102 not realizable

8 7 7 7 4 3 1 1 1 1 1 1, DS* = 100 not realizable

8 7 7 7 4 2 2 1 1 1 1 1, DS* = 99

Other sequences 8 7 7 7 x x x x x x x x do not have bigger DS*.

8 7 7 6 6 2 1 1 1 1 1 1, DS* = 101 not realizable

8 7 7 6 5 3 1 1 1 1 1 1, DS* = 98

Other sequences 8 7 7 6 x x x x x x x x do not have bigger DS*.

8 7 7 5 5 4 1 1 1 1 1 1, DS* = 96

Other sequences 8 7 x x x x x x x x x x do not have bigger DS*.

8 6 6 6 6 4 1 1 1 1 1 1, DS* = 94

Other sequences 8 x x x x x x x x x x x do not have bigger DS*.

7 7 7 7 7 1 1 1 1 1 1 1, DS* = 105 can't be 3-optimal

7 7 7 7 6 2 1 1 1 1 1 1, DS* = 100 can't be 3-optimal

7 7 7 7 5 3 1 1 1 1 1 1, DS* = 97

Other sequences 7 7 7 7 x x x x x x x x do not have bigger DS*.

7 7 7 6 6 3 1 1 1 1 1 1, DS* = 96

Other sequences 7 x x x x x x x x x x x do not have bigger DS*.

6 6 6 6 6 6 1 1 1 1 1 1, DS* = 90

Other sequences 6 x x x x x x x x x x x do not have bigger DS*.

5 5 5 5 5 5 5 3 1 1 1 1, DS* = 73

Other sequencse 5 x x x x x x x x x x x do not have bigger DS*.

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