The Laplacian Spectrum of Graphs

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There are several people who deserve my thanks for their contribution to this endeavor. First of all, my supervisor, Michael Doob, who first introduced me to this subject and helped me in numerous ways throughout. Lynn Batten and William Kocay gave me their crucial support and encouragement during this project. Rolland Gaudet has yet to see this thesis, but without him it would never have existed. My friends and family gave me love and understanding; windows and paintbrushes. Dad liked it right from the beginning. B.I. gave me essential food for thought. Glenn provided the soundtrack all the way through.

quand on a avalé le bœuf, il ne faut pas s'arretêr à la queue

ABSTRACT

In this thesis we investigate the spectrum of the Laplacian matrix of a graph. Although its use dates back to Kirchhoff, most of the major results are much more recent. It is seen to reflect in a very natural way the structure of the graph, particularly those aspects related to connectedness. This can be intuitively understood as a consequence of the relationship between the Laplacian matrix and the boundary of a set of vertices in the graph. We investigate the relationship between the spectrum and the isoperimetric constant, expansion properties, and diameter of the graph. We consider the problem of integral spectra, and see how the structure of the eigenvectors can be used to deduce more information on both the spectrum and the graph, particularly for trees. In closing, we mention some alternatives to and generalisations of the Laplacian.

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Chapter 1

Introduction

1.1 Definitions and examples

Let $G(V, E)$ be a graph with vertex set V of cardinality n and edge set E of cardinality m. Unless otherwise noted, all graphs will be undirected and finite. Let d_j be the degree of vertex j. We will use δ for the minimum degree and Δ for the maximum degree. We will indicate adjacency of vertices by $i \sim j$ for $ij \in E(G)$.

Let A be the $n \times n$ $\{0, 1\}$ adjacency matrix such that $A_{ij} = 1$ if and only if $ij \in E(G)$. Let D be the $n \times n$ diagonal matrix with $D_{jj} = d_j$. We define

Definition 1.1.1. $L = D - A$

to be the *(combinatorial) Laplacian* matrix associated with the graph, and we will write $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$ for its eigenvalues (see also Section 8.1). Unless otherwise noted, all eigenvectors and eigenvalues will be with respect to the Laplacian matrix (not the ordinary adjacency matrix). Furthermore, we will abuse the language and write "eigenvalue of G" for "eigenvalue of $L(G)$".

Let K be the $n \times m$ incidence matrix, where the columns are indexed by the edges and the rows are indexed by the vertices. Choose an (arbitrary) orientation on each edge, and for each column, place $+1$ in the row corresponding to the positive end and -1 in the row corresponding to the negative end; all other entries are zero. It can be seen directly that $L = KK^t$. If we let λ be any eigenvalue of L and x a corresponding eigenvector, we have:

$$\lambda ||x||^2 = \langle \lambda x, x \rangle = \langle KK^t x, x \rangle = \langle K^t x, K^t x \rangle = ||K^t x||^2 \geq 0$$

and thus L is positive semi-definite. Furthermore, as the row sums of L are all zero, the all-ones vector is an eigenvector with eigenvalue $\lambda_1 = 0$. Note that by the definition of L, we have

$$(Lx)_j = d_j x_j - \sum_{i \sim j} x_i,$$

allowing us to express the eigenvalue condition at each vertex as

$$(d_j - \lambda)x_j = \sum_{i \sim j} x_i$$

Using the well-known Courant-Fischer inequalities, we may characterise the eigenvalues by

$$\lambda_2 = \min_x \frac{\langle x, Lx \rangle}{\langle x, x \rangle} \qquad \text{and} \qquad \lambda_n = \max_x \frac{\langle x, Lx \rangle}{\langle x, x \rangle}$$

where x ranges over all non-zero column vectors of size n that are orthogonal to the all-ones vector. (One may also give similar descriptions of the other eigenvalues, where x ranges over appropriate subspaces; we will not need them here.) Thus we have that

$$\lambda_2 \leq \frac{\langle x, Lx \rangle}{\langle x, x \rangle} \leq \lambda_n$$

$$\langle x, Lx \rangle = \sum_{ij \in E(G)} (x_i - x_j)^2$$

and thus

$$\lambda_2 = \min_x \frac{\sum_{ij \in E(G)} (x_i - x_j)^2}{\sum_{j \in V(G)} (x_j)^2} \tag{1.1}$$

and

$$\lambda_n = \max_x \frac{\sum_{ij \in E(G)} (x_i - x_j)^2}{\sum_{j \in V(G)} (x_j)^2} \tag{1.2}$$

where again x is orthogonal to the all-ones vector.

An alternative formulation is

$$\lambda_2 = \min_x \max_{t \in \mathbb{R}} \frac{\sum_{ij \in E(G)} (x_i - x_j)^2}{\sum_{j \in V(G)} (x_j - t)^2} \tag{1.3}$$

where x now ranges over all non-constant vectors. This can be seen by observing that for a given vector x, the value of t that maximises the ratio is $t = \sum x_j/n$, and that thus the vector y defined by $y_j = x_j - t$ is orthogonal to the all-ones vector and $y_i - y_j = x_i - x_j$; furthermore, all vectors orthogonal to the all-ones vector may be obtained in this manner.

Fiedler [15] also gave the following characterisation.

$$\lambda_2 = \min_x \frac{2n \sum_{ij \in E(G)} (x_i - x_j)^2}{\sum_{i \in V} \sum_{j \in V} (x_i - x_j)^2} \tag{1.4}$$

We will also make frequent and tacit use of the Cauchy interlacing inequalities (see, e.g., [30]). Specifically, for any Hermitian matrix B, let $B_{[r]}$ be the matrix formed by deleting the r^{th} row and r^{th} column from B. Let $\alpha_1 \leq \alpha_2 \leq \cdots \leq \alpha_n$ be the eigenvalues of B and let $\beta_1 \leq \beta_2 \leq \cdots \leq \beta_{n-1}$ be the eigenvalues of $B_{[r]}$. Then

$$\alpha_i \leq \beta_i \leq \alpha_{i+1} \text{ for } 1 \leq i \leq n-1$$

We note that for the case of regular graphs, $L = dI - A$ where d is the common vertex degree. So if we let $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$ be the eigenvalues of A, we see that $\lambda_j = d - \mu_j$. So the Laplacian spectrum for regular graphs tells us nothing we didn't already know from the spectrum of A. This allows us to restate any theorem (for regular graphs) on the eigenvalues of A as a theorem on the eigenvalues of L.

For instance, we can prove using L that given a d-regular graph G, the largest eigenvalue of the adjacency matrix is d, and it is simple (see Theorem 1.3.4).

As another example, consider the matrix K_+, the unoriented incidence matrix. Its entries are the absolute value of the corresponding entries in the matrix K. Thus the eigenvalues of $K_+{K_+}^t$ are no smaller than the eigenvalues of KK^t. But the eigenvalues of $K_+{K_+}^t$ are the same as the eigenvalues of ${K_+}^tK_+$. A direct computation shows that ${K_+}^tK_+ = 2I + B$, where B is the adjacency matrix of the line graph of G. Thus we have a relationship between the Laplacian eigenvalues of a graph and the adjacency eigenvalues of its line graph. Furthermore, since the eigenvalues of $K_+{}^tK_+$ are nonnegative, and the smallest eigenvalue of a line graph is at least -2. This gives a connection with the theory of *root systems* [6].

In general, there is no simple relationship between the eigenvalues of A and the eigenvalues of L. However, we do have the following. Given a graph G, construct the graph G' by adding an appropriately weighted loop to each vertex such that G' is d-regular. We then have that $L(G) = L(G') = dI - A(G')$. So the Laplacian spectrum of a graph does reduce to the adjacency spectrum of *some* (weighted) graph.

We also see here an interesting property of L, namely that although every graph has a unique Laplacian matrix, this matrix does not in general uniquely determine a graph: the Laplacian tells us nothing about how many loops were to be found in the original graph. It is interesting to note that this missing information may be characterised as exactly that aspect of a graph that is completely irrelevant to issues of connectedness.

Furthermore, consider a set $X \subseteq V$, and define the column-vector $x = (x_j)$ by $x_j = 1$ for $x \in X$ and $x_j = 0$ for $x \notin X$. Let $y = Lx$. By the definition of L, we see that $y_j > 0$ means that vertex j is in X and is connected to y_j vertices not in X, $y_j < 0$ means that vertex j is not in X and is connected to $|y_j|$ vertices in X, and $y_j = 0$ means that vertex j is in [or not in] X and is only connected to vertices in [or not in] X. In other words, Lx tells us exactly how the set X is connected to the rest of the graph. (If we let $X = V$, we note that there are no vertices of the first two types, and thus see again that 0 is an eigenvalue). This interpretation can be thought of as analogous to the following property of A: given a set X of vertices with x being the characteristic vector of X, then Ax corresponds to the (multi-)set of neighbours of X. More correctly (and generally), A^kx corresponds to the multiset of endpoints of paths of length k originating in X. So we see that A directly models paths, whereas L directly models boundaries. Of course, since the graph is uniquely determined by either of them (modulo loops), they both contain directly or indirectly the same information. We will not dwell on these properties further for the moment[1], except to note that they provide some intuitive sense of why the matrix L should be associated with connectedness properties of the graph.

It should be noted that most results carry over quite well to the case of

[1] Actually, this interpretation will come up in connection with the isoperimetric constant of the graph; see Section 2.1.

weighted graphs (or graphs with multiple edges). Here we would use the weighted adjacency matrix A^*, where A^*_{ij} is the weight of the edge between i and j (zero weight being interpreted as no edge), and the degree of a vertex is the sum of the weights of the edges adjacent to it. This gives, in a straightforward manner, that $L^* = D^* - A^*$. Of course, the unweighted Laplacian is really a special case of this, with all weights being either zero or one. This thesis will concentrate principally on the eigenvalues of L (in particular λ_2), and their relation to other graph properties, stressing properties relating to "connectedness".

1.2 Historical background

One of the motivators of the study of graph eigenvalues was the study of vibrations of membranes. This has its origins in Kac's provocative paper [22] and is closely tied in with the study of eigenvalues and eigenfunctions on Riemannian manifolds.

Consider a membrane in the xy plane, with the vertical displacement being $z = z(x, y)$. Letting t be the time-variable and c the speed of the wave[2], the wave equation (see e.g. [16]) gives

$$\frac{\partial^2 z}{\partial x^2} + \frac{\partial^2 z}{\partial y^2} = \frac{1}{c^2}\frac{\partial^2 z}{\partial t^2} \tag{1.5}$$

If we assume that the membrane behaves like a spring in that there is a restoring force proportional to the displacement, Hooke's Law gives

$$\frac{\partial^2 z}{\partial t^2} = -kz \tag{1.6}$$

By approximating the membrane using a discrete grid of particles of spacing w, we may approximate the partial derivative by

$$\frac{\partial z(x,y)}{\partial x} \approx \frac{z(x,y) - z(x-w,y)}{w} \tag{1.7}$$

$$\frac{\partial z(x+w,y)}{\partial x} \approx \frac{z(x+w,y) - z(x,y)}{w} \tag{1.8}$$

[2]The speed of a wave depends only on the medium (in this case the membrane), not on the "shape" of the wave.

This gives that

$$\frac{\partial^2 z(x,y)}{\partial x^2} \approx \frac{(1.8)-(1.7)}{w}$$
$$= \frac{z(x+w,y)+z(x-w,y)-2z(x,y)}{w^2} \tag{1.9}$$

Substituting (1.9) (and the analogous expression for $\partial^2 z/\partial y^2$) into (1.5), and using (1.6), we have that

$$4z(x,y) - z(x+w,y) - z(x-w,y) - z(x,y+w) - z(x,y-w) \approx \frac{kw^2}{c^2} z(x,y) \tag{1.10}$$

This says that z is an eigenfunction of the Laplacian matrix of the grid graph with eigenvalue kw^2/c^2. This explains the term "Laplacian" for the matrix L, as it functions as the discrete analogue of the continuous Laplacian operator. There is nothing special about the membrane; a similar example would hold in one or three dimensions. In fact, an approach quite similar to this (in one dimension) is commonly used in introductory physics texts to show that the stable modes of vibration (i.e.: eigenfunction/eigenvalues) of a string are precisely sinusoidal curves (see e.g. [16]). Nor is there anything special about the grid graph; it is just a simple way to discretize the surface. We would have gotten the Laplacian of *whatever* graph we had chosen.

1.3 Basic properties of the eigenvalues

One of the earliest uses of the matrix L proper was the Matrix-Tree Theorem, due to Kirchhoff (in fact, L is sometimes called the Kirchhoff matrix). It states that the cofactors of L give the number of spanning trees of the graph. For notation, let $L_{[i,j]}$ be the submatrix L with the i^{th} row and j^{th} column removed, and let $L_{[A,B]}$ be the submatrix of L with the set A of rows and the set B of columns removed. Denote the number of spanning trees of G by $t(G)$. Then we may state that:

Theorem 1.3.1. $(-1)^{i+j}\det(L_{[i,j]}) = t(G)$

Proof. This can be proved by considering the incidence matrix K, where $L = KK^t$. Note that if G is connected and not a tree, then G has at least n

edges, i.e., K is a either a square matrix or a "wide" matrix. First consider $\det(L_{[j,j]})$. It can be seen that

$$\det(L_{[j,j]}) = \det((K_{[j,\emptyset]})(K_{[j,\emptyset]})^t)$$

Now applying Cauchy's determinant formula to this product, we obtain that

$$\det(L_{[j,j]}) = \sum_M \det((K_{[j,M]})(K_{[j,M]})^t) = \sum_M \det(K_{[j,M]}) \det(K_{[j,M]})^t) \quad (1.11)$$

where M denotes a set of columns whose deletion from $K_{[j,\emptyset]}$ leaves a square matrix and the sum is over all such sets M. Note that M can be viewed as a set of edges, with $|M| = |E(G)| - (|V(G)| - 1)$. Denote by G' the subgraph of G obtained by removing the edges of M; G' has $n-1$ edges. Now for any given set M, we see that $K_{[\emptyset,M]}$ represents the incidence matrix of G'. Since G' has n vertices and $n-1$ edges, we see that G' represents a spanning tree if and only if it contains no cycles and if and only if it is connected. Therefore, $\det(K_{[j,M]}) = 0$ exactly when G' is not a spanning tree. Furthermore, $\det(K_{[j,M]}) = \pm 1$ exactly when G' is a spanning tree. Since $\det(K_{[j,M]})^t) = \det(K_{[j,M]}))$, the sum in (1.11) will exactly count the number of connected acyclic subgraphs of G with $n-1$ edges: i.e., the number of spanning trees. □

It can be shown that in fact all of the cofactors are equal; since we have shown the validity of the theorem on the cofactors of the diagonal, it is true for all of them.

By looking at the linear coefficient in the characteristic polynomial of L (e.g. [9]), we see that in terms of eigenvalues we have:

Corollary 1.3.2. $\prod_{j=2}^{n} \lambda_j = n\, t(G)$

We can thus incidentally observe (once again) that $\lambda_2 = 0$ if and only if G is disconnected.

This can be regarded as a consequence of a more general theorem. We will first establish some notation. Let G be a graph on n vertices, and let $J \subseteq V(G)$. Define the graph $G_{[J]}$ to be the graph obtained by replacing all the vertices of J with a single vertex, which is adjacent to exactly those vertices in $G \backslash J$ that are adjacent (in G) with some vertex of J. Note that this may produce multiple edges (if some vertices in J share a common neighbour not in J) or loops (if some vertices in J are adjacent to each other). Write $t(G)$ for the number of spanning trees of G. This leads to the following characterisation, due to Kel'mans ([25], [9], p38).

Theorem 1.3.3. *Let $x^n + c_{n-1}x^{n-1} + \cdots + c_1 x$ be the characteristic polynomial of $L(G)$. Then*

$$c_i = (-1)^n \sum_{\substack{J \subset V(G) \\ |J| = i}} t(G_J)$$

Some of the first modern results suggested that the value λ is related to the "connectedness" of the graph (Fiedler called it the "algebraic connectivity"). Informally, large values of λ_2 are associated with graphs that are hard to disconnect. In fact, by ordering the vertices such that L is in block form with the blocks corresponding to the connected components of G, we see not only that $\lambda_2 = 0$ if and only if G is disconnected, but furthermore that

Theorem 1.3.4. *The number of connected components of G is equal to the multiplicity of 0 as an eigenvalue*

A matrix A is said to be *reducible* if there exists a permutation matrix P such that

$$P^T A P = \begin{pmatrix} B & 0 \\ D & C \end{pmatrix} \tag{1.12}$$

where B and C are square matrices. Otherwise it is *irreducible.* Furthermore, if A is reducible, then there exists a permutation matrix P such that $P^t A P$ has the form

$$\begin{pmatrix} A_{1,1} & 0 & \cdots & 0 & 0 & \cdots & 0 \\ 0 & A_{2,2} & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & & \ddots & & & & \vdots \\ 0 & 0 & \cdots & A_{s,s} & 0 & \cdots & 0 \\ A_{s+1,1} & A_{s+1,2} & \cdots & A_{s+1,s} & A_{s+1,s+1} & \cdots & 0 \\ \vdots & & & & & \ddots & \vdots \\ A_{t,1} & A_{t,2} & \cdots & A_{t,s} & A_{t,s+1} & \cdots & A_{t,t} \end{pmatrix}$$

with the matrices $\{A_{k,1}, A_{k,2}, \ldots, A_{k,k-1}\}$ not all zero for any fixed value of $k > s$. This is a *normal form* of the matrix (see [44]). It is not necessarily unique, as permutations among and within blocks are possible.

So as a corollary to Theorem 1.3.4, we have that

Corollary 1.3.5. *A graph G is connected if and only if the matrix $L(G)$ is irreducible. Furthermore, if G is disconnected, then a normal form of the (reducible) matrix L is obtained by any ordering of the vertices that lists the vertices in order of components.*

If L is decomposable, then partition the vertices according to the submatrices B and C in form (1.12). The zero block then indicates an absence of edges between the two parts of this partition, i.e., the graph is disconnected. It can easily be seen that by listing the vertices by connected component that the block submatrix corresponding to each connected component is irreducible and that all off-diagonal blocks are zero. In fact, this is not just a normal form, it is a block diagonal form.

There is a nice relationship between the eigenvalues of a graph and of its complement. If we let $L(G)$ stand for the Laplacian of a graph G, and G^c stand for the complement of the graph G, then we see that $L(G^c) + L(G) = nI - J$, and hence that $L(G^c) = nI - J - L(G)$, where J is the all-ones matrix. If x is an eigenvector of $L(G)$ orthogonal to the all-ones vector, with eigenvalue λ, then since $Jx = 0$, we see that x is also an eigenvector of $L(G')$ with eigenvalue $n - \lambda$. This was first obtained by Kel'mans [23],[24] in the following result, where $P_G(x)$ stands for the characteristic polynomial of the Laplacian matrix of G:

Theorem 1.3.6. $(n-x)P_{G^c}(x) = (-1)^n x P_G(n-x)$

Corollary 1.3.7. $\lambda_j(G^c) = n - \lambda_{n+2-j}(G)$ *for* $2 \leq j \leq n$

We also get an upper bound on Laplacian eigenvalues [25].

Corollary 1.3.8. $\lambda_n \leq n$ *with equality if and only if* G^c *is disconnected*

Hence we have $\lambda_2(G) = 0 \iff \lambda_n(G^c) = n \iff$ G is disconnected. So the spectrum is, in a sense, symmetric, and questions about λ_2 of a graph are equivalent to questions about λ_n of its complement.

By looking at the trace of L, we have that $\sum_{j=1}^n d_j = \sum_{j=1}^n \lambda_j$, and thus $\lambda_2 \leq \frac{n}{n-1}\bar{d} \leq \lambda_n$. However, we can do better than this. Fiedler [13] shows that

Theorem 1.3.9. $\lambda_2 \leq \frac{n}{n-1}\delta$ *and* $\frac{n}{n-1}\Delta \leq \lambda_n$

Thus the range of the non-zero eigenvalues of a connected graph is (approximately) at least as great as the range of the vertex degrees. Obviously, by Theorem 1.3.4 and Corollary 1.3.8, we also have $\lambda_2 \leq n$ with equality if and only if the graph is complete. He further established the following result [13], with $v(G)$ representing the vertex connectivity of the graph.

Theorem 1.3.10. $\lambda_2 \leq v(G)$

Proof. To show this, we first note that if G_1 and G_2 are edge disjoint graphs on the same set of vertices, then $L(G_1) + L(G_2) = L(G_1 \cup G_2)$. Writing $\mathbf{j}$ for the all-ones vector, this gives that

$$\begin{aligned}
\lambda_2(G_1 \cup G_2) &= \min_{x \perp \mathbf{j}} \frac{\langle x, L(G_1 \cup G_2)x\rangle}{\langle x, x\rangle} \\
&= \min_{x \perp \mathbf{j}} \left(\frac{\langle x, L(G_1)x\rangle}{\langle x, x\rangle} + \frac{\langle x, L(G_2)x\rangle}{\langle x, x\rangle} \right) \\
&\geq \min_{x \perp \mathbf{j}} \frac{\langle x, L(G_1)x\rangle}{\langle x, x\rangle} + \min_{x \perp \mathbf{j}} \frac{\langle x, L(G_2)x\rangle}{\langle x, x\rangle} \\
&= \lambda_2(G_1) + \lambda_2(G_2) \qquad (1.13)
\end{aligned}$$

where the minimum is as usual over all non-zero vectors orthogonal to the all-ones vector. Thus removing edges does not increase λ_2. Now given a graph G and a vertex $j \in V(G)$, define $H = G\backslash\{j\}$, and define G' to be the graph with vertex set $V(G)$ and edge set $E(H) \cup \{ij \mid i \in V(G)\}$. (This may be seen as $G' = H \vee j$; see Theorem 1.4.5.) If x is an eigenvector of $L(H)$ with eigenvalue α, then the vector x' formed by the entries of x with one additional zero entry is seen to be an eigenvector of $L(G')$ with eigenvalue $\alpha + 1$. This gives

$$\lambda_2(G) \leq \lambda_2(G') \leq \lambda_2(H) + 1$$

By induction, we have that

$$\lambda_2(G) \leq \lambda_2(G\backslash\{v_1, v_2, \dots, v_k\})$$

So if the removal of some k vertices disconnects G, then $\lambda_2(G) \leq k$, which is exactly the result. Since the edge connectivity $b(G) \geq v(G)$, we also have that $\lambda_2 \leq b(G)$. □

In the same paper, he also established the following bounds relative to the edge connectivity, $e = e(G)$.

Theorem 1.3.11.

$$\lambda_2 \geq 2e(1 - \cos(\pi/n))$$
$$\lambda_2 \geq 2[\cos(\pi/n) - \cos(2\pi/n)] - 2\cos(\pi/n)(1 - \cos(\pi/n))\Delta$$

The second bound is better if and only if $2e > \Delta$. It is relevant to note in connection with this bound that $2(1 - \cos(\pi/n)) = \lambda_2(P_n)$, where P_n is the path on n vertices. A path being, in a sense, the "most nearly disconnected" connected graph, we see that, for fixed n, λ_2 is minimal for "most nearly disconnected" graphs, i.e., it is minimal on P_n.

We give values of λ_2 for certain graphs.

path	$P_n \lambda_2$	$= 2(1 - \cos(\pi/n))$
cycle	$C_n \lambda_2$	$= 2(1 - \cos(2\pi/n))$
cube	$Q_m \lambda_2$	$= 2$
complete	$K_n \lambda_2$	$= n$
completebipartite	$K_{m,n} \lambda_2$	$= \min\{m, n\}$
star	$S_n = K_{1,n-1} \lambda_2$	$= 1$

We note that, informally, graphs which are more connected have a larger λ_2.

1.4 Operations on graphs

We have already seen that removal of edges from a graph does not increase λ_2. We will now consider more precisely what happens to λ_2 under various graph operations.

Recall that the *Cartesian product* of two graphs G_1 and G_2 is defined as the graph $G_1 \times G_2$, with vertex-set $V(G_1) \times V(G_2)$; (i_1, j_1) and (i_2, j_2) are connected by an edge if and only if $i_1 = i_2$ and $j_1 \sim_{G_2} j_2$, or $j_1 = j_2$ and $i_1 \sim_{G_1} i_2$.

Lemma 1.4.1. $\lambda_2(G_1 \times G_2) = \min\{\lambda_2(G_1), \lambda_2(G_2)\}$

We note that a similar statement can be made about the eigenvalues of the adjacency matrix. In fact, the proof is quite general, depending only on the fact that $L(G_1 \times G_2) = L(G_1) \otimes I + I \otimes L(G_2)$, where I represents an appropriately-sized identity matrix and $\otimes$ represents the Kronecker product. It can be shown from this that the set of eigenvalues of $G_1 \times G_2$ is exactly

$\{\lambda_i(G_1) + \lambda_j(G_2) \mid 1 \le i \le n_1, 1 \le j \le n_2\}$. Furthermore, if x is an eigenvector of $L(G_1)$ corresponding to $\lambda_i(G_1)$, and y is an eigenvector of $L(G_2)$ corresponding to $\lambda_j(G_2)$, then $x \otimes y$ is an eigenvector of $L(G_1 \times G_2)$ corresponding to $\lambda_i(G_1) + \lambda_j(G_2)$.

In particular, if we take the product of G with itself, then λ_2 remains constant. Thus, given any graph, we can build arbitrarily large graphs with the same λ_2.

The *line graph* of G, denoted $l(G)$[3], is the graph whose vertices correspond to the edges of G, with two vertices of $l(G)$ being adjacent if and only if the corresponding edges of G share a common vertex. The *subdivision graph* of G, denoted by $s(G)$, is the graph obtained by replacing every edge in G with a copy of P_2 ("subdividing" each edge). The *total* graph of G, denoted by $t(G)$, is the graph whose vertices correspond to the union of the set of vertices and edges of G, with two vertices of $t(G)$ being adjacent if and only if the corresponding elements are adjacent or incident in G.

Let G be a d-regular graph, with n vertices and m edges. It is shown in [25] that

Theorem 1.4.2.

$$
\begin{aligned}
P_{l(G)}(x) &= (x-2d)^{m-n} P_G(x) \\
P_{s(G)}(x) &= (-1)^m (2-x)^{m-n} P_G(x(d+2-x)) \\
P_{t(G)}(x) &= (-1)^m (d+1-x)^n (2d+2-x)^{m-n} P_G\left(\frac{x(d+2-x)}{d+1-x}\right)
\end{aligned}
$$

where $P_G(x)$ represents the characteristic polynomial of the Laplacian matrix of the graph G. Note that, if G is d-regular with $d > 1$ (i.e. not a disjoint union of copies of K_2), then the eigenvalues of $l(G)$ are exactly the eigenvalues of G with the addition of the (multiple) eigenvalue $2d$, which was not an eigenvalue of G (Theorem 2.2.4). If G is 1-regular (i.e., a disjoint union of copies of K_2), then $2d = 2$ is an eigenvalue of G and the leading term in the expression for the characteristic polynomial for $l(G)$ "takes it away" instead of adding it to the spectrum.

Of course, as this theorem applies only to regular graphs, equivalent statements are possible in terms of the adjacency matrix (see [9]).

[3] We avoid the more customary $L(G)$ as this is reserved for the Laplacian matrix of G.

A *bipartite* (r,s)*-semiregular* graph is a bipartite graph with bipartition $V(G) = U \cup W$, such that all vertices in U have degree r and all vertices in W have degree s. In [46], Mohar shows that

Theorem 1.4.3. *Let G be a bipartite (r,s)-semiregular graph. Then $P_{l(G)}(x) = (-1)^m (r+s-x)^{m-n} P_G(r+s-x)$.*

We will define the *(disjoint) union* of two graphs G_1, G_2 to be the graph with vertex-set $V(G_1) \cup V(G_2)$ and edge-set $E(G_1) \cup E(G_2)$ and will denote it by $G_1 + G_2$. Note that this is a disconnected graph, and therefore $\lambda_2(G_1 + G_2) = 0$. In fact, one may easily prove

Theorem 1.4.4. *Given graphs G_1 and G_2 with spectra $0 = \alpha_1 \leq \alpha_2 \leq \ldots \leq \alpha_{n_1}$ and $0 = \beta_1 \leq \beta_2 \leq \ldots \leq \beta_{n_2}$, then the spectrum of $G_1 + G_2$ is the multiset $\{\alpha_1, \alpha_2, \ldots, \alpha_{n_1}, \beta_1, \beta_2, \ldots, \beta_{n_2}\}$.*

Define the *join* of two graphs G_1, G_2 to be $G_1 \vee G_2 = (G_1^c + G_2^c)^c$. This is the union of the two graphs, with every vertex in G_1 connected to every vertex in G_2. We note that $G_1 \vee G_2$ is always connected. It is obvious from the definition that the diameter of $G_1 \vee G_2$ is at most 2, with diameter 1 if and only if G_1 and G_2 are both complete graphs. The join of two graphs may be thought of as maximally attaching the two graphs together. In fact, since the complement of $G_1 \vee G_2$ is disconnected, we see that $n_1 + n_2$ must be an eigenvalue.

The matrix $L(G_1 \vee G_2)$ has a particularly nice block structure. The upper-left block is the matrix $L(G_1) + n_2 I$, the lower-left block is the matrix $L(G_2) + n_1 I$, and the other two blocks are $-J$. From this we may readily deduce the spectrum of $G_1 \vee G_2$, by exhibiting a complete set of eigenvectors. If x is an eigenvector of $L(G_1)$ corresponding to λ_i, $1 \leq i \leq n_1 - 1$, then the vector x', defined by $x'_k = x_k, 1 \leq k \leq n_1$ and $x'_k = 0$ otherwise, can be seen to be an eigenvector of $L(G_1 \vee G_2)$ with eigenvalue $\lambda_i + n_2$. Similarly, we obtain the eigenvalues $\lambda_j + n_1$ for $1 \leq j \leq n_2 - 1$. The all-ones vector gives, as usual, the eigenvalue 0, and the eigenvector whose value is $-n_1$ on the vertices of G_1 and n_2 on the vertices of G_2 gives the eigenvalue $n_1 + n_2$.

We have proved the following theorem, due to Merris [41]

Theorem 1.4.5. *Given graphs G_1 and G_2 with spectra $0 = \alpha_1 \leq \alpha_2 \leq \ldots \leq \alpha_{n_1}$ and $0 = \beta_1 \leq \beta_2 \leq \ldots \leq \beta_{n_2}$, then the spectrum of $G_1 \vee G_2$ is the multiset $\{0, \alpha_i + n_2, \beta_j + n_1, n_1 + n_2 \mid 1 \leq i \leq n_1 - 1, 1 \leq j \leq n_2\}$.*

In particular, $\lambda_2(G_1 \vee G_2) = \min\{\lambda_2(G_1), \lambda_2(G_2)\}$..

We note that this theorem gives a simple way of determining the Laplacian spectrum of a complete bipartite graph, since $K_{m,n} = {K_m}^c \vee {K_n}^c$.

Merris [41] notes as a corollary of this that

Corollary 1.4.6. *If x is an eigenvector corresponding to λ with $0 < \lambda < n$, then $x_j = 0$ whenever $d_j = n - 1$*

Proof. To see this result, let G be a graph, and j a vertex of degree $n - 1$. We see that $G = (G \backslash \{j\}) \vee \{j\}$. Thus, by Theorem 1.4.5, we have that the vector y, which takes the value $n-1$ at vertex j and 1 otherwise, corresponds to the eigenvalue n. The all-ones vector e corresponds to the eigenvalue 0. If x is an eigenvector corresponding to the eigenvalue λ, $0 < \lambda < n$, then x is orthogonal to both y and e, and hence is orthogonal to $x - e$. Hence $x_j = 0$. □

We therefore have that the number of eigenvalues less than n (including multiplicities) is no more than the number of vertices of degree less than $n-1$, and hence that the multiplicity of n is at least equal to the number of vertices of degree $n-1$. We can do better than this. Recall that the multiplicity of 0 is equal to the number of connected components, and that the multiplicity of n is equal to the number of connected components in the complement. Since vertices of degree $n - 1$ in a graph correspond exactly to isolated points in the complement, we have that the total number of eigenvalues (counting multiplicities) strictly between 0 and n is exactly the number of vertices of degree inclusively between 1 and $n - 2$.

We see that the union and join operations preserve "integrality". That is, if G_1 and G_2 have only integers in their spectra, then the same can be said of $G_1 \vee G_2$ and $G_1 \cup G_2$. Merris observes that any graph that can be expressed as a series of unions and joins of isolated vertices will have only integral eigenvalues; he refers to these as *decomposable* graphs. Note that for decomposable graphs, the final sentence of the preceeding paragraph says that the number of vertices of degree between 1 and $n - 2$ gives the number of eigenvalues between 1 and $n - 1$. In particular, we have that all connected decomposable graphs have $\lambda_2 \geq 1$. The fact that λ_2 is bounded away from zero for this class of graphs is intuitively consistent, as connected decomposable graphs were necessarily constructed with a join as the final operation, meaning that the resulting graph is highly connected.

1.5 Bounds on eigenvalues

Anderson and Morley [1] gave one of the first bounds on λ_2, as

Theorem 1.5.1. $\lambda_n \leq \max\limits_{i\sim j}(d_i + d_j)$

We omit the proof of this result.

Using the relationship between the Laplacian spectrum of a graph and its complement, we can of course write

$$\lambda_2 \geq \max_{i\sim j}(d_i + d_j) - (n-2)$$

In a similar spirit, Li and Zhang [27] show that

Theorem 1.5.2. $\lambda_n \leq 2 + \sqrt{(d_i + d_j - 2)(d'_i + d'_j - 2)}$

where d_i, d_j are the degrees of the endpoints of the edge with the largest number of adjacent vertices, and d'_i, d'_j are the degrees of the endpoints of the edge (not including the previous edge) with the (next) largest number of adjacent vertices.

Merris noted the following bound [42] (which he says is usually better than Theorem 1.5.2), where m_i represents the average degree of all the neighbours of the vertex i

Theorem 1.5.3. $\lambda_n \leq \max\limits_{i\sim j}(m_i + d_j)$

Li and Zhang [28] were able to improve their bound to

Theorem 1.5.4. $\lambda_n \leq \max\limits_{i\sim j}\frac{d_i(d_i+m_i)+d_j(d_j+m_j)}{d_i+d_j}$

Proof. To prove this result, we recall that $L = KK^t$, where K is the oriented vertex-edge incidence matrix. It is well known that KK^t and K^tK share the same nonzero eigenvalues. So λ_n is in fact the largest eigenvalue of K^tK. It is also well known that the largest eigenvalue of K^tK is no greater than the largest eigenvalue of ${K_+}^tK_+$, where K_+ is the unoriented vertex-edge incidence matrix (it's entries are just the absolute value of the corresponding entries of K^tK). A simple calculation shows that ${K_+}^tK_+ = 2I + B$, where B is the adjacency matrix of the line graph of the original graph. Let y be a vector of m components, where $m = |E(G)|$. We then have that

$$\lambda_n \leq \max \frac{((2I+B)y)_u}{y_u}$$

Choose $x_u = d_i + d_j$, where the edge u joins vertices i and j. We then have

$$\begin{aligned}((2I+B)y)_u &= 2(d_i+d_j) + \sum_{a\sim i}(d_i+d_a) - (d_i+d_j) + \sum_{b\sim j}(d_j+d_b) - (d_j+d_i) \\ &= d_i^2 + \sum_{a\sim i} d_a + d_j^2 + \sum_{b\sim j} d_b \\ &= d_i(d_i+m_i) + d_j(d_j+m_j)\end{aligned}$$

The result follows. □

Given the "standard" nature of the proof, it is perhaps somewhat surprising that this result was not published until 1998, while the observations on K^tK and $K_+{}^tK_+$ were made specifically in the context of Laplacian eigenvalues as early as 1971 in [1].

We note the role of the average degree, and the average degree among neighbours in these bounds. In fact, the quantity $d_i m_i$ has been termed the 2-degree of the vertex, as it gives the number of paths of length 2 originating from the vertex.

Chapter 2

Isoperimetric Inequalities

2.1 Introduction

Let $X \subset V(G)$. Define ∂X to be the set of edges of G with exactly one endpoint in X; this is sometimes referred to as the edge boundary of X, and is useful in analysing cut-set problems. We define the *isoperimetric constant* of a graph to be

Definition 2.1.1. $h(G) = \min_{|X| \leq n/2} \frac{|\partial X|}{|X|}$

We can interpret the quantity $|\partial X|/|X|$ as the average boundary degree of X. More precisely, given a graph G and a subset of vertices X, create a new multigraph G' by coalescing X onto a single new vertex x, preserving multiple edges but deleting any loops that would be formed. The degree of x is then precisely $|\partial X|$. Thus $|\partial X|/|X|$ is the average contribution of the vertices in X to the degree of x.

The isoperimetric constant can be understood as a measure of how easy it is to disconnect a large part of the graph. To a terrorist with an eye to knocking out the phone system, this is the reciprocal of the "bang for the buck". We note that like λ_2, we have that $h(G) = 0$ if and only if G is disconnected. We will see that $\lambda_2(G)$ and $h(G)$ are in fact quite closely related. It should be noted, however, that $h(G)$ is quite affected by local properties, since it finds the weakest part of the graph. In other words, "most" of the graph could be quite well-connected, with only one weak link, and the isoperimetric constant would reflect only this weak link. As an example of this, let G be the graph composed of two copies of K_n joined by a single edge, and let $H = P_{2n}$. We then have $h(G) = 1/n = h(H)$. Intuitively, one of these is more connected than the other, and in fact $\lambda_2(G) = n$ (This is a consequence of Theorem 6.1.1) and $\lambda_2(P_{2n}) = 2(1-\cos(\pi/2n))$. We give values of h for certain graphs.

path	$P_n h$	$= 1/\lfloor n/2 \rfloor$
cycle	$C_n h$	$= 2/\lfloor n/2 \rfloor$
cube	$Q_n h$	$= 1$
complete	$K_n h$	$= \lceil n/2 \rceil$
completebipartite	$K_{m,n} h$	$= \lceil mn/2 \rceil / \lfloor (m+n)/2 \rfloor$
star	$S_n = K_{1,n-1} h$	$= 1$

We have the following elementary bounds on $h(G)$.

$$\begin{aligned}
&h(G) \leq \delta \\
&h(G) \leq \min_{i \sim j} \frac{d_i + d_j - 2}{2} \text{ if } n \geq 4 \\
&h(G) \leq \lceil n/2 \rceil \\
&h(G) \geq \frac{1}{\lfloor n/2 \rfloor} \text{ if } G \text{ is connected}
\end{aligned}$$

The first two may be seen by considering X to be a (single) minimal degree vertex and a pair of connected vertices, respectively. The third comes from considering that $|\partial X| \leq (|X|)(n - |X|)$. The fourth is a consequence of the fact $|\partial X| \geq 1$ and $|X| \leq n/2$.

Chung [7] gives an alternative characterisation of the isoperimetric constant similar to (1.3), namely that

$$h = \min_{x} \max_{t \in \mathbb{R}} \frac{\sum_{ij \in E(G)} |x_i - x_j|}{\sum_{j \in V(G)} |x_j - t|} \tag{2.1}$$

where x ranges over all non-constant vectors. So h is just λ_2 measured with a different norm. Note that the value of t that achieves the maximum may be taken as the median of the values $\{x_j\}$. If n is odd, this is unique; if n is even, then t may be taken to be any value in the closed interval between the two median values of the set $\{x_j\}$. Recall that in (1.3) the value t was uniquely determined to be the mean of the values $\{x_j\}$.

Recall the interpretation of Lx given in Section 1.1, namely that given a $\{0,1\}$-vector x (i.e., the characteristic vector of a subset X of vertices) Lx describes exactly the boundary of X. We see that

$$\frac{\langle x, Lx\rangle}{\langle x, x\rangle} = \frac{|\partial X|}{|X|}$$

In other words, we may give the equivalent definition of

$$h(G) = \min \frac{\langle x, Lx\rangle}{\langle x, x\rangle}$$

where the minimum is over all $\{0,1\}$-vectors x with $\langle x, x\rangle \leq n/2$ — or equivalently over all subsets X of vertices with $|X| \leq n/2$. This has obvious similarities with the definition of λ_2, however, it should be noted that the sets of vectors over which x ranges in these definitions are disjoint. Also, though the set of vectors orthogonal to the constant vector is certainly a vector space, the set of $\{0,1\}$-vectors x with $\langle x, x\rangle \leq n/2$ is certainly not.

Computationally, determining λ_2 amounts to minimising a quadratic form over a vector space, while determining h amounts to minimising a quadratic form over a set. So it's not surprising that determining h seems to be in general exponential [45]. In fact, in that same paper, Mohar does show that the determination of h for general graphs with multiple edges is NP-hard.

2.2 Bounds on $h(G)$

A first approximation, due to Mohar [45] gives that the isoperimetric number is bounded by approximately half the average degree:

$$h(G) \leq \frac{2m\lceil n/2\rceil}{n(n-1)}$$

This is not entirely unexpected, as for sets X of a single vertex, we have exactly that $|\partial X|$ is the (average) degree of that vertex, and for sets X where $|X| > 1$, unless the subgraph induced by X has no edges, then $|\partial X|$ will be at most the average degree of the vertices in X.

Proof. To show this result, we will, following Mohar, define the quantities

$$h_r(G) = \min_{|X|=r\leq n/2} \frac{|\partial X|}{|X|}$$

Consider the r-subsets of $V(G)$; there are $\binom{n}{r}$ of them. Fix an edge $ij \in E(G)$; there are $2\binom{n-2}{r-1}$ r-subsets X with $ij \in \partial X$. Therefore,

$$\sum_{|X|=r} |\partial X| = m\, 2\binom{n-2}{r-1}$$

This gives that

$$h_r \leq \frac{\text{average } \{|\partial X|\}}{r} = \frac{m\, 2\binom{n-2}{r-1} / \binom{n}{r}}{r} = \frac{2m(n-r)}{n(n-1)}$$

and thus

$$h(G) = \min_{1 \leq r \leq n/2} h_r(G) \leq \frac{2m\lceil n/2 \rceil}{(n(n-1)}$$

$\square$

Informally, we see that both λ_2 and $h(G)$ tend to increase as the G becomes "more connected", and decrease as it becomes "less connected". For a given n, they are both maximal (only) for K_n and minimal for P_n (though h is also minimal on other graphs, such as two copies of $K_{n/2}$ joined by a single edge). The link between them can be made explicit by the following two theorems, due to Mohar [45]:

Theorem 2.2.1. $\lambda_2/2 \leq h(G)$

Theorem 2.2.2. $h(G) \leq \sqrt{\lambda_2(2\Delta - \lambda_2)}$ *for* $G \neq K_1, K_2, K_3$

Note that $2\Delta \geq \lambda_2$ is a positive quantity for graphs on $n \geq 3$ vertices (in fact, we will shortly establish a stronger result), so this bound is well-formed. By simply observing $2\Delta - \lambda_2 \leq 2\Delta$, we have a weaker form of Theorem 2.2.2 which is (sometimes) easier to use.

Corollary 2.2.3. $\frac{h^2(G)}{2\Delta} \leq \lambda_2$

Proof. To show Theorem 2.2.1, let X be a set that achieves $h(G)$, i.e. such that $h(G) = |\partial X|/|X|$. Let $a = |X| \leq n/2$ and $b = n - |X|$. Define the vector

$$x_j = \begin{cases} a & \text{if } j \notin X \\ -b & \text{if } j \in X \end{cases}$$

We have that x is orthogonal to the all-ones vector, and hence that

$$\begin{aligned}
\lambda_2 &\leq \frac{\langle x, Lx \rangle}{\langle x, x \rangle} \\
&= \frac{\sum_{i \sim j}(x_i - x_j)^2}{\sum_{j \in V(G)}(x_j)^2} \\
&= \frac{\sum_{ij \in \partial X}(x_i - x_j)^2}{\sum_{j \in V(G)}(x_j)^2} \\
&= \frac{|\partial X|(a+b)^2}{ab^2 + ba^2} \\
&= |\partial X|(\frac{1}{a} + \frac{1}{b}) \leq |\partial X|\frac{2}{a} = 2h(G)
\end{aligned}$$

□

To prove Theorem 2.2.2, we will need the following

Lemma 2.2.4. *For a complete graph, $\lambda_2 = n = \Delta + 1$. Otherwise, $\lambda_2 \leq \Delta$.*

Proof. We have already noted that $\lambda_2 = n$ for complete graphs; it is a simple consequence of (among other things) the fact that the complement of a complete graph has n components.

If the graph is not regular, then by Theorem 1.3.9, we have

$$\lambda_2 \leq \frac{n}{n-1}\delta = \delta + \frac{\delta}{n-1} < \delta + 1 \leq \Delta$$

If the graph is regular but not complete, then it contains P_3 as an induced subgraph. Let μ_2 be the second largest eigenvalue of the adjacency matrix A of the graph. Applying the interlacing theorem, we see that μ_2 must be larger than the second largest eigenvalue of the adjacency matrix of P_3, i.e., $\mu_2 \geq 0$. however, since the graph is regular, $L = D - A = \Delta I - A$, and thus $\Delta - \lambda_2 = \mu_2$, giving that $\lambda_2 \leq \Delta$. □

We note parenthetically that there is a gap in the permissible values of λ_2. If it is larger than the maximal degree, then it must be exactly one more than the maximal degree.

Proof. The following proof of Theorem 2.2.2 is due to Mohar [45]. We first note some special cases. Obviously, if G is disconnected, then $h(G) = \lambda_2(G) = 0$ and the theorem holds. If $G = K_n, n \geq 4$, then we have that

$$\sqrt{\lambda_2(2\Delta - \lambda_2)} = \sqrt{n(2(n-1)-n)} = \sqrt{n(n-2)} \geq n-2 \geq \lceil n/2 \rceil = h(G)$$

Also, if $\lambda_2 > \delta$ and the graph is not complete, then by Lemma 2.2.4

$$\sqrt{\lambda_2(2\Delta - \lambda_2)} > \sqrt{\delta\Delta} > \delta \geq h(G)$$

So we may assume that G is connected, not a complete graph, and that $\lambda_2 \leq \delta$. Let f be an eigenvector of λ_2. Define the set $W = \{j \mid f_j > 0\}$. We may assume that $|W| \leq n/2$ (otherwise negate f). Define a vector g by $g_j = f_j$ if $j \in W$ and $g_j = 0$ otherwise. Denote by $E(W)$ the set of edges of the induced subgraph of the vertex set W. Recalling that the eigenvalue condition for λ_2 may be written at each vertex as

$$\lambda_2 f_j = d_j f_j - \sum_{i \sim j} f_i$$

we see that

$$\begin{aligned}
\lambda_2 \sum g_j^2 = \lambda_2 \sum_{j \in W} f_j^2 &= \sum_{j \in W} (\lambda_2 f_j) f_j \\
&= \sum_{j \in W} (d_j f_j - \sum_{i \sim j} f_i) f_j \\
&= \sum_{j \in W} \sum_{i \sim j} (f_j - f_i) f_j \\
&= \sum_{ij \in E(W)} [(f_j - f_i) f_j + (f_i - f_j) f_i] + \sum_{\substack{j \in W \\ ij \in \partial W}} (f_j - f_i) f_j \\
&= \sum_{i \sim j} (g_i - g_j)^2 - \sum_{\substack{j \in W \\ ij \in \partial W}} f_i f_j \qquad (2.2)
\end{aligned}$$

Also, note that

$$\begin{aligned}(2\Delta-\lambda_2)\sum g_j^2 = (2\Delta-\lambda_2)\sum_{j\in W} f_j^2 &= \sum_{j\in W}(2\Delta f_j - \lambda_2 f_j)\, f_j \\ &= \sum_{j\in W}\left(2\Delta f_j - d_j f_j + \sum_{i\sim j} f_i\right) f_j \\ &\geq \sum_{j\in W}\left(d_j f_j + \sum_{i\sim j} f_i\right) f_j \\ &= \sum_{i\sim j}(g_i+g_j)^2 + \sum_{ij\in\partial W} f_i f_j\end{aligned}$$

Combining these two, and writing $A = \sum_{ij\in\partial W}(f_i f_j)$, we have

$$\begin{aligned}&\lambda_2(2\Delta-\lambda_2)\left(\sum g_j^2\right) \geq \\ &\qquad \sum_{i\sim j}(g_i-g_j)^2\sum_{i\sim j}(g_i+g_j)^2 - A\left(A + 4\sum_{ij\in E(W)} f_i f_j\right)\end{aligned} \tag{2.3}$$

Observe that $A \leq 0$. Also note that since $\lambda_2 \leq \delta$, we have

$$\begin{aligned}A + 4\sum_{ij\in E(W)} f_i f_j &= 2\sum_{ij\in E(W)} f_i f_j + \sum_{j\in W}\sum_{i\sim j} f_i f_j \\ &= 2\sum_{ij\in E(W)} f_i f_j + \sum_{j\in W}(d_j-\lambda_2) f_j^2\end{aligned} \tag{2.4}$$

Denote $B = \sum_{i\sim j}|g_i^2 - g_j^2|$. We then have

$$\begin{aligned}B^2 &\leq \sum_{i\sim j}(g_i-g_j)^2\sum_{i\sim j}(g_i+g_j)^2 \\ &\leq \lambda_2(2\Delta-\lambda_2)\left(\sum g_j^2\right) + A\left(A + 4\sum_{ij\in E(W)} f_i f_j\right) \\ &\leq \lambda_2(2\Delta-\lambda_2)\left(\sum g_j^2\right)^2\end{aligned} \tag{2.5}$$

We now obtain a lower bound on B. Let the distinct values of the components of g be $0 = t_0 < t_1 < \cdots < t_m$. Define the set $V_k = \{j \mid g_j \geq t_k\}$.

We note that $|V_0| = n$ and that $|V_k| \le |V_1| \le |W| \le n/2$ for $k \ge 1$.

$$\begin{aligned}
B &= \sum_{k=1}^{m} \sum_{\substack{i\sim j \\ g_i<g_j=t_k}} (g_j^2 - g_i^2) \\
&= \sum_{k=1}^{m} \sum_{ij\in\partial V_k} (t_k^2 - t_{k-1}^2) \\
&= \sum_{k=1}^{m} |\partial V_k|(t_k^2 - t_{k-1}^2) \\
&\ge h(G) \sum_{k=1}^{m} |V_k|(t_k^2 - t_{k-1}^2) \\
&= h(G) \sum g_j^2 \qquad (2.6)
\end{aligned}$$

Putting these two bounds together we get

$$\left(h(G) \sum g_j^2\right)^2 \le B^2 \le \lambda_2(2\Delta - \lambda_2) \left(\sum g_j^2\right)^2$$

which completes the proof. □

As a general comment on the discipline, it is interesting to note that the vectors f and g were also used in proving results on magnifier graphs [2] (Theorem 3.2.3 of the present paper).

Note that $2\Delta - \lambda_2 > \Delta$ is never "small": for a complete graph, $2\Delta - \lambda_2 = n-2$ and otherwise $2\Delta - \lambda_2 \ge \Delta$. So for $\sqrt{\lambda_2(2\Delta - \lambda_2)}$ to be small we need to have λ_2 small. Thus by combining Theorem 2.2.1 and Theorem 2.2.2, we have

$$\lambda_2/2 \le h(G) \le \sqrt{\lambda_2(2\Delta - \lambda_2)}$$

In other words, small values of λ_2 force the graph to have a poorly-connected subset, and a graph with no poorly-connected subset has a large λ_2. We can formalise this for a given infinite family of graphs G_r by

$$\lim_{r\to\infty} h(G_r) = 0 \iff \lim_{r\to\infty} \lambda_2(G_r) = 0$$

It is relevant to note that, in general, there is no known efficient way to calculate $h(G)$ for a given graph. Although it seems to be a difficult quantity to calculate, it is not been formally proved that there is no polynomial algorithm to determine $h(G)$ in general. As noted above, it is NP-hard for graphs with multiple edges. Computing λ_2, however, is much easier. Thus we may use λ_2 to obtain an easily computable upper bound for $h(G)$. This is a recurring theme, in fact. Although λ_2 does not *directly* measure most graph properties, we will see that it often provides useful (and easily computable) bounds.

Theorem 2.2.1 can be seen to be tight for the cube graphs, where we have $\lambda_2 = 2$ and $h = 1$. Corollary 2.2.3 can be seen to be roughly tight to (within a constant factor) for a path or a complete graph, for instance:

$$\frac{h^2(P_n)}{2\Delta(P_n)} = \frac{\left(\frac{1}{\lfloor n/2 \rfloor}\right)^2}{2 \times 2} \approx \frac{1}{n^2}$$

$$\lambda_2(P_n) = 2(1 - \cos(\pi/n)) = 2 - 2(1 - \frac{(\pi/n)^2}{2!} + \frac{(\pi/n)^4}{4!} + \cdots) \approx \frac{\pi^2}{n^2} \quad (2.7)$$

$$\frac{h^2(K_n)}{2\Delta(K_n)} = \frac{\lceil n/2 \rceil^2}{2(n-1)} \approx \frac{n}{8}$$

$$\lambda_2(K_n) = n$$

In general, however, this is not always the case. For example, if G is the graph formed by joining two copies of K_n with a single edge, then $\lambda_2(G) = n$ while $h(G) = 1/n$.

It is useful to note (by observing the final inequality in the proof of Theorem 2.2.1) that if the set X that achieves h is such that $|X|$ is much less than $n/2$, we may (almost) state $\lambda_2 < h$. Informally, for a graph to have a large value of λ_2, not only should h be large, but also any set that achieves h should be as close as possible to half the total number of vertices in size.

Note that in Theorem 2.2.1 we needn't insist that X achieves $h(G)$, so in fact for arbitrary $|X|$ we have (following the proof of Theorem 2.2.1) that

$$\lambda_2 \leq |\partial X|(\frac{1}{|X|} + \frac{1}{n - |X|}) \leq \lambda_n \quad (2.8)$$

For a given set X, we define the edge density of X to be

$$\rho(X) = \frac{|\partial X|}{|X|(n - |X|)}$$

This represents the ratio of edges to vertex pairs ("potential edges") between X and its complement. It is a relative measure of the extent to which X is connected to its complement.

Given X, ∂X is uniquely defined. If the graph is connected, then ∂X is the edge boundary only of X (or the complement of X). If the graph is disconnected, it is possible for two distinct non-complementary sets X_1 and X_2 to have $\partial X_1 = \partial X_2$. Thus if G is connected, and Y is a minimal set of edges that disconnects the graph, then $Y = \partial X$ for a unique X (up to complementation) and we see that $\rho(X)$ depends only on Y.

We see then that the bounds (2.8) gives rise to bounds on the edge-density in a graph:

$$\frac{\lambda_2}{n} \leq \rho(X) \leq \frac{\lambda_n}{n}$$

Also, letting X be a set that achieves $h(G)$, we have, in light of Theorem 2.2.1, that

$$\rho(X) = \frac{h(G)}{n - |X|} \leq \frac{\sqrt{\lambda_2(2\Delta - \lambda_2)}}{n/2}$$

and we see that the minimal edge density in the graph is bounded above by λ_2. This is an extremely important observation, as the value of λ_2 allows us to conclude the existence of a "weak link" in the graph, where weakness is measured in terms of edge density. For a graph to have no set X with low edge density, it is necessary (though not sufficient) that λ_2 be large relative to n.

Chapter 3

Expanders

3.1 Introduction

The isoperimetric constant was motivated by a desire to find the "weakest" point of a graph, the part that is (for its size) least connected to the rest of the graph. We may ask essentially the same question in reverse: Can we construct a graph such that any "small" set of vertices is well-connected to the rest of the graph? Here we are looking for graphs with large growth rate, i.e., the number of vertices at distance k from some (fixed but arbitrary) point increases rapidly with k. This leads to several related notions, including concentrators, superconcentrators, magnifiers... all based on essentially this one idea.

Such graphs are useful in computer science. Expander graphs are used in parallel sorting algorithms, as well as graph pebbling algorithms (see [3] and the references therein). According to [2] they are quite common (e.g. almost all regular bipartite graphs on n inputs and n outputs are expanders for some value of c). They are also used to build superconcentrators, which are used in computer science (again, see the references in [3]). Explicit constructions, though possible ([17], [31]) are more difficult and may have expansion properties that actually compare quite poorly with the expectation for a random graph [2]. Although this means that random guessing is the "best" way, the explicit calculation of the expansion properties of any given graph can be quite difficult. This dilemma can be resolved using the Laplacian eigenvalues of the graph.

3.2 Relations with eigenvalues

An (n, Δ, c)-*expander* graph is a bipartite graph on two sets of vertices I and O ("inputs" and "outputs"), with $|I| = |O| = n$, the maximal vertex degree is Δ, and for every subset X of I with $|X| \leq n/2$ we have

$$|N(X)| \geq (1 + c(1 - |X|/n))|X|$$

where $N(X)$ is the neighbourhood of X: the set of vertices adjacent to a vertex in X. It is a *strong* (n, Δ, c)-*expander* if the result holds for all subsets X of I.

It turns out that the expansion properties of a graph are related to the Laplacian eigenvalues of the graph. This has direct practical consequences. By randomly generating graphs, we are almost sure that the graphs will be expanders; by checking the value of λ_2, we can establish a bound on the amount of expansion. That is the essential result of [2]. To demonstrate this, we will need to consider magnifiers. An (n, Δ, c)-*magnifier* graph is a graph on n vertices, with maximal degree Δ, such that for every subset X of vertices with $|X| \leq n/2$ we have

$$|N(X) - X| \geq c|X|$$

This is essentially the non-bipartite version of an expander graph. Were it not for the fact that the applications are more in terms of expanders, this might well be regarded as the more "fundamental" definition. The relation between the two can be made more explicit by observing that magnifiers give rise to expanders. Specifically, [2] we see by direct calculation that

Lemma 3.2.1. *Let G be an (n, Δ, c)-magnifier on vertices $\{v_1, v_2, \ldots, v_n\}$. Form the graph H with inputs $\{x_1, x_2, \ldots, x_n\}$ and outputs $\{y_1, y_2, \ldots, y_n\}$ such that the edges of H are exactly the pairs $\{(x_i y_i)\}$ for $i = 1, 2, \ldots, n$ and the pairs $\{(x_i y_j)\}$ where $(v_i v_j)$ is an edge of G. (This is the* extended double cover *of G.) Then H is an $(n, \Delta + 1, c)$-expander.*

Alon establishes the relationship between magnifiers and eigenvalues by the following two lemmas (the notation is slightly changed from the original paper). [2]

Theorem 3.2.2. *Given a graph G on n vertices with maximal degree Δ, then G is an (n, Δ, c)-magnifier with $c = 2\lambda_2/(\Delta + 2\lambda_2)$*

Theorem 3.2.3. *Given an (n, Δ, c)-magnifier, then $\lambda_2 \geq c^2/(4 + 2c^2)$*

Thus a graph with good magnification properties (which means a graph such that any small subset is well connected to the rest of the graph) is more or less the same as a graph with large λ_2. We have as a straightforward consequence, that given an (n, Δ, c)-magnifier, we can *prove* (by computing eigenvalues), that it is an (n, Δ, c')-magnifier with $c' = c^2/(c^2 + \Delta(2 + c^2))$. This is relevant in that if we are generating graphs randomly, we don't know what c is explicitly even though we may be fairly certain that it is large. This makes the random generation and subsequent verification (by eigenvalues) of magnifier graphs an efficient process.

The proof of Theorem 3.2.2 depends on the following lemma from [3]. Define the *distance* between two sets of vertices A and B as the length of the shortest path that starts in A and ends in B.

Lemma 3.2.4. *Given two disjoint sets of vertices A and B such that the distance between them is $d > 1$. Let $a = |A|/n$ and $b = |B|/n$. Then*

$$b \leq \frac{(1-a)}{1 + \lambda_2\, ad^2/\Delta}$$

Informally, this says that if λ_2 is large, then "large" sets of vertices cannot be "far" apart.

Proof. To show Theorem 3.2.2, let X be a subset of vertices such that $|X| \leq n/2$. Using Lemma 3.2.4 with $A = X$ and $B = V(G) - (X \cup N(X))$, we obtain

$$1 - \frac{|X| + |N(X) - X|}{n} \leq \frac{1 - |X|/n}{1 + \lambda_2(|X|/n)2^2/\Delta}$$

$$|N(X) - X| \geq n\left[1 - |X|/n - \frac{1 - |X|/n}{1 + 4\lambda_2\,|X|/(n\Delta)}\right]$$

$$|N(X) - X| \geq n(1 - |X|/n)\left[1 - \frac{1}{1 + 4\lambda_2\,|X|/(n\Delta)}\right]$$

$$|N(X) - X| \geq |X|(1 - |X|/n)\frac{4\lambda_2}{\Delta + 4\lambda_2\,|X|/n}$$

For $|X| \leq n/2$, this gives that

$$|N(X) - X| \geq |X|\frac{2\lambda_2}{\Delta + 2\lambda_2}$$

which says that the graph is an (n, Δ, c)-magnifier with $c = 2\lambda_2/(\Delta + 2\lambda_2)$. $\square$

Proof. To proof of Theorem 3.2.3 is a little trickier. We define, as we did in the proof of Theorem 2.2.2, the vector f to be an eigenvector of λ_2 with at most $n/2$ positive entries, the set $W = \{j \mid f_j > 0\}$, the set $E(W)$ to be the set of edges both of whose endpoints are in W, and the vector g by $g_j = f_j$ if $j \in W$ and $g_j = 0$ otherwise.

Making use of prior work, we find that (2.2) gives the following bound for λ_2:

$$\lambda_2 \geq \frac{\sum_{ij \in E(W)} (g_i - g_j)^2}{\sum_{j \in V(G)} {g_j}^2} \tag{3.1}$$

We now construct a network, with an eye towards applying the well-known max-flow min-cut theorem. The network has vertex set $\{s, t\} \cup X \cup Y$, where s is the source, t is the sink, X is a copy of W and Y is a copy of $V(G)$. The arcs are defined as follows:

1. The arc (s, i) has capacity $1 + c$ for every $i \in X$
2. The arc (i, j) has capacity 1 if $ij \in W$ or if $i = j$, and 0 otherwise
3. The arc (j, t) has capacity 1 for every $j \in Y$

The cut consisting of all arcs (s, i) has capacity $|W|(1 + c)$; the claim is that this is minimal. Let C be some cut that does not include all arcs originating from the source. Let U be the set of arcs of the form (s, i) that are not in C. Consider the set $\{j \in Y \mid (i, j)$ is an arc for some $i \in U\}$. But the graph is a magnifier. Therefore, this set has cardinality at least $(1 + c)|U|$. Since C is a cut, it must contain at least one arc incident to each element of this set. Thus the total capacity of C is at least

$$|W - U| \cdot (1 + c) + (1 + c)|U| \cdot 1 \geq |W|(1 + c)$$

The max-flow min-cut theorem gives that there exists an orientation $\bar{E}$ of the $E(G)$ and a function α defined on the directed edges such that

1. $0 \leq \alpha(i, j) \leq 1$ for all (i, j)
2. $\sum_j \alpha(i, j) = 1 + c$ if $i \in W$, and 0 otherwise

3. $\sum_i \alpha(i,j) \le 1$

One can check that the function α satisfies

$$\begin{aligned}
\sum_{ij\in\bar{E}} \alpha^2(i,j)(g_i+g_j)^2 &\le 2\sum_{ij\in\bar{E}} \alpha^2(i,j)({g_i}^2+{g_j}^2) \\
&\le 2\sum_{i\in V(G)} {g_i}^2\Big(\sum_j \alpha^2(i,j) + \sum_j \alpha^2(j,i)\Big) \\
&\le 2(2+c^2)\sum_{i\in V(G)} {g_i}^2 \qquad (3.2)
\end{aligned}$$

and

$$\begin{aligned}
\sum_{ij\in\bar{E}} \alpha(i,j)({g_i}^2-{g_j}^2) &= \sum_{i\in V(G)} {g_i}^2\Big(\sum_j \alpha(i,j) - \sum_j \alpha(j,i)\Big) \\
&\ge c\sum_{i\in V(G)} {g_i}^2 \qquad (3.3)
\end{aligned}$$

Combining (3.1), (3.2), and (3.3), we obtain

$$\begin{aligned}
\lambda_2 &\ge \frac{\sum_{ij\in E(W)}(g_i-g_j)^2}{\sum_{j\in V(G)} {g_j}^2} \\
&= \frac{\sum_{ij\in E(W)}(g_i-g_j)^2 \sum_{ij\in\bar{E}} \alpha^2(i,j)(g_i+g_j)^2}{\sum_{j\in V(G)} {g_j}^2 \sum_{ij\in\bar{E}} \alpha^2(i,j)(g_i+g_j)^2} \\
&\ge \frac{\left(\sum_{ij\in\bar{E}} \alpha(i,j)|{g_i}^2-{g_j}^2|\right)^2}{2(2+c^2)\left(\sum_{j\in V(G)} {g_j}^2\right)^2} \\
&\ge \frac{1}{4+2c^2}\left(\frac{\sum_{ij\in\bar{E}} \alpha(i,j)({g_i}^2-{g_j}^2)}{\sum_{j\in V(G)} {g_j}^2}\right)^2 \\
&\ge \frac{c^2}{4+2c^2}
\end{aligned}$$

□

In the same paper, Alon also establishes the following two results, which we reproduce here without proof:

Theorem 3.2.5. *If G is an (n, Δ, c) strong expander, then G is a $(2n, \Delta, c/16)$-magnifier.*

Theorem 3.2.6. *If G is a Δ-regular bipartite graph on the vertex sets I and O with $|I| = |O| = n$, and G is a $(2n, \Delta, c)$-magnifier then G is a $(n, \Delta, 2c/((d+1)(c+1)))$ strong expander.*

It is remarked that the constant 16 is not optimal. Combining this with previous results, this gives

Corollary 3.2.7. *If G is an (n, Δ, c) strong expander, then $\lambda_2 \geq \frac{c^2}{1024+c^2}$.*

If G is a Δ-regular bipartite graph on the vertex sets I and O with $|I| = |O| = n$, then G is a $(n, \Delta, \frac{4\lambda_2}{(\Delta+1)(\Delta+4\lambda_2)})$-expander.

Alternatively, he also derives the following result, which is in principle the same thing, but with a better bound.

Theorem 3.2.8. *If G is a Δ-regular bipartite graph on the vertex sets I and O with $|I| = |O| = n$, then G is a $(n, \Delta, \frac{(2\Delta-\lambda_2)\lambda_2}{\Delta^2})$-expander.*

3.3 Vertex expansion

One can view the properties of expanders as being similar to the properties of the isoperimetric constant h. One can define the *vertex boundary* of a set X as being the set $\delta X = \{y \in V(G) \mid y \notin X, y \sim x \in X\}$. We can then give the alternative definition of the parameter h' in an (n, Δ, h')-magnifier as

Definition 3.3.1. $h' = \min\limits_{|X| \leq n/2} \frac{|\delta X|}{|X|}$

where this definition includes the rather uninteresting case where $h' = 0$.

We can see trivially that $|\delta X| \leq |\partial X|$, so that $h' \leq h$. Thus by Theorem 2.2.2 (or the weaker version, Corollary 2.2.3) that

$$h'(G) \leq \sqrt{\lambda_2(2\Delta - \lambda_2)} \text{ for } G \neq K_1, K_2, K_3$$
$$\frac{h'^2(G)}{2\Delta} \leq \lambda_2$$

These bounds can sometimes be tight to within a constant factor: for example, for the path, we have $h'(P_n) = h(P_n)$, and (2.7) applies to $h'(P_n)$ as well as to $h(P_n)$. However, for the complete graph, we obtain

$$\frac{(h'(K_n))^2}{2\Delta(K_n)} = \frac{\lceil n/2 \rceil^2 / \lfloor n/2 \rfloor^2}{2(n-1)} \approx \frac{1}{2(n-1)} \qquad \ll \qquad \lambda_2(K_n) = n$$

In fact, we see directly from the definition that for any graph, $h' \leq 1$.

Considering any graph, we see that the magnification constant h' is bounded below by

$$h' = \min \frac{|N(X) - X|}{|X|} = \min \frac{|\delta X|}{|X|} \geq \min \frac{|\partial X|/\Delta}{|X|} = \frac{h}{\Delta}$$

where the minimum is taken over all subset X of vertices with $|X| \leq n/2$. So we also have the bound

$$h' \geq \frac{\lambda_2}{2\Delta}$$

This bound can be tight to within a constant factor. For example, for the graph H composed of two copies of K_n joined by a single edge and for a path we have

$$\begin{aligned} h'(H) = 1 \quad &\geq \quad \frac{\lambda_2(H)}{2\Delta(H)} = \frac{n}{2n} = \frac{1}{2} \\ h'(P_n) = h(P_n) = \frac{1}{\lfloor n/2 \rfloor} \quad &\geq \quad \frac{\lambda_2(P_n)}{2\Delta(P_n)} = \frac{2(1 - \cos(\pi/n))}{2 \times 2} \approx \frac{\pi^2}{4n^2} \end{aligned}$$

Note that as a corollary to Theorem 3.2.8 and Theorem 2.2.2, we obtain a lower bound on h', allowing us to give

$$\left(\frac{h}{2}\right)^2 \leq h' \leq h.$$

Chapter 4

Other Graph Parameters

4.1 Diameter and mean distance

Due to the way in which the Laplacian matrix measures the boundary of a subset of vertices, we should not be surprised to find that it is related to the diameter.

As a first relationship, we have that (writing D for the diameter of the graph)

Theorem 4.1.1.

$$\lambda_2 \geq \frac{1}{nD}$$

Proof. To prove this, we use the "standard" Rayleigh quotient formulation, adapted from [7] (where it was proved in the context of the matrix $\mathcal{L}$, see Section 8.1). Let x be a vector achieving λ_2 in (1.1), and let u be a vertex such that $|x_u| = \max_i |x_i|$. Since x is orthogonal to the all-ones vector, there is another vertex v such that $x_u x_v < 0$. Let P be a shortest path joining u to v. Let t be the length of P. We then have:

$$\begin{aligned}\lambda_2 &= \frac{\sum_{i\sim j}(x_i - x_j)^2}{\sum_{j\in V(G)}(x_j)^2} \\ &\geq \frac{\sum_{ij\in P}(x_i - x_j)^2}{n(x_u)^2} \\ &\geq \frac{(x_u - x_v)^2/t}{n(x_u)^2} \\ &\geq \frac{1}{nt} \\ &\geq \frac{1}{nD}\end{aligned}$$

where we used the Cauchy-Schwarz inequality in the third line. □

Another bound, due to Nilli [49] gives that

Theorem 4.1.2.

$$\lambda_2 \leq \Delta - 2\sqrt{\Delta - 1} + \frac{2\sqrt{\Delta - 1} - 1}{\lfloor D/2 \rfloor}$$

Proof. To prove this result, consider two edges at a distance of at least $2t+2$. Define the set V_0 to be the the set containing the two vertices of one of these edges, and U_0 to be the set containing the two vertices of the other edge. Let $V_k, 1 \leq k \leq t$ be the set of all vertices of distance k from V_0, and let $U_k, 1 \leq k \leq t$ be the set of all vertices of distance k from U_0. We note that these are all disjoint, and that furthermore there is no edge joining a vertex of the set $\bigcup_{k=0}^{t} V_k$ with a vertex of the set $\bigcup_{k=0}^{t} U_k$. Also, we have $|V_k| \leq (\Delta-1)|V_{k-1}|$ and $|V_k| \leq (\Delta-1)|V_{k-1}|$ for $1 \leq k \leq t$. For given $a, b \in \mathbb{R}$, define a n-vector x on the vertices by $x_j = a(\Delta - 1)^{k/2}$ for $j \in V_k, 0 \leq k \leq t$, $x_j = b(\Delta - 1)^{k/2}$ for $j \in U_k, 0 \leq k \leq t$, and $x_j = 0$ otherwise. Note that we may choose a, b so as to make $\sum j \in V(G)x_j = 0$; in other words, we may choose x to be orthogonal to the all-ones vector. Thus

$$\lambda_2 \leq \frac{\sum_{i\sim j}(x_i - x_j)^2}{\sum_{j\in V(G)}(x_j)^2}$$

It is a simple calculation to determine that $\sum_{j\in V(G)}(x_j)^2 = A_1 + B_1$ where

$$A_1 = a^2 \sum_{k=0}^{t} \frac{|V_k|}{(\Delta - 1)^k} \qquad B_1 = b^2 \sum_{k=0}^{t} \frac{|U_k|}{(\Delta - 1)^k}$$

The number of edges connecting vertices in V_k to vertices in V_{k+1} is at most $\Delta - 1$, and there are no edges from V_t to any U_k for $0 \leq k \leq t$. So we have $\sum_{i \sim j}(x_i - x_j)^2 = A_2 + B_2$ where

$$A_2 \leq a^2|V_t|(\Delta - 1)\left(\frac{1}{(\Delta-1)^{t/2}} - 0\right)^2 + a^2 \sum_{k=0}^{t-1} |V_k|(\Delta - 1)\left(\frac{1}{(\Delta-1)^{k/2}} - \frac{1}{(\Delta-1)^{(k+1)/2}}\right)^2$$

with a similar expression for B_2

We obtain an upper bound for the quantity A_2/A_1, observing that the same bound holds by symmetry for B_2/B_1, and therefore will be an upper bound for $(A_2 + B_2)/(A_1 + B_1)$, which is itself an upper bound for λ_2.

Note that $|V_k| \leq (\Delta - 1)|V_{k-1}|$ implies $|V_k|/(\Delta-1)^k \leq |V_{k-1}|/(\Delta-1)^{k-1}$, and we have

$$\begin{aligned}
A_2 &\leq a^2 \frac{|V_t|}{(\Delta-1)^t}(\Delta - 1) + a^2 \sum_{k=0}^{t-1} \frac{|V_k|}{(\Delta-1)^k}(\Delta - 2\sqrt{\Delta - 1}) \\
&= a^2 \frac{|V_t|}{(\Delta-1)^t}\left((2\sqrt{\Delta-1} - 1) + (\Delta - 2\sqrt{\Delta-1})\right) \\
&\qquad + a^2 \sum_{k=0}^{t-1} \frac{|V_k|}{(\Delta-1)^k}(\Delta - 2\sqrt{\Delta - 1}) \\
&\leq \frac{A_1}{t+1}(2\sqrt{\Delta-1} - 1) + A_1(\Delta - 2\sqrt{\Delta-1})
\end{aligned}$$

Thus we have

$$\frac{A_2}{A_1} \leq \frac{1}{t+1}(2\sqrt{\Delta-1} - 1) + (\Delta - 2\sqrt{\Delta-1})$$

which establishes the bound on λ_2. □

Theorem 4.1.2 has, as a corollary, a result which was first obtained by another method by Alon and Boppana [2], namely that given an infinite family of Δ-regular graphs, that

$$\limsup \lambda_2 \leq \Delta - 2\sqrt{\Delta - 1}$$

This bound is important in that it is, asymptotically, best possible. Lubotzky, Phillips, and Sarnak gave an explicit construction for the so-called Ramanujan graphs, that have $\lambda_2 \geq \Delta - 2\sqrt{\Delta - 1}$ [29]. These are graphs with large girth, small diameter, and large λ_2. In fact, we see that the conditions "small diameter" and "large λ_2" are essentially the same thing.

Alon and Millman [3] show that

Theorem 4.1.3.

$$D \leq 2 \log_2 n \sqrt{2\Delta/\lambda_2}$$

By combining Theorem 4.1.1 and Theorem 4.1.3, we see that for a given number of vertices, the diameter is small for large values of λ_2 and large for small values of λ_2. Noting that $\lambda_2 = 0$ means that $D = \infty$ (the graph is disconnected) and $\lambda_2 = n$ means that the graph is a complete graph, we are not surprised to discover that these results are approximated for nearly extremal values of λ_2. Theorem 4.1.1 gives $\lambda_2 \approx 0 \Rightarrow D$ large and Theorem 4.1.3 gives $\lambda_2 \approx n \Rightarrow D$ small .

In fact, we can do better than either Theorem 4.1.3 or Theorem 4.1.1. Mohar establishes the following two upper bounds on the diameter [47]. They are not, in general, comparable, although he says the second is "in most cases, much stronger than" the first. The second also represents a better bound than Theorem 4.1.3.

Theorem 4.1.4.

$$D \leq 2 \left\lceil \frac{\Delta + \lambda_2}{4\lambda_2} \log(n-1) \right\rceil$$

For the proof see [46]. The second bound is valid for any $\alpha > 1$ (he provides tables giving "good" choices for α).

Theorem 4.1.5.

$$D \leq 2 \left\lceil \sqrt{\frac{\lambda_n}{\lambda_2} \frac{\alpha^2 - 1}{4\alpha} + 1} \log_\alpha(n/2) \right\rceil$$

The proof of Theorem 4.1.5 will follow trivially from the following two lemmas. We will use the notation established previously, that $B_k(w)$ will be the set of vertices at distance at most k from some (fixed) vertex w. Also, we will write e_k for the number of edges with exactly one endpoint in B_k.

Lemma 4.1.6. *Let $r > 1$ and $k \geq 0$ be integers and let w be some (fixed) vertex of G. Define $b = |B_k|$ and $c = |V \backslash B_{k+r}| = n - |B_{k+r}|$. Then*

$$(r-1)^2 < \frac{\lambda_n}{4\lambda_2} \frac{(n-b-c)(b+c)}{bc}$$

Proof. Note that B_k and $V \backslash B_{k+r}$ are two sets of vertices separated by a distance r.

We define a vector

$$x_j = \begin{cases} t & \text{if } j \in B_k \\ t + r - 1 & \text{if } j \notin B_{k+r} \\ t + i - 1 & \text{if } j \in B_{k+i} \backslash B_{k+i-1} \end{cases}$$

We can choose the value of t to make x orthogonal to the all-ones vector, and can thus apply (1.1). Direct computation shows that

$$\begin{aligned} \langle x, x \rangle &= \sum_i {x_i}^2 \\ &> bt^2 + c(t + r - 1)^2 \\ &> b \left(\frac{-c(r-1)}{b+c} \right)^2 \left(\frac{-c(r-1)}{b+c} + r - 1 \right)^2 \\ &= \frac{bc(r-1)^2}{b+c} \langle x, Lx \rangle \qquad = \sum_{ij \in E(G)} x_i - {x_j}^2 \\ &= \sum_{i=k+1}^{k+r-1} e_i \end{aligned}$$

We need an upper bound on the quantity $\sum_{i=k+1}^{k+r-1} e_i$. Consider the subgraph H induced by $B_{k+r} \backslash B_k$. The interlacing inequalities give that $\lambda_n(H) \leq \lambda_n(G)$. Define the following vector on H

$$y_j = \begin{cases} +1 & \text{if } j \in B_{2i+1} \backslash B_2 i \text{ for some } i \\ -1 & \text{otherwise} \end{cases}$$

It may readily be seen that by (1.2), we now have

$$\lambda_n(H) \geq \frac{\sum_{ij \in E(G)} y_i - {y_j}^2}{n - b - c} = \frac{4 \sum_{i=k+1}^{k+r-1} e_i}{n - b - c}$$

which establishes the desired result. $\square$

Lemma 4.1.7. *Let $r > 1$ and $k \geq 0$ be integers and let w be some (fixed) vertex of G. Define $b = |B_k|$ and $c = |V \backslash B_{k+r}| = n - |B_{k+r}|$. If $n - c \leq \alpha b \leq n/2$ then*

$$r < \sqrt{\frac{\lambda_n}{\lambda_2} \frac{\alpha^2 - 1}{4\alpha}} + 1$$

Proof. Note that since $b + c \geq n - \alpha b + b$ and $n - \alpha b + b \geq n/2$ we have

$$(n - (b + c))(b + c) \leq (n - \alpha b + b)(\alpha b - b)$$

Note that the left-hand side appears in Lemma 4.1.6. Using Lemma 4.1.6, we obtain the result. □

Proof. The proof of Theorem 4.1.5 follows for basically the same reasons as the other bounds on the diameter. We simply determine how far out from (a fixed but arbitrary) w we have to go in order to include at least half the vertices.

If $r \geq \sqrt{\frac{\lambda_n}{\lambda_2} \frac{\alpha^2-1}{4\alpha}} + 1$, then by Lemma 4.1.7 either we have $|B_k| > n/2$ or $|B_{k+r}| \geq \alpha |B_k|$. Thus, for such an r, we are guaranteed to find at least half the vertices within a distance of $r\lceil \log_\alpha(n/2) \rceil$ from w. Note that w is a fixed but arbitrary vertex; the result follows trivially. □

As a consequence of the work that gave the two bounds on the diameter, we also have the following two bounds on the mean distance in the graph.

Theorem 4.1.8.

$$\bar{d} \leq \frac{n}{n-1} \left(\left\lceil \frac{\Delta + \lambda_2}{4\lambda_2} \log(n-1) \right\rceil + \frac{1}{2} \right)$$

The second is again valid for any $\alpha > 1$.

Theorem 4.1.9.

$$\bar{d} < \frac{n}{n-1} \left\lceil 1 + \sqrt{\frac{\lambda_n}{\lambda_2} \frac{\alpha^2 - 1}{4\alpha}} \right\rceil \left(\frac{1}{2} + \log_\alpha(n/2) \right)$$

Also in [47], we have the following lower bound on the diameter, due to McKay (compare with Theorem 4.1.1).

Theorem 4.1.10.

$$\lambda_2 \geq \frac{4}{nD}$$

Mohar extends this to a lower bound on the mean distance.

Theorem 4.1.11.

$$(n-1)\bar{d} \geq \frac{2}{\lambda_2} + \frac{n-2}{2}$$

4.2 Expansion

Given the tight connection between expansion and λ_2, it is not surprising that we can directly relate the expansion properties of the graph to λ_2. For instance, the following is mentioned in [8] without proof:

Proposition 4.2.1. *Given an (n, Δ, c)-magnifier, the diameter D is bounded by*

$$\left\lfloor \frac{D-1}{2} \right\rfloor \leq \frac{\log(n/2)}{\log(1+c)}$$

Proof. The proof is somewhat similar to the proof of Theorem 4.1.2 in style, in that we consider nested balls of consecutive radius. Letting $B_k(v)$ be the set of vertices at distance less than or equal to k from vertex v, we see that as long as $|B_k(v)| \leq n/2$,

$$\frac{|B_k(v)|}{|B_{k-1}(v)|} \geq 1 + c$$

Consider two vertices u and v at distance D. We must have $|B_{\lfloor (D-1)/2 \rfloor}(u)| \leq n/2$ or $|B_{\lfloor (D-1)/2 \rfloor}(v)| \leq n/2$ (or both); without loss of generality, assume $|B_{\lfloor (D-1)/2 \rfloor}(v)| \leq n/2$. Thus

$$|B_{\lfloor (D-1)/2 \rfloor}(v)| = \frac{|B_{\lfloor (D-1)/2 \rfloor}(v)|}{|B_0(v)|} \geq (1+c)^{\lfloor (D-1)/2 \rfloor}$$

The result follows. □

A similar result, proved using a similar technique, gives a bound based on the isoperimetric constant [45]

Theorem 4.2.2. *Given a graph with maximal degree Δ and isoperimetric constant h, the diameter D is bounded by*

$$D \leq 2 \left\lceil \frac{\log(n/2)}{\log \frac{\Delta+h}{\Delta-h}} \right\rceil$$

Proof. This is proved by considering the growth of the graph, i.e., the ratio of the number vertices at distance k to the number vertices at distance $k-1$. Letting $B_k(v)$ be the set of vertices at distance less than or equal to k from vertex v, we see that as long as $|B_k(v)| \leq n/2$,

$$\Delta |B_k(v) - B_{k-1}(v)| \geq h\left(|B_k(v)| + |B_{k-1}(v)|\right)$$

and thus that

$$\frac{|B_k(v)|}{|B_{k-1}(v)|} \geq \frac{\Delta + h}{\Delta - h}$$

□

4.3 Trees

For trees, we have the result that says that λ is bounded by the largest path in the tree. Doob shows that [9]

Theorem 4.3.1. *Let G be a graph with diameter D, and let μ be the smallest eigenvalue of its adjacency matrix Then $-2 \leq \mu \leq -2\cos(\frac{\pi}{D+1})$*

By virtue of the relation between the Laplacian spectrum of a graph and the adjacency spectrum mentioned in the proof of Theorem 1.5.4, we can translate this into Laplacian terms as

$$\lambda_2 \leq 2\left(1 - \cos(\pi/(D+1))\right) = \lambda_2(P_{D+1})$$

Comparing this with Theorem 1.3.11, we can give the range of permissible λ_2 for trees.

Corollary 4.3.2. *Let T be a tree on n vertices with diameter D. Then $\lambda_2(P_n) \leq \lambda_2(T) \leq \lambda_2(P_{D+1})$.*

We will close this section with a direct connection between the mean distance and the Laplacian spectrum, which Mohar attributes to McKay [47]

Theorem 4.3.3. *For any tree on n vertices we have*

$$(n-1)\bar{d} = 2\sum_{i=2}^{n} \frac{1}{\lambda_i}$$

Proof. Let the characteristic polynomial of $L(T)$ be $x^n + c_{n-1}x^{n-1} + \cdots + c_2x^2 + c_1x$. By Corollary 1.3.2, $c_1 = n$, and by the more general Theorem 1.3.3, we have that c_2 is the number of spanning trees of all graphs H_{ij} obtained by identifying any pair of vertices i and j. If we identify two vertices of a tree, we create a graph with exactly one cycle, whose length is the distance (in T) between the two vertices. Thus the number of spanning trees in H_{ij} is the distance (in T) between i and j. So c_2 is exactly the sum of all the distances between any pair of vertices.

Furthermore, by writing the coefficients in terms of the roots (eigenvalues), we see that $c_1 = \prod_{i>1} \lambda_i$, and c_2 is the sum of all products of $n-2$ eigenvalues taken from $\lambda_2, \lambda_3, \ldots, \lambda_n$. Simplifying, we obtain,

$$\sum_{i=2}^{n} \frac{1}{\lambda_i} = \left|\frac{c_2}{c_1}\right| = \frac{\sum_{i,j\in V(G)} d(i,j)}{n} = \frac{n-1}{2}\bar{d}$$

□

Chapter 5

Integral Spectra

5.1 Pendant vertices and multiplicities

We will use the term *pendant vertex* for a vertex of degree 1 and *quasipendant vertex* for a vertex adjacent to a pendant vertex.

We recall the eigenvalue condition at a vertex:

$$(d_j - \lambda)x_j = \sum_{i \sim j} x_i$$

We have as an immediate consequence

Lemma 5.1.1. *Let x be an eigenvector corresponding to λ_2, and suppose there is a pendant vertex v such that $x_v = 0$. Let u be the vertex adjacent to v. Then $x_u = 0$.*

Thus pendant vertices are never isolated zeroes of eigenvectors.

In the same vein, we may observe that if x is an eigenvector corresponding to $\lambda = 1$, then x is always zero on quasi-pendant vertices. Inspired by this observation, let us consider the following scenario. Start with a graph that has (at least) two pendant vertices attached to a common (quasipendant) vertex. For concreteness, take P_3, the simplest such example. Define a vector to be $+1$ and -1, respectively on the two pendant vertices and 0 on the quasipendant vertex. This is an eigenvector corresponding to $\lambda = 1$ for P_3. We can see, either by Theorem 6.1.1 or by directly verifying the eigenvalue condition at each vertex, that we may adjoin whatever other graph we wish to the quasipendant vertex and extend the vector to be 0 on on the rest of the graph. The result is an eigenvector corresponding to $\lambda = 1$ for the new graph (note that although $\lambda_2(P_3) = 1$, $\lambda = 1$ is not necessarily $\lambda_2(G)$). Such a vector, with exactly one $+1$, one -1, and all other entries 0, corresponding to the eigenvalue $\lambda = 1$ is termed a *Faria vector.* Denote by $m_G(\lambda)$ the multiplicity of λ as an eigenvalue of $L(G)$. It is a matter of counting to see that

Theorem 5.1.2. *$m_G(1) \geq p(G) - q(G)$, where $p(G)$ is the number of pendant vertices of G and $q(G)$ is the number of quasipendant vertices of G.*

This was first observed (as a corollary to other results) by Faria in [12], where she refers to $p(G) - q(G)$ as the "star degree" of the graph. This result "explains" why 1 is often an eigenvalue, and so often a multiple eigenvalue of trees (see Appendix A). There is a similar result for the adjacency matrix of trees. Specifically, using $\tilde{m}_G(\mu)$ for the multiplicity of μ as an eigenvalue of $A(G)$, we have ([9], p.258).

Theorem 5.1.3. $p(T) - q(T) \leq \tilde{m}_T(0) \leq p(T) - 1$

For trees, we can add an upper bound to Faria's inequality to obtain the following theorem [21].

Theorem 5.1.4. $p(T) - q(T) \leq m_T(1) \leq p(T) - 1$

It is worth recalling that as trees are not regular we do not expect a direct relationship between the two spectra. The similarity between Theorem 5.1.3 and Theorem 5.1.4 is thus a little unusual.

Proof. The lower bound is already established. Let v be a pendant vertex and u be the quasipendant vertex adjacent to v, Let x be an eigenvector corresponding to 1. If $x_v = 0$, then the eigenvalue condition at vertex v gives that $x_u = 0$ as well. Then we could define a new tree T' by removing vertex v (and edge uv) from T; the vector x' obtained by restricting x to T' would be an eigenvector of T' corresponding to 1. But this new vector would be 0 on u, a pendant vertex of T' (though not of T). As x cannot be identically zero on T, we see that there must be at least two pendant vertices of T on which it is non-zero. If $m_G(1) > p(T) - 1$, then we would have at least $p(T)$ linearly independent eigenvectors corresponding to 1 from which we could form a combination that would be zero on $p(T) - 1$ (pendant) vertices. $\square$

More strikingly, we have the following theorem for integral eigenvalues for trees [21].

Theorem 5.1.5. *Let $\lambda > 1$ be an integer eigenvalue for some tree T on n vertices, and x be a corresponding eigenvector. Then*

1. *λ divides n*

2. *$x_i \neq 0$ for $1 \leq i \leq n$*

3. *$m_T(\lambda) = 1$*

Proof. The characteristic polynomial is always an integer polynomial, with leading coefficient ± 1. Factoring the characteristic polynomial as $xf(x)$, we see that λ must divide the constant term of $f(x)$, which is the linear term of the characteristic polynomial, which is, by Corollary 1.3.2, equal to n (a tree has exactly one spanning tree). Thus λ must divide n.

Assume some coordinate of x is zero. We may assume it is $x_n = 0$. We then obtain the following block structure for $L(T)$,

$$L(T) = \begin{pmatrix} A_1 & 0 & \cdots & 0 & C \\ 0 & A_2 & \cdots & 0 & C \\ \vdots & & \ddots & & \vdots \\ 0 & 0 & \cdots & A_d & C \\ R & R & R & R & d \end{pmatrix}, \tag{5.1}$$

where $d = d_n$ is the degree of vertex n, and the R's [C's] represent appropriately sized row [column] matrices whose only nonzero entry is a -1 in the column [row] corresponding to the vertex in that block that is adjacent to vertex n. Since $x_n = 0$ and x is not identically zero, we see that the restriction of x to one of the blocks must give an eigenvector of some A_i (the only reason it might not be an eigenvector would be because it is identically zero. Thus $\lambda > 1$ is an integer eigenvalue of, say, B_1. If we consider the set of vertices corresponding to the block B_1, we see that B_1 is equal to $L(T_1)$, the Laplacian matrix that these vertices induce on T, plus a single 1 added to one of the diagonal elements (the vertex adjacent on T to vertex n). So $\det B_1 = \det L(T_1) + \det L_1$, where L_1 is the matrix obtained by deleting the row and column corresponding to the vertex adjacent (in T) to vertex n from $L(T_1)$. Since $\det L_1 = 1$ (Matrix-Tree Theorem) and $\det L(T_1) = 0$, we have that $\det B_1 = 1$. But again, the characteristic polynomial of B_1 is an integer polynomial with leading coefficient ± 1 and constant coefficient 1. So the only possible nonnegative rational eigenvalue is $+1$, which λ is not. Thus no coordinate of x can be zero.

If $m_T(1) > 1$, then we could construct (by linear combination) an eigenvector corresponding to 1 that had any desired coordinate equal to zero. $\square$

This can be extended somewhat [20].

Theorem 5.1.6. *Let G be a graph with n vertices and t spanning trees. If λ is a positive integral eigenvalue, then $\lambda \mid nt$. If, furthermore, G is Laplacian integral, then $\lambda^k \mid nt$, where $k = m_G(\lambda)$*

Proof. As in the proof of Theorem 5.1.5, write the characteristic polynomial as $xf(x)$, and observe that Theorem 1.3.1 and Corollary 1.3.2 give that the constant term of $f(x)$ is $f(0) = nt = \prod_{i=2}^{n} \lambda_i$. Again, we see that λ must divide $f(0)$, so $\lambda \mid nt$. Also, if all eigenvalues are integers, then λ^k is contained in the product $\prod_{i=2}^{n} \lambda_i$, and hence $\lambda^k \mid nt$. $\square$

Certain types of pruning give us information about multiplicities of eigenvalues in terms of multiplicities of eigenvalues in subgraphs. As one example [21],

Theorem 5.1.7. *Let G be a graph and let $S_k = K_{1,k-1}$ be the star graph on k vertices. Let G' be a graph obtained by joining, in any manner, G and S_k with a single edge. Then $m_G(k) = m_{G'}(k)$.*

In practice, this allows one to "prune off" copies of S_k from a graph. For instance, we see that $m_{P_5}(k) = m_{P_3}(k)$, since P_5 can be obtained by joining P_2 and P_3 with a single edge. Note that this process of joining with a single edge is not uniquely well-defined, in that there is another graph not isomorphic to P_5 that can be obtained by joining P_3 and P_2 by a single edge. We can give the following

Corollary 5.1.8. *$m_{P_n}(2) = 1$ if $2|n$ and 0 otherwise. $m_{P_n}(3) = 1$ if $3|n$ and 0 otherwise.*

A companion to Theorem 5.1.7 is [21]

Theorem 5.1.9. *Let G be any graph, and P_3 be the path on three vertices. Let G_1 be a graph obtained by joining any vertex G to a pendant vertex of P_3 with a single edge. Then $m_G(1) = m_{G'}(1)$.*

Theorem 5.1.10. *Let G' be a graph obtained by joining any vertex G to the quasipendant vertex of P_3 with a single edge. Then $m_G(1) \leq m_{G'}(1) \leq m_G(1) + 2$, where all three possibilities for $m_{G'}(1)$ can occur.*

The proofs given in [21] examine directly the kernels of the eigenspaces of the two graphs. We will not prove either of these results yet, as they will follow from Theorem 6.1.1 by considering the structure of the eigenvectors.

As an example, we note that Theorem 5.1.7 allows us to prune off copies of P_2 from the first graph of Figure 5.1 to obtain C_4. Indeed, since the eigenvalues of C_4 are $0, 2, 2, 4$, we have that $m_G(2) = 2$. Using both Theorem 5.1.7 and Theorem 5.1.9, we may prune off copies of P_3 from the first graph in Figure 5.2 to obtain C_6. The eigenvalues of C_6 are $0, 1, 1, 3, 3, 4$, giving that $m_G(3) = 2$ and $m_G(1) = 2$.

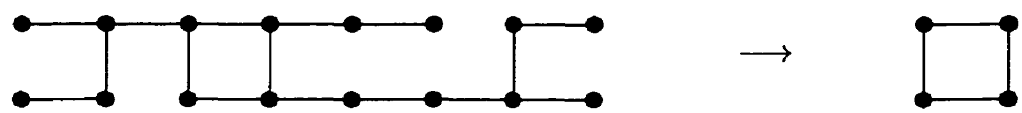


Figure 5.1: pruning off P_2's to see $m_G(2) = m_{C_4}(2)$

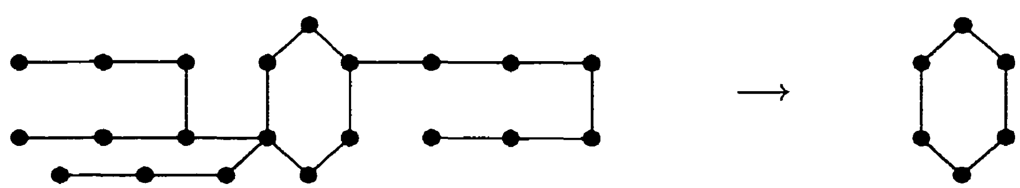


Figure 5.2: pruning off P_3's to see $m_G(3) = m_{C_6}(3)$ and $m_G(1) = m_{C_6}(1)$

In considering Theorem 5.1.10, we note that, with the exception of $G = K_1, G' = K_{1,3}$, we have

$$p(G) - q(G) \leq p(G') - q(G') \leq p(G) - q(G) + 1$$

so that Faria vectors alone cannot account for all three cases. Examples for the three possibilities for Theorem 5.1.10 are shown in Figures 5.3-5.5, where the open circles correspond to the P_3 that is to be pruned. Note that all

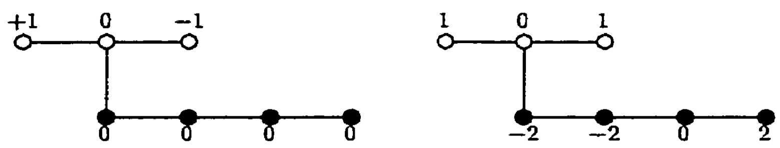


Figure 5.3: pruning P_3 from G' to give $G = P_4$: $m_{G'}(1) - m_G(1) = 2 - 0 = 2$

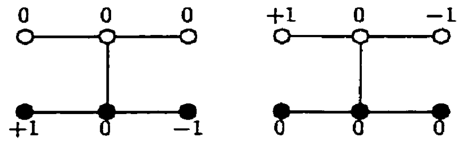


Figure 5.4: pruning P_3 from G' to give $G = P_3$: $m_{G'}(1) - m_G(1) = 2 - 1 = 1$

but one of the vectors shown is a Faria vector, and that this one is linearly independent from the Faria vector.

To close this section, we will mention two more results that, while not dealing directly with integral eigenvalues, seem to be connected [21]. For an interval I, we write $m_G(I)$ for the total number of eigenvalues of G, counting multiplicities, in I.

Proposition 5.1.11. *Let G be a graph, with $p(G)$ pendant vertices and $q(G)$ quasipendant vertices. Then $q(G) \leq m_G[0, 1)$ and $q(G) \leq m_G(1, \infty)$.*

Furthermore, by Theorem 5.1.2, we may write $q(G) \leq m_G[0, 1) \leq n - p(G)$ and $q(G) \leq m_G(1, \infty) \leq n - p(G)$. Note that this last observation explains why 1 tends to be a "middle" eigenvalue of trees (see Appendix A).

Proposition 5.1.12. *Let T be a tree with diameter D. Then $\lceil D/2 \rceil \leq m_T(0, 2)$ and $\lceil D/2 \rceil \leq m_T(2, \infty)$*

5.2 Degree sequences

The degree sequence of a graph may be thought of simply as a sequence of nonnegative integers. Of course, not every sequence of positive integers is in fact the degree sequence of some graph. For instance, [3, 0, 0, 0] and [1, 1, 1, 1] are both obviously not degree sequences. It is perhaps less obvious (without drawing pictures) that [5, 4, 3, 3, 2, 1] is, or that [5, 4, 4, 2, 2, 1] is not. We will

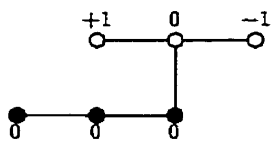


Figure 5.5: pruning P_3 from G' to give $G = P_3$: $m_{G'}(1) - m_G(1) = 1 - 1 = 0$

adopt the convention that the degree sequence is arranged in nonincreasing order. Certainly, we have as necessary conditions that the first element must be less than the number of elements in the sequence, and that the sum of all the elements must be even.

More precisely, let $\rho = [\rho_1, \rho_2, \dots, \rho_s]$ be a sequence of nonnegative integers arranged in nonincreasing order, which we will refer to as a *partition*. Define the *transpose* of a partition as ρ^*, where ${\rho^*}_i = |\{j \mid \rho_j \geq i\}|$. The *Ferrers diagram* of ρ consists of rows (left-justified) of boxes, with ρ_i boxes in the i^{th} row. Thus the Ferrers diagram of the transpose of a partition is the (visual) transpose of the Ferrers diagram of the original partition. If ρ represents the degree sequence of a graph, then the number of boxes in the i^{th} row of the Ferrers diagram is the degree of vertex i, while the number of boxes in the i^{th} row of the Ferrers diagram of the transpose is the number of vertices with degree at least i. The *trace* of a partition ρ is $\text{tr}(\rho) = |\{i \mid \rho_i \geq i\}|$; this is the length of the "diagonal" of the Ferrers diagram for ρ (or ρ^*). Figure 5.6 illustrates this for the partition $\rho = \{5, 4, 3, 3, 2, 1\}$.

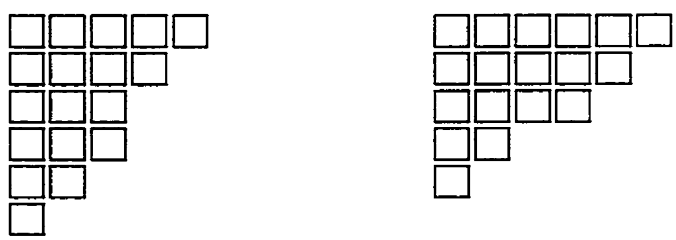


Figure 5.6: a Ferrers diagram for $[5, 4, 3, 3, 2, 1]$ and its transpose $[6, 5, 4, 2, 1]$, (both) having trace 3

The following theorem from [50] determines whether or not a given partition corresponds to an actual degree sequence.

Theorem 5.2.1. *The partition $\rho = [\rho_1, \rho_2, \dots, \rho_s]$ represents a (simple loopless) graph if and only if $\sum_{i=1}^{k} \rho^*{}_i \geq \sum_{i=1}^{k}(\rho_i + 1)$ for $1 \leq k \leq \operatorname{tr}(\rho)$.*

Thus we see that $\rho = \{5, 4, 3, 3, 2, 1\}$ does indeed correspond to a graph; it is shown in Figure 5.7. In fact, we see that for ρ, the inequalities in Theorem 5.2.1 are in fact equalities. Any partition for which $\rho_i + 1 = \rho^*{}_i, 1 \leq k \leq \operatorname{tr}(\rho)$ is said to be a *maximal* partition. The graph corresponding to this partition is said to be a *threshold graph.* Note that (if we ignore isolated vertices) for a threshold graph we always have $\Delta = n - 1$, so threshold graphs are always connected.

In general, the degree sequence does not determine a graph; this is easy to see, even in the case of regular graphs, or trees. However, if we ignore isolated vertices, threshold graphs are uniquely determined by their degree sequence [50]. This is important in light of the following theorem of [35]

Theorem 5.2.2. *Let G be a threshold graph with no isolated vertices. Then the transpose of its degree sequence is equal to its (nonzero) Laplacian spectrum.*

Thus threshold graphs are characterised by their Laplacian eigenvalues, which are furthermore integers. We may also conclude that all threshold graphs have $\lambda_2 \geq 1$. As an example, the star graphs $K_{1,n-1}$ are threshold graphs, and hence are Laplacian integral graphs that are characterised by their spectra and furthermore have $\lambda_2(K_{1,n-1}) = 1$.

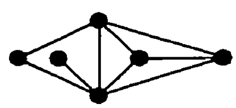


Figure 5.7: (the) threshold graph with degree sequence $[5, 4, 3, 3, 2, 1]$

The inequalities of Theorem 5.2.1 are reminiscent of the technique of *majorisation.* More precisely, given two sequences $a = [a_1, a_2, \dots, a_n]$ and $b = [b_1, b_2, \dots, b_n]$ then a majorises b if

$$\sum_{i=1}^{k} a_i \geq \sum_{i=1}^{k} b_i \text{ for } 1 \leq k \leq n.$$

Define $d(G) = [\Delta = d_1, d_2, \dots, d_n = \delta]$ to be the degree sequence of the graph, with the vertices ordered so that $d(G)$ is nonincreasing. Note that elsewhere in the present paper we were not assuming any special ordering of the vertices. It follows from a result of Schur [32] that the spectrum majorises the degree sequence, that is that

Theorem 5.2.3. $\sum_{i=1}^{k} \lambda_{n+1-i} \geq \sum_{i=1}^{k} d_i$ *for* $1 \leq k \leq n$.

This gives, among other things, that $\lambda_n \geq \Delta$. By Theorem 1.3.9 we already had that $\lambda_n \geq \Delta + \Delta/(n-1)$, and in [20] it was shown that $\lambda_n \geq \Delta+1$. This can in fact be strengthened [18] (as was conjectured in [20]) to

Theorem 5.2.4. *Let G be a (simple, loopless) connected graph on vertices $\{1, 2, \dots, n\}$, ordered so that $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n = \delta$. Let t_k be the number of components of the graph induced on the vertices $\{1, 2, \dots, k\}$. Then $\sum_{i=1}^{k} \lambda_{n+1-i} \geq t_k + \sum_{i=1}^{k} d_i$ for $1 \leq k \leq n$.*

We omit the proof of this result.

Write $d(G)^*$ for the transpose of the degree sequence $d(G)$. We have that $d(G)^*$ majorises $d(G)$, and that the spectrum majorises $d(G)$. Theorem 5.2.1 and Theorem 5.2.4 suggest that the second majorisation is at least as strong as the first. It has been conjectured [20] that

Conjecture 5.2.5. *$d(G)^*$ majorises the Laplacian spectrum for connected graphs.*

The first inequality ($n = d^*_1 \geq \lambda_n$) is certainly true, but the others are not established. This conjecture would give as a straightforward consequence we would have the following, which we can in fact show that [20]

Proposition 5.2.6. *d^*_1, the number of vertices of degree $n-1$, is at most λ_2*

Proof. Let $k = d^*_1$, the number of vertices of degree $n-1$. If $k = n$, then $G = K_n$ and $\lambda_2 = n$. Otherwise, we see immediately that G^c has at least $k+1$ components, the largest having no more than $n-k$ vertices. Thus $\lambda_n(G^c) \leq n-k$ and Corollary 1.3.7 gives that $\lambda_2(G) \geq k$. □

Recall that the $\geq k+1$ components of G^c give that the multiplicity of 0 as an eigenvalue of G^c is at least $k+1$, and hence the multiplicity of n as an eigenvalue of G is at least k.

In investigating this conjecture, Merris derives the following

Theorem 5.2.7. *Let G be a connected graph, and let u be a cut-vertex of G. If the largest component of $G\backslash\{u\}$ has r vertices, then $\lambda_{n-1} \leq r+1$.*

Corollary 5.2.8. *Let G be a connected graph on $n > 2$ vertices. Suppose that u is a quasipendant vertex with k pendant neighbours. Then $\lambda_{n-1} \leq n-k$.*

Corollary 5.2.9. *Let G be a connected graph with integral Laplacian spectrum on $n > 2$ vertices, with p pendant vertices. Then in fact all p pendant vertices are adjacent to the same quasipendant vertex and hence $\lambda_{n-1} \leq n-p$.*

It is interesting to compare this result with Theorem 5.1.4, where p functions as a bound on the *multiplicity* if an eigenvalue. Also, looking at the complements of the graphs and making use of Corollary 1.3.7, we may rephrase these as

Corollary 5.2.10. *Let G be a connected graph on $n > 2$ vertices. Suppose that there are k vertices of degree $n-2$ that are adjacent to the same set of neighbours (i.e. they are all not adjacent to the same vertex) Then $\lambda_3 \geq k$*

Let G be a connected graph with integral Laplacian spectrum on $n > 2$ vertices, with p vertices of degree $n-2$. Then in fact they all are adjacent to the same neighbours (i.e. they are all not adjacent to the same vertex) and $\lambda_3 \geq p$

5.3 Cospectral graphs

It had once been conjectured that two graphs are isomorphic if and only if they are adjacency-cospectral. This was strongly answered answered in the negative by [51].

Theorem 5.3.1. *Let t_n be the number of nonisomorphic trees on n vertices. Let r_n be the number of trees T on n vertices for which there exists a tree T' that is cospectral to T. Then $\lim_{n\to\infty} r_n/t_n = 1$.*

In fact, even more can be said. Recall that the *distance matrix* of a graph is the $n \times n$ matrix whose ij^{th} entry gives the length of a shortest path between vertices i and j. We have the following result of [33],

Theorem 5.3.2. *Let t_n be the number of nonisomorphic trees on n vertices. Let r_n be the number of trees T on n vertices for which there exists a tree T' such that simultaneously:*

1. T and T' are adjacency-cospectral

2. T and T' are distance-cospectral

3. T and T' are Laplacian-cospectral.

Then $\lim_{n\to\infty} r_n/t_n = 1$.

It is perhaps relevant to note that in the same paper, it is shown that given any two trees T_1 and T_2, there is some matrix B that can be expressed as some polynomial function of the matrices D and A, such that T_1 and T_2 are not B-cospectral.

Generalising the concept of the characteristic polynomial to the immanantal polynomials, we can extend Theorem 5.3.2 to [4]

Theorem 5.3.3. *Let t_n be the number of nonisomorphic trees on n vertices. Let r_n be the number of trees T on n vertices for which there exists a tree T' such that simultaneously for every character χ of S_n*

1. $d_\chi(xI - A(T)) = d_\chi(xI - A(T'))$

2. $d_\chi(xI - L(T)) = d_\chi(xI - L(T'))$

Then $\lim_{n\to\infty} r_n/t_n = 1$.

We may conclude that trees that are uniquely determined by their Laplacian spectrum (such as the star graph) are, in some sense, exceptional objects.

Thus it is not surprising to find large collections of cospectral graphs. Merris [39] gives an explicit construction of such, which we reproduce here.

Theorem 5.3.4. *For infinitely many n, there exist a family of 2^k q-connected, nonisomorphic, Laplacian integral, Laplacian cospectral graphs on n vertices, where $k > n/(2\log_2 n)$ and $q > n - \log_2 n$.*

Merris [38] proves that there are exactly 2^{n-2} (nonisomorphic connected) threshold graphs on n vertices. Thus we have an easy example of an infinite family of graphs that are chacterised by their Laplacian spectra. This is also useful in the following proof of cospectral graphs.

Proof. The proof is by construction. Let G be a threshold graph on n vertices with degree sequence $[\Delta = n - 1 = d_1, d_2, \dots, d_n]$. Thus the eigenvalues of G are

$$[\lambda_n = d_1{}^* = n, \lambda_{n-1} = d_2{}^*, \dots, \lambda_2 = d_{n-1}{}^*, \lambda_1 = 0].$$

Define the graph $\tilde{G}$ to be the graph formed by adding a single pendant vertex to a vertex of degree $n-1$ of G (there may be more than one such vertex in G). The new graph $\tilde{G}$ may be seen to also be a threshold graph on $n-1$ vertices. In particular, the eigenvalues of $\tilde{G}$ are

$$[n+1, \lambda_{n-1}, \lambda_{n-2}, \dots, \lambda_2, 1, 0].$$

Now if H is another (distinct) threshold graph on n vertices with eigenvalues

$$[\mu_n = d_1{}^* = n, \mu_{n-1} = d_2{}^*, \dots, \mu_2, 0],$$

then we see that the graphs $G+\tilde{H}$ and $\tilde{G}+H$ have as their (common) spectra

$$[n+1, n, \lambda_{n-1}, \lambda_{n-2}, \dots, \lambda_2, \mu_{n-1}, \mu_{n-2}, \dots, \mu_2, 1, 0, 0].$$

Thus we have constructed a pair of Laplacian integral cospectral graphs.

Now consider the set of all nonisomorphic threshold graphs on k vertices, $\{G_r\}$. There are, as remarked above, 2^{k-2} such graphs. Let I be any set of 2^{k-3} distinct values chosen from $\{1, 2, 3, \dots, 2^{k-2}\}$. Define the graph

$$K_I = \sum_{r \in I} G_r{}' + \sum_{r \notin I} G_r.$$

The number of vertices of K_I is $n = 2^{k-3}k + 2^{k-3}(k+1) = 2^{k-3}(2k+1)$. We see by induction that the eigenvalues of K_I are independent of the particular choice of I. Assuming $k > 3$, the number of such choices is

$$\begin{aligned} \binom{2^{k-2}}{2^{k-3}} &= \frac{(2^{k-3}+1) \cdot (2^{k-3}+2), \dots, 2^{k-2}}{1 \cdot 2 \dots 2^{k-3}} \\ &> 2^{(2^k-3)} \end{aligned}$$

Furthermore, if $n \geq 8$, then

$$\begin{aligned} 2\log_2 n &= 2(k-3) + 2\log_2(2k+1) \\ &> 2k+1 \end{aligned} \tag{5.2}$$

giving $2^{k-3} = n/(2k+1) > n/(2\log_2 n)$, and thus there are at least

$$2^{(2^k-3)} > 2^{n/(2\log_2 n)}$$

choices for I, each leading to a distinct graph K_I.

We note that these graphs are very disconnected. However, due to Corollary 1.3.7, the set of graphs ${K_I}^c$ are a set of connected Laplacian integral nonisomorphic cospectral graphs. Furthermore, as the maximum eigenvalue of K_I is $k+1$, we have that $\lambda_2({K_I}^c) = n-(k+1) > n-\log_2 n$, for $k \geq 8$. As ${K_I}^c$ is not complete, Theorem 1.3.10 allows us to conclude that the vertex connectivity is at least $n - \log_2 n$.

$\square$

Chapter 6

Eigenvectors

6.1 Edge principle

Certain operations are more properly looked at in the context of the eigenvectors associated with the eigenvalues. An important result (which can be used to obtain Theorem 5.1.7 and Theorem 5.1.9)is the Edge Principle obtained by Merris [41].

Theorem 6.1.1. *Let G be a graph, and x an eigenvector with corresponding eigenvalue λ such that $x_u = x_v$ for some $u \neq v$. Let G' be the graph obtained by either removing or adding or the edge uv (depending on whether it is or is not an edge of G). Then x is an eigenvector of G' with corresponding eigenvalue λ.*

It should be emphasized that this theorem does not state that $\lambda_2(G) = \lambda_2(G')$. This is not the case, as can be seen by the following simple example (Figure 6.1. Take two (disjoint) copies of any graph (say P_3); call this graph G. Add an edge between any two corresponding vertices; call this graph G'. Clearly $\lambda_2(G) = 0 < \lambda_2(G')$.

Figure 6.1: $\lambda_2(G) = 0 < \lambda_2(G')$

The eigenvector illustrated in Figure 6.1 is an eigenvector of the graph P_3 corresponding to $\lambda_2(P_3) = 1$. This is obviously an eigenvalue of $G = P_3 + P_3$. The result of the Edge Principle is that $\lambda_2(P_3) = 1$ is an eigenvalue of G' as well. In fact, we see as an easy consequence that the set of eigenvalues of P_{2n} contains the set of eigenvalues of P_n. Note that Theorem 5.1.7 gives that 3 is an eigenvalue of G', and Theorem 5.1.9 also gives that 2 is an eigenvalue of G'.

Proof. Proving the Edge Principle is a simple matter of checking the eigenvalue conditions at each vertex. For any vertex $j \neq u, v$, and noting that d_j is both the degree in G and in G' of vertex j, we see that the condition

$$(d_j - \lambda)x_j = \sum_{i \sim j} x_i$$

is identical for the two graphs. Consider the case where uv is not an edge of G. Noting here d_j for the degree in G of vertex j, the eigenvalue condition for G is

$$(d_u - \lambda)x_u = \sum_{i \sim_G u} x_i$$

and that for G' is

$$((d_u + 1) - \lambda)x_u = \sum_{i \sim_{G'} u} x_i = \sum_{i \sim_G u} x_i + x_v$$

which are easily seen to be equivalent as $x_u = x_v$. The conditions for v are the same (by symmetry). $\square$

We have the following obvious corollaries:

Corollary 6.1.2. *Let G be a given graph. Let H be the graph formed by joining two copies of G with a single edge between corresponding vertices.*

If λ is an eigenvalue of G with multiplicity k, then λ is an eigenvalue of H with multiplicity at least k. Furthermore, any eigenvector x of G may be extended to an eigenvector of H by taking two copies of x.

Corollary 6.1.3. *Let G be a given graph. Let H be the Cartesian product of two copies of G.*

If λ is an eigenvalue of G with multiplicity k, then λ is an eigenvalue of H with multiplicity at least k. Furthermore,any eigenvector x of G may be extended to an eigenvector of H by taking two copies of x.

We also have

Corollary 6.1.4. *Let λ be an eigenvalue of G with eigenvector x such $x_j = 0$. Let G' be the graph formed by joining some arbitrary graph H to vertex j of G with a single edge.*

Then λ is an eigenvalue of G' with eigenvector x' such that $x'_i = x_i$ for $i \in V(G)$ and $x'_i = 0$ otherwise.

To see this result, we need merely observe that, for the purposes of Theorem 6.1.1 the all-zero vector behaves like an eigenvector of H for *any* eigenvalue. Furthermore, if there are k linearly independent eigenvectors for an eigenvalue λ, then there are at least $k-1$ linearly independent eigenvectors for this same eigenvalue such that they are all zero for any arbitrarily chosen (but fixed) vertex of the graph. So we have

Corollary 6.1.5. *Let λ be an eigenvalue of G of multiplicity k. Let G' be the graph formed by joining some arbitrary graph H to some vertex of G.*

Then λ is an eigenvalue of G' of multiplicity at least $k-1$; the corresponding eigenvectors can be chosen so as to be eigenvectors of λ on G, and zero on H.

In fact, we may even prove Theorem 5.1.7 and Theorem 5.1.9 using the Edge Principle. This is essentially the same as the argument given originally in [21].

Proof. Note first that k is a simple eigenvalue (actually, the largest eigenvalue) of S_k. If we list the pendant vertices first and the central vertex last, then a corresponding eigenvector is $(1, 1, \dots, 1, -k+1)$. Thus given any nonzero constant c and any fixed vertex j of S_k, there is a unique eigenvector of S_k corresponding to k that takes on the value c at j.

Let G be any graph on n vertices, and let G' be a graph on $n+k$ vertices formed by joining a vertex of G with a vertex of S_k, the star graph on k vertices. Order the vertices such that G is listed first, then S_k, and such that the added edge connects the n^{th} and $(n+1)^{st}$ vertices. Consider a basis of eigenvectors $\{x^{(1)}, x^{(2)}, \dots, x^{(a)}\}$ for G corresponding to k. We may define extensions of these to G', $\{y^{(1)}, y^{(2)}, \dots, y^{(a)}\}$ by the following. If $x^{(i)}_n = 0$, then $y^{(i)} = 0$ on S_k. If $x^{(i)}_n = c \neq 0$, then define $y^{(i)}$ on S_k by $y^{(i)}_{n+1} = c$ and such that the extension is the unique eigenvector (of S_k) with $y^{(i)}_{n+1} = c$. By the edge principle, this is an eigenvector of G'. It may easily be seen that the $y^{(i)}$'s are linearly independent.

Conversely, let $\{y^{(1)}, y^{(2)}, \dots, y^{(b)}\}$ be a basis of eigenvectors for G' corresponding to k. List the vertices of G' as before. Then it may be seen by multiplying $y^{(i)}$ with the rows $\{n+1, n+2, \dots, n+k\}$ of $L(G')$ that the last k coordinates of $y^{(i)}$ either form an eigenvector of S_k, or else are all zero. In either case, by considering the n^{th} row of $L(G')$, we see that $y^{(i)}_{n+1} = y^{(i)}_n$. Note that if $y^{(i)}$ is identically zero on S_k, then it cannot be identically zero on G. Thus by the edge principle, removing the edge between S_k and G results in a graph for which $y^{(i)}$ is still an eigenvalue corresponding to k, and thus its restriction to G is also an eigenvalue corresponding to k. The restrictions of the $y^{(i)}$'s will all be linearly independent. □

Theorem 5.1.9 may be proved using similar techniques. In fact, we may generalise this in the following

Corollary 6.1.6. *Let H be any graph with a simple eigenvalue λ. Let u be a vertex of H such that an eigenvector x corresponding to λ is nonzero on u. Let G be any graph, and let G' be the graph formed by joining an arbitrary vertex of G to u. Then the multiplicity of λ as an eigenvalue of G is equal to the multiplicity of λ as an eigenvalue of G'.*

The proof follows the same lines as the argument just given.

Theorem 5.1.9 may be proved in a similar way

Proof. Let v be the quasipendant vertex of P_2, and let u be the vertex of G' that is adjacent (in G') to u. If there are k linearly independent eigenvectors of G corresponding to 1, then we may assume that $k-1$ of them are 0 on u. The vector x that takes on the values ± 1 on the two pendant vertices and 0 at v is an eigenvector of P_3 corresponding to 1. Thus, by the edge principle, we obtain $k-1$ linearly independent eigenvectors of G' corresponding to 1. Extending x to be 0 on G gives one more.

For the other inequality, assume we have $k+2$ linearly independent eigenvectors of G' corresponding to 1. They must all be 0 at vertex v, as v is a quasipendant vertex of G'. We may assume that one of these, is the extension of x that is 0 on G. Using this vector, we may assumer that the remaining $k+1$ vectors are 0 on P_3. Furthermore, of the remaining $k+1$ vectors, we may assume that k of these are 0 on vertex u. Thus we have k eigenvectors of G' corresponding to 1 that are all 0 on vertices u and P_3. Thus the restrictions of these vectors to G give k linearly independent eigenvectors of G corresponding to 1. □

6.2 Further principles

In a similar vein, Merris gives the following result, which he refers to as the Principle of Reduction and Extension [41].

Theorem 6.2.1. *Let G be a graph and X be a non-empty subset of vertices of G. Define the graph $G\{X\}$ to have vertex set $X \cup \{i \in V(G) \mid i \sim X\}$, and edge set $\{ij \in E(G) \mid i \in X \text{ or } j \in X\}$. Suppose x is an eigenvector of $G\{X\}$ corresponding to λ such that x is nonzero only on X. Then x extends to an eigenvector of G (the extension being zero) corresponding to λ.*

Proof. $G\{X\}$ can be thought of as the graph induced on X with the addition of its boundary: $V(G\{X\}) = X \cup \delta X$ and $E(G\{X\}) = E(X) \cup \partial X$. The proof is a simple consequence of the Edge Principle. We may further remark that the multiplicity of λ as an eigenvalue of G is at least as great as the multiplicity of λ as an eigenvalue of $G\{X\}$. □

A further technique is the Alternating Principle

Theorem 6.2.2. *Let G be a graph, and let x be an eigenvector corresponding to λ. Let X be the set of vertices on which x is nonzero. Suppose the vertices of X can be paired up in such a way that if i, j are two paired vertices then $x_i = -x_j$. Suppose further that all paired vertices are adjacent [not adjacent]. Let G' be the graph obtained by deleting [adding] the edges between paired vertices. Then x is an eigenvector of G' corresponding to $\lambda - 2$ [$\lambda + 2$].*

Proof. The eigenvalue condition is the same in G and G' for vertices not in X. If $u \in X$, then it is paired with a vertex $v \in X$. Writing d_i for the degree in G of vertex i, the eigenvalue condition in G is

$$(d_u - \lambda)x_u = \sum_{i \sim_G u} x_i$$

and the eigenvalue condition in G' is

$$((d_u \pm 1) - (\lambda \pm 2))x_u = \sum_{i \sim_{G'} u} x_i = \sum_{i \sim_G u} x_i \pm x_v$$

which are easily seen to be equivalent. □

Given a graph G and some subset X of its vertices, we may define a contraction to be a graph G' with vertex-set $(V(G)\backslash X) \cup \{u\}$ and edge-set $E(G\backslash X) \cup \{iu \mid i \sim v \text{ for some } v \in X\}$. We identify the set X with a new vertex u, which is joined to exactly those vertices in $V(G)\backslash X$ that the vertices of the set X were.

Theorem 6.2.3. *Let x be an eigenvector of G corresponding to λ, with two vertices a and b such that they have no common neighbours and $x_i = x_j = 0$. Define the graph G' to have vertex set $(V(G)\backslash\{a,b\}) \cup \{u\}$, and edge set $E(G\backslash\{a,b\}) \cup \{iu \mid i \sim a \text{ or } i \sim b\}$. Define the vector x' to be the vector obtained by deleting the i^{th} (or j^{th}) coordinate of x. Then x' is an eigenvector of G' corresponding to λ.*

Proof. Proving this is a simple matter of checking the eigenvalue condition at each vertex. It should be noted that if we consider the weighted Laplacian, then we may remove the condition that contracted vertices have no common neighbours by defining the weight of edges iu (where u is the new vertex) to be the sum of the weights over all edges ix, with $x \in X$. $\square$

6.3 Constructions

These principles may be used to generate eigenvectors (and hence eigenvalues) for certain graph constructions. Using these principles, as well as Theorem 1.4.5, Merris determines a pair of non-isomorphic cospectral graphs G_1 and G_2. We give his construction here (slightly modified) as an example of the application of these principles.

Let $H_1 = H_2 = K_{2,3} = {K_2}^c \vee {K_3}^c$. Then by Theorem 1.4.5, we have that the spectrum of H_1 is $\{0, 2, 2, 3, 5\}$. Eigenvectors illustrating these eigenvalues are shown in Figure 6.2.

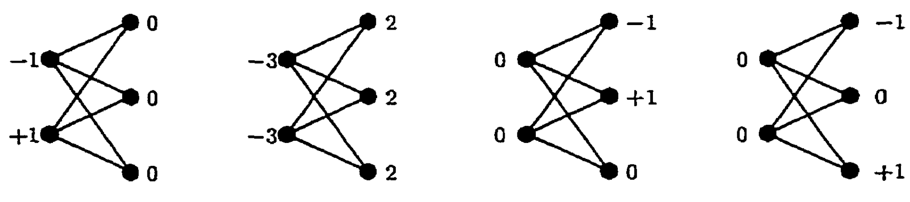


Figure 6.2: $\lambda_2 = 3, 5, 2, 2$

Consider the graph H shown in Figure 6.3, obtained by adding three edges to $H_1 + H_2$. Using the Principle of Reduction and Extension, the first eigenvector of Figure 6.2 gives two linearly independent eigenvectors of H corresponding to 3. Using the edge principle, the remaining eigenvectors of Figure 6.2 give eigenvectors corresponding to 5, 2, and 2. Using the Alternating Principle, the last two also give two linearly independent eigenvectors corresponding to 4. By observing that H may be written as C_{10} with the addition of five edges, as shown in Figure 6.4 (the eigenvector shown corresponds to the eigenvalue 4 of C_{10}), the Alternating Principle gives the eigenvalue 6 for H as well. As usual, $\lambda_1(H) = 0$, and the remaining eigenvalue may be determined (by counting spanning trees or otherwise) to be 1.

Thus

$$\text{spectrum}(H) = \{6, 5, 4, 4, 3, 3, 2, 2, 1, 0\}$$

We note that H is one of exactly 13 cubic, connected, graphs with integral (Laplacian) spectra [5].

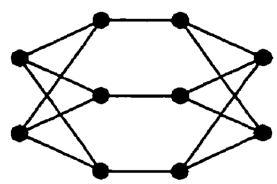


Figure 6.3: The graph H

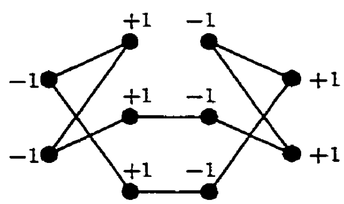


Figure 6.4: Adding five edges to C_{10} would give H

We already have that the spectrum of $K_{2,3}$ is $\{5, 3, 2, 2, 0\}$. Using Theorem 1.4.4 and Corollary 1.3.7, one can easily determine the spectrum of

$G_1 = K_{2,3} + (K_{2,3} + K_1)^c$ to be the same as that of $G_2 = H + K_1$. Comparing the degree sequences, we have

$$\begin{aligned} \text{degree}(G_1) &= 5, 3^5, 2^5 \\ \text{degree}(G_2) &= 3^{10}, 0. \end{aligned}$$

Furthermore, G_1 is decomposable but not bipartite, while G_2 is bipartite but not decomposable. As $\lambda_n < n$, the complements of these graphs are connected and cospectral.

Chapter 7

Trees

7.1 Characteristic vertices

We note firstly a straightforward though useful:

Theorem 7.1.1. *$\lambda_2(T) \leq 1$ for any tree T with equality if and only if $T = K_{1,n-1}$, the star on n vertices.*

The inequality is a simple consequence of Theorem 1.3.10. The equality is obtained in [34]. It is not surprising that $\lambda_2(T)$ should be maximal (over trees) when $T = S_n$, as the star is the best-connected tree. It is also easy to see that the same inequality applies to the isoperimetric constant, i.e. $h(T) \leq 1$ for any tree T with equality only when $T = K_{1,n-1}$. It is a recurrent theme: the second-smallest eigenvalue of L mimics the behaviour of the isoperimetric constant. Consider the set of eigenvectors corresponding to λ_2. It may happen that for some eigenvector x and some vertex j that $x_j = 0$. If the multiplicity of λ_2 is greater than one, this is guaranteed to happen. Depending on which eigenvector x we pick, this may (or may not) be true for any given vertex. The following result of Fiedler strengthens this somewhat [14].

Theorem 7.1.2. *Let T be a tree such that $\lambda_2(T)$ is a multiple eigenvalue. then for any eigenvector x of T corresponding to λ_2, there is a vertex j such that $x_j = 0$.*

We will denote by $\xi(G)$ be the set of eigenvectors of $L(G)$ corresponding to $\lambda_2(G)$. These are commonly referred to as "Fiedler vectors" (or "characteristic valuations" in some papers). The following theorem describes the structural possibilities of the elements of $\xi(G)$ [15].

Theorem 7.1.3. *Let T be a tree, and x an eigenvector corresponding to λ_2. There are two possibilities for x.*

Case 1: If $x_j \neq 0$ for all vertices j, then there exists a unique edge $\{u, v\}$ such that $x_u > 0$ and $x_v < 0$. The values of x along any path originating at u and not including v are increasing, while the values of x along any path originating at v and not including u are decreasing.

Case 2: If $Z = \{j \in V(T) \mid x_j = 0\} \neq \emptyset$, then the graph induced on T by Z is connected, and there exists a unique vertex $w \in Z$ such that w is adjacent to a vertex not in Z. The values of x along any path starting at w are either strictly increasing, strictly decreasing, or identically zero.

We will refer to the vertices u, v (or w) in Theorem 7.1.3 as the *characteristic vertices* of the tree. *The* [characteristic vertices] is justified by the following theorem of Merris, which establishes that they are in fact independent of the choice of eigenvector x and hence an invariant of the tree [34].

Theorem 7.1.4. *Let T be a tree, and x, y be eigenvectors corresponding to λ_2. Then j is a characteristic vertex of T with respect to x if and only if j is a characteristic vertex of T with respect to y.*

Proof. To prove this, we first note that if λ_2 is a simple eigenvalue, then x and y are multiples of each other and the result is obvious.

Define the sets $X_f = \{j \in V(T) \mid f_j = 0\}$ and $X = \bigcap_{f \in \xi(T)} X_f$. If X were empty, then there would be a vector $f \in \xi(T)$ that is never zero, contradicting Theorem 7.1.2. So X is non-empty. As T is connected, there is (at least) one vertex in X that is connected to a vertex not in X. If there were two distinct vertices $\{w_1, w_2\}$ in X and two (not necessarily distinct) vertices $\{v_1, v_2\}$ not in X such that $w_1 \sim v_1$ and $w_2 \sim v_2$, then there would be a vector $f \in \xi(T)$ such that $f_{v_1}, f_{v_2} \neq 0$, contradicting Theorem 7.1.3. It remains to show that w is *a* characteristic vertex for any $g \in \xi(T)$; clearly there can be no other characteristic vertex.

Let $g \in \xi(T)$ have a characteristic vertex j, with $j \neq w$. By Theorem 7.1.3 there exists a vertex i such that $i \sim j$ and $g_i \neq 0$. Since w is the unique vertex of X connected to a vertex not in X, it follows that $j \notin X$. Thus there exists $h \in \xi(T)$ such that $h_j \neq 0$. Since $0 = g_w = g_j \neq g_i$, the (unique) path from w to i passes through j; it follows (by Theorem 7.1.3) that h_i is nonzero as well. Comparing g and h, we can take a linear combination of them (and hence an element of $\xi(T)$) which will be zero on i but nonzero on j, again contradicting Theorem 7.1.3. Thus $j = w$, the unique characteristic vertex of T. □

Define $F(G)$ to be the set of characteristic vertices of G. If there is one characteristic vertex, then we will say T is a *type 1* tree, and if there are two characteristic vertices, then we will say that T is a *type 2* tree. These definitions correspond of course to the two cases in Theorem 7.1.3 (though not in that order). Note as a corollary of this that if T is of type 2, then λ_2 is a simple eigenvalue; the converse does not hold. Thus the eigenspace corresponding to λ_2 is less interesting for type 2 trees, and we will concentrate principally on type 1 trees.

It should be noted that $F(G)$ need not coincide with either the centre or the centroid of a graph, despite the apparent similarities.

Given a vertex j, define $R(j)$ to be the length of the longest path starting at j. Then j is a *centre* point if

$$R(j) = \min_{i \in V(G)} R(i)$$

A *branch* rooted at j is a maximal connected subtree containing exactly one edge incident with j. Define $W(j)$ to be the maximum number of edges in any branch rooted at j. A vertex j is a *centroid* point if

$$W(j) = \min_{i \in V(G)} W(i)$$

The set F shares some characteristics with both the centre and the centroid. All of these are either a single vertex or a pair of adjacent vertices. However, F need not coincide with the centre or the centroid of a graph. In Figure 7.1 the centre is at u, the centroid is at v, and the characteristic vertices are marked F.

7.2 Trees with a single characteristic vertex

Let us consider type 1 trees. These include (but are not limited to) all trees where λ_2 is a multiple eigenvalue. Motivated by the fact that the (unique) characteristic vertex is a graph invariant, we may speak of *the* branches of

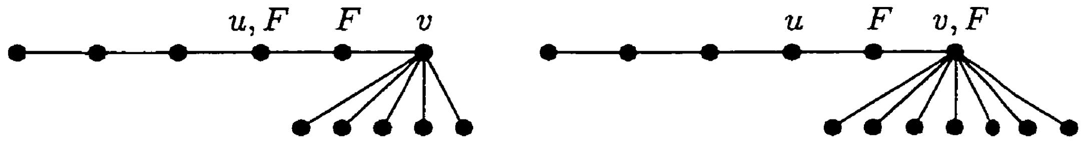


Figure 7.1: characteristic vertices

the tree (at the characteristic vertex). As a consequence of Theorem 7.1.4, we may describe the branches as *passive* if every $x \in \xi(T)$ is identically zero on that branch, or *active* if some $x \in \xi(T)$ is not identically zero on that branch. Note that a given eigenvector x may be partly or completely zero on an active branch. Since $x \in \xi(T)$ is of constant sign on each branch, and is orthogonal to the all-ones vector, there must be (at least) two active branches: one positive and one negative.

For the adjacency matrix, there is a simple and obvious relationship between subgraphs and submatrices: by deleting some set of rows and the same set of columns, we obtain the adjacency matrix of the subgraph obtained by deleting that same set of vertices. This is not true for Laplacian matrices, unless the deleted vertices all have degree zero. However, if we consider the rooted branches of a tree, we almost have the same relationship. More precisely, let T be a tree, and consider a branch B at v (we do not for the moment assume anything special about v). There is exactly one vertex in B that is adjacent (in T) to v; call this vertex the *root* of B and denote it $r(B)$. The vertex $r(B)$ is uniquely determined by v. Note that we do not include the vertex v in B. Define the matrix

$$(\hat{L}(B))_{ij} = \begin{cases} (L(B))_{ij} + 1 & \text{if } i = j = r(B) \\ (L(B))_{ij} & \text{otherwise} \end{cases}$$

This is almost the same as $L(B)$. In fact, the determinant of $\hat{L}(B)$ is exactly the sum of the determinant of $L(B)$ and the determinant of the matrix obtained by deleting the row and column corresponding to $r(B)$ from $L(B)$. The determinant of $L(B)$ is zero, as it is a Laplacian matrix, and the determinant of the deleted matrix is exactly the number of spanning trees of B. We have proved [19]

Lemma 7.2.1. $\det(\hat{L}(B)) = 1$

Consider a type 1 tree. Label its characteristic vertex w, and let $d = d_w$ be the degree of w. If we now consider the set of all branches of T at w, $\{B_1, B_2, \dots, B_d\}$, then we see that w is adjacent to (exactly) the vertices $\{r(B_1), r(B_2), \dots, r(B_d)\}$. We may order the vertices of T such that the vertices of B_1 are listed first (with $r(B_1)$ last among these), followed by the vertices of B_2 (with $r(B_2)$ last among these), and so on, with w listed last of all. This gives the following block structure

$$L(T) = \begin{pmatrix} \hat{L}(B_1) & 0 & \cdots & 0 & C \\ 0 & \hat{L}(B_2) & \cdots & 0 & C \\ \vdots & & \ddots & & \vdots \\ 0 & 0 & \cdots & \hat{L}(B_d) & C \\ R & R & R & R & d \end{pmatrix} \tag{7.1}$$

where the R's [C's] represent appropriately sized row [column] matrices whose only nonzero entry is a -1 in their last column [row].

This form allows us to deduce results on the multiplicity of λ_2, as well as possibilities for the sets of active and passive branches, and hence the automorphism group of the tree.

7.3 Multiplicity

In this section we will deal with type 1 trees. We will always consider branches to be rooted at $r(B)$, the vertex of the branch adjacent to the characteristic vertex. We will label the characteristic vertex w and denote its multiplicity (and hence the number of branches at w) by d, and order the vertices according to form (7.1).

The following theorem [19] describes the relationship between λ_2 and active branches.

Theorem 7.3.1. *A branch B is active if and only if $\lambda_2(T)$ is an eigenvalue of $\hat{L}(B)$. Furthermore, if $\lambda_2(T)$ is an eigenvalue of $\hat{L}(B)$ then it is the smallest eigenvalue of $\hat{L}(B)$ and it is simple.*

Proof. Let the active branches (at w) be $\{B_1, B_2, \dots, B_k\}$ and the passive branches be $\{B_{k+1}, B_{k+2}, \dots, B_d\}$, so that the active branches are listed first in form 7.1. By Theorem 7.1.3, there exist eigenvectors $f^{(1)}, f^{(2)}, \dots, f^{(k)}$ corresponding to λ_2 such that $f^{(i)}$ takes on the value 1 at $r(B_i)$ and all other coordinates of $f^{(i)}$ are greater than 1. Thus there is an eigenvector f that is non-zero on every active branch. Following the ordering of the vertices induced by 7.1, we may write f as

$$f = (x^{(1)}, x^{(2)}, \ldots, x^{(k)}, 0^{(k+1)}, 0^{(k+2)}, \ldots, 0^{(d)}, 0)$$

where each $x^{(i)}$ corresponds to an active branch, each $0^{(i)}$ corresponds to a passive branch, and the final 0 corresponds to w. Block multiplication gives that each $x^{(i)}$ is an eigenvector of $\hat{L}(B_i)$ corresponding to $\lambda_2(T)$. By dividing each $x^{(i)}$ by their last coordinate (i.e., the coordinate corresponding to $r(B_i)$), we obtain rescaled eigenvectors $y^{(i)}$ that take on the value 1 at $r(B_i)$ and are strictly greater than 1 on the rest of $r(B_i)$. More importantly, the vectors $y^{(i)}$ are entrywise positive eigenvectors of the matrices $\hat{L}(B_i)$. These matrices are irreducible (Theorem 1.3.5) positive definite M-matrices (see, e.g., [44]), and so letting A_i be the inverse of $\hat{L}(B_i)$, we see that A_i is entrywise nonnegative. Thus we have $A_i y^{(i)} = \lambda_2^{-1} y^{(i)}$ and λ_2^{-1} is the (simple) maximal eigenvalue of A_i. Therefore λ_2 is the (simple) minimal eigenvalue of $\hat{L}(B_i)$.

Suppose now that λ_2 is an eigenvalue of $\hat{L}(B_i)$ for some $i > k$, i.e., for a passive branch. Let $z^{(i)}$ be a corresponding eigenvector. If the last coordinate of $z^{(i)}$ is zero, then the vector

$$(0^{(1)}, 0^{(2)}, \ldots, 0^{(i-1)}, z^{(i)}, 0^{(i+1)}, \ldots, 0^{(d)}, 0)$$

is an eigenvector of L corresponding to λ_2 which is nonzero on a passive branch, and thus a contradiction. If the last coordinate of $z^{(i)}$ is nonzero, then we may (by rescaling) assume that it is -1. Define $z^{(1)}$ to be the vector whose only nonzero coordinate is a -1 in the last position. Then the vector

$$(0^{(1)}, 0^{(2)}, \ldots, 0^{(i-1)}, z^{(i)}, 0^{(i+1)}, \ldots, 0^{(d)}, 0)$$

is an eigenvector of L corresponding to λ_2 which is nonzero on a passive branch, and thus also a contradiction. ☐

As a corollary we have [19]

Corollary 7.3.2. *Let L_w be the matrix obtained by deleting the last row and column of L (i.e., the row and column corresponding to w). Then the number of active branches of T is equal to the multiplicity of λ_2 as an eigenvalue of L_w.*

Proof. This is a simple consequence of the structure of L_w: it is the direct sum of the matrices $\hat{L}(B_i), 1 \leq i \leq d$. Since λ_2 is a simple eigenvalue of $\hat{L}(B)$ if B is active, and not an eigenvalue of $\hat{L}(B)$ if B is passive, the result is immediate. □

We also have a direct relationship between the number of active branches and the multiplicity of λ_2 as an eigenvalue of $L(T)$ [19].

Theorem 7.3.3. *Let m be the multiplicity of λ_2 as an eigenvalue of L. Then there are exactly $m+1$ active branches.*

Proof. Let the vectors $f, x^{(i)}, y^{(i)}$ be as in the proof of Theorem 7.3.1. It can then be seen that the set of vectors $\{f_i\}, 2 \leq i \leq k$, where

$$f_i = (-y^{(1)}, 0^{(2)}, \dots, 0^{(i-1)}, y^{(i)}, 0^{(i+1)}, \dots, 0^{(d)}, 0)$$

forms a set of linearly independent eigenvectors of L corresponding to λ_2.

Now suppose that we have $g \in \xi(T)$. By Theorem 7.1.3, we may write g as

$$(g^{(1)}, g^{(2)}, \dots, g^{(k)}, 0^{(k+1)}, 0^{(k+2)}, \dots, 0^{(d)}, 0).$$

Block multiplication with (7.1) gives that each (nonzero) $g^{(i)}$ is an eigenvector of $\hat{L}(B_i)$ corresponding to the (simple) eigenvalue λ_2. Thus $g^{(i)} = c_i y^{(i)}$ for some constants c_i. In fact, the c_i are exactly the last coordinate of the $g^{(i)}$. Multiplying g by the last row in (7.1), we see that the sum of the c_i is zero, and hence that

$$g = \sum_{i=2}^{k} c_i f_i.$$

Thus $\{f_1, f_2, \dots, f_k\}$ forms a basis for $\xi(T)$, which gives the result. □

Note that we have as an obvious corollary that there are always at least two active branches, which was already deduced by more direct observations.

More importantly, Theorem 7.3.1 and Corollary 7.3.2 allow us to deduce

Corollary 7.3.4. *The multiplicity of λ_2 as an eigenvalue of L_w is one more than the multiplicity of λ_2 as an eigenvalue of L.*

As a corollary, we have [19]

Corollary 7.3.5. *λ_2 is the smallest eigenvalue of L_w. Equivalently, if B is a passive branch, then the smallest eigenvalue of $\hat{L}(B)$ is greater than λ_2.*

Proof. Writing m for the multiplicity of λ_2 as an eigenvalue of $L(T)$, we have the following eigenvalues for $L(T)$:

$$\lambda_1 < \lambda_2 = \lambda_3 = \cdots = \lambda_{m+1} < \lambda_{m+2} \leq \cdots \leq \lambda_n.$$

If we let the eigenvalues of L_v be

$$\alpha_1 \leq \alpha_2 \leq \cdots \leq \alpha_{n-1}$$

then the Cauchy interlacing inequalities give that

$$\alpha_1 \leq \lambda_2 \leq \alpha_2 \leq \cdots \leq \alpha_m \leq \lambda_{m+1}\alpha_{m+1}.$$

Since $\lambda_{m+1} = \lambda_2$, this gives $\alpha_2 = \alpha_3 = \cdots = \alpha_m$. Corollary 7.3.4 then gives that $\alpha_1 = \alpha_{m+1} = \lambda_2$, and thus the smallest eigenvalue of L_w is λ_2. The word "Equivalently" is justified by Theorem 7.3.1. This gives the result. □

7.4 Structural operations on trees

We may use the characteristic vertex to determine the effects of certain pruning and grafting of vertices. The following theorem of Merris [34] allows us to remove vertices without changing properties related to λ_2.

Theorem 7.4.1. *Let $x \in \xi(T)$ be an eigenvector corresponding to λ_2. Suppose there is a pendant vertex v such that $x_v = 0$. Let u be the vertex adjacent to v. Define T_v to be the tree obtained by deleting vertex v and the edge uv from T. Define y to be the restriction of x to T_v. Then $x_u = 0$, $\lambda_2(T_v) = \lambda_2(T)$, $y \in \xi(T_v)$, and $F(T) = F(T_v)$*

Note that in order to have an eigenvector $x \in \xi(T)$ and a pendant vertex j such that $x_j = 0$, the tree must be of type 1. Theorem 7.1.3 guarantees one positive and one negative branch. The vertex j then makes a minimum of four vertices.

Proof. The first result is true by Lemma 5.1.1.

Order the vertices of T so that v is last and u is second last. Define L_v to be the matrix obtained by removing the last row and column from L, and

L_u to be the matrix obtained by removing the last row and column from L_v, giving the forms:

$$L = \begin{pmatrix} & & & & 0 \\ & L_v & & & \vdots \\ & & & & 0 \\ & & & & -1 \\ 0 & \cdots & 0 & -1 & 1 \end{pmatrix} \quad \text{and} \quad L_v = \begin{pmatrix} & & & a_{1,n-1} \\ & L_u & & a_{2,n-1} \\ & & & \vdots \\ a_{n-1,1} & a_{n-1,2} & \cdots & a_{n-1,n-1} \end{pmatrix}.$$

Since $x_v = 0$ we see that y is an eigenvector of L_v corresponding to $\lambda_2(T)$, and furthermore since $x_u = x_v = 0$, that $L_v y = L(T_v)y$ and hence $\lambda_2(T)$ is an eigenvalue both of L_v and $L(T_v)$. Denote the eigenvalues by

eigenvalues of $L(T)$	$0 = \lambda_1 < \lambda_2 \leq \lambda_3 \leq \cdots \leq \lambda_n$
eigenvalues of $L(T_v)$	$0 = \mu_1 < \mu_2 \leq \mu_3 \leq \cdots \leq \mu_n$
eigenvalues of L_v	$0 < \alpha_1 < \alpha_2 \leq \alpha_3 \leq \cdots \leq \alpha_n$
eigenvalues of L_u	$0 < \beta_1 < \beta_2 \leq \beta_3 \leq \cdots \leq \beta_n$

Since L_v is a principal submatrix of $L(T)$, and L_u is a principal submatrix of both L_v and $L(T_v)$, the interlacing inequalities give

$$0 = \lambda_1 \leq \alpha_1 \leq \beta_1 \leq \mu_2 \quad \text{and} \quad \lambda_2 \leq \alpha_2 \leq \beta_2 \leq \mu_3 \tag{7.2}$$

Now λ_2 is a (nonzero) eigenvalue of $L(T_v)$, so if $\lambda_2 \neq \mu_2$ then (7.2) gives that

$$0 = \lambda_1 < \alpha_1 \leq \beta_1 \leq \mu_2 < \lambda_2 = \alpha_2 = \beta_2 = \mu_3 \leq 1,$$

with the final inequality a consequence of Theorem 7.1.1.

Denote the characteristic polynomials by

$$\begin{aligned} q(x) &= \det(xI - L(T)) \\ r(x) &= \det(xI - L(T_v)) \\ a(x) &= \det(xI - L_v) \\ b(x) &= \det(xI - L_u). \end{aligned}$$

These polynomials are not independent. We have from the structure of the matrices that

$$q(x) = (x-1)a(x) - b(x) \quad \text{and} \quad a(x) = r(x) - b(x), \tag{7.3}$$

giving that

$$q(x) = (x-1)r(x) - xb(x) \tag{7.4}$$

By examining signs, we will show that it is impossible to have $\mu_2 < \lambda_2$. We may first note that (7.3) gives that any common root of $a(x)$ and $b(x)$ is also a root of $q(x)$, and (7.4) gives that any common root of $r(x)$ and $b(x)$ is also a root of $q(x)$. Thus we may sharpen (7.4) to

$$0 = \lambda_1 < \alpha_1 < \beta_1 < \mu_2 < \lambda_2 = \alpha_2 = \beta_2 = \mu_3 \leq 1$$

The polynomial $q(x)$ is of degree n, the polynomial $r(x)$ is of degree $n-1$, and the polynomial $b(x)$ is of degree $n-2$. The leading coefficients are all $+1$. So we may use (7.4) to construct sign diagrams for these polynomials.

If n is even we have:

	$(0, \beta_1)$	(β_1, μ_2)	(μ_2, λ_2)
$q(x)$	$-$	$-$	$-$
$r(x)$	$+$	$+$	$-$
$b(x)$	$+$	$-$	$-$

If n is odd all signs are reversed.

Observing that $x-1$ is negative on $(0, \lambda_2)$, we see that (7.4) gives a contradiction on the interval (μ_2, λ_2). Thus we may confidently assert that this interval does not exist, and $\mu_2 = \lambda_2$.

We may determine the characteristic vertex of T using x and Theorem 7.1.3; we may determine the characteristic vertex of T_v using y and Theorem 7.1.3. As vertex v cannot be the characteristic vertex (Lemma 5.1.1), the two characteristic vertices are necessarily the same. □

We have as a corollary that passive branches may be removed without changing λ_2. Indeed, by removing passive branches, we conserve $\xi(T)$, except of course that the excess coordinates (which are all zero) are removed. Note however that this theorem does not only apply to passive branches.

As an example, the three graphs in Figure 7.2 show the result of successively removing two pendant vertices, together with an eigenvector corresponding to $\lambda_2 = (3-\sqrt{5})/2$ in each case.

Though we can arbitrarily remove passive branches, we cannot always add to them. Merris presents a partial converse to Theorem 7.4.1 [34].

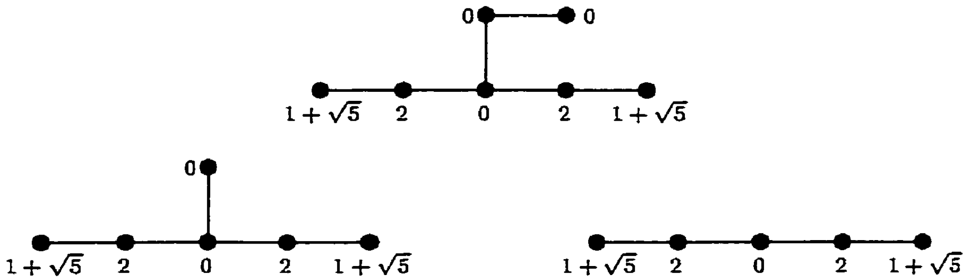


Figure 7.2: pruning vertices

Theorem 7.4.2. *Let T be a type 1 tree. Let $x \in \xi(T)$ and $u \in V(T)$ such that $x_u = 0$. Let T' be the tree obtained by adding a new pendant vertex v adjacent to u, and let x' be the extension of x to T' by defining $x'_v = 0$. Then x' is an eigenvector of T' with eigenvalue $\lambda_2(T)$. Furthermore, if $\lambda_2(T) = \lambda_2(T')$, then $x' \in \xi(T')$ and $F(T) = F(T')$.*

Proof. Since $x'_v = 0$, we see directly that $L(T')x' = \lambda_2(T)x'$. If $\lambda_2(T) = \lambda_2(T')$, then by definition we have $x' \in \xi(T')$. In this case, the characteristic vertices must coincide for the same reasons given at the end of the proof of Theorem 7.4.1. We note parenthetically that since $\lambda_2(T) > 0$ and $\lambda_2(T') > 0$, we must always have $\lambda_2(T) \geq \lambda_2(T')$. □

This is illustrated in Figure 7.3, where we show the result of grafting a pendant vertex onto the first tree of Figure 7.2. Two eigenvectors are shown: the eigenvector of Theorem 7.4.2, and the eigenvector corresponding to λ_2 of the new tree.

Figure 7.3: adding a new passive vertex; $\lambda_3 = (3-\sqrt{5})/2$ and $\lambda_2 \approx 0.2434$

However, we can always add pendant vertices to the characteristic vertex, as demonstrated by the following result from [19]:

Theorem 7.4.3. *Let T be a type 1 tree with characteristic vertex w. Let $x \in \xi(T)$. Let T' be the tree obtained by adding a new pendant vertex v adjacent to w, and let x' be the extension of x to T' by defining $x'_v = 0$. Then x' is an eigenvector of T' with eigenvalue $\lambda_2(T)$. Furthermore, $\lambda_2(T) = \lambda_2(T')$, $x' \in \xi(T')$, and $F(T) = F(T')$.*

Proof. By Theorem 7.4.2, we need merely show that $\lambda_2(T') \geq \lambda_2(T)$.

Let L_w be the matrix obtained from $L(T)$ by deleting the row and column corresponding to w; Let L'_w be the matrix obtained from $L(T')$ by deleting the row and column corresponding to w. Thus we have the forms

$$L(T) = \begin{pmatrix} L_w & C \\ R & d_w \end{pmatrix}, \quad L(T') = \begin{pmatrix} L'_w & C \\ R & d_w + 1 \end{pmatrix}, \quad L'_w = \begin{pmatrix} L_w & 0 \\ 0 & 1 \end{pmatrix}$$

where the R's [C's] represent appropriately sized row [column] matrices whose only nonzero entries indicate the vertices of T adjacent to w. Obviously the eigenvalues of L'_w are precisely the eigenvalues of L_w with the extra eigenvalue 1. Corollary 7.3.5 gives that the smallest eigenvalue of L_w is $\lambda_2(T)$, which is thus also the smallest eigenvalue of L'_w. As L'_w is a principal submatrix of $L(T')$, the interlacing inequalities give that this can be no larger than $\lambda_2(T')$, i.e., that $\lambda_2(T) \leq \lambda_2(T')$. □

Hence without further ado, the graph shown in Figure 7.4 has $\lambda_2 = (3 - \sqrt{5})/2$.

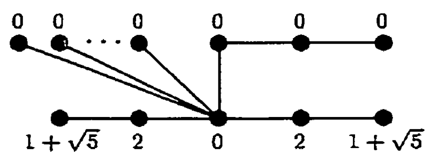


Figure 7.4: adding pendant vertices to the char. vertex; $\lambda_2 = (3 - \sqrt{5})/2$

Furthermore, we have

Corollary 7.4.4. *Let $T \neq S_n$ be a type 1 tree with characteristic vertex w, with a pendant vertex p adjacent to w. Then $x_p = 0$ for all $x' \in \xi(T')$.*

Proof. Let B be the branch of T containing only p. Then $\hat{L}(B)$ is the 1×1 matrix (1), with the single eigenvalue 1. Since $T \neq S_n$, $\lambda_2(T) < 1$ and thus $\lambda_2(T)$ is not an eigenvalue of $\hat{L}(B)$. By Theorem 7.3.1, B is a passive branch, and hence $x_p = 0$ for all $x' \in \xi(T')$. □

Thus we may add pendant vertices to the characteristic vertex without changing λ_2; the eigenvectors corresponding to λ_2 will extend to zero on the newly added pendant vertices. Furthermore, (with the exception of $T = S_n$) any pendant vertices adjacent to the characteristic vertex got there by virtue of Theorem 7.4.3. This gives a complete "explanation" of pendant vertices adjacent to the characteristic vertex.

In fact, given any two type 1 trees T_1 and T_2, we can form a new type 1 tree T by identifying the two characteristic vertices of T_1 and T_2. It can readily be seen that the result will be a type 1 tree with the characteristic vertex being the amalgamated characteristic vertices of the two original trees. Furthermore, if we take an eigenvector of T_1, and extend it to an eigenvector of T by defining it to be 0 on T_2, we obtain an eigenvector of T. We can do the same for eigenvectors of T_2. Thus $\lambda_2(T) \leq \min\{\lambda_2(T_1), \lambda_2(T_2)\}$. We can do better. If we take a set of (non-zero) linearly independant eigenvectors for T_1 and T_2, and extend them in the above manner to eigenvectors of T, then the extensions are all linearly independant as well. So not only is $\lambda_2(T) = \min\{\lambda_2(T_1), \lambda_2(T_2)\}$, but in fact the non-zero spectrum of T is simply the collection of all non-zero eigenvalues of T_1 and T_2.

7.5 Structure of the automorphism group

Recall that an automorphism is a bijective mapping $\phi : V(G) \to V(G)$ such that ij is an edge if and only if $\phi(i)\phi(j)$ is an edge. Of course, the automorphisms form a (permutation) group under composition. We will refer to this group as $\Gamma(G)$.

We had previously mentioned the Faria vectors of a graph. These are eigenvectors (corresponding to 1) all of whose only non-zero entries are a $+1$ and a -1 respectively, on two pendant vertices which are adjacent to a common vertex. There are (Theorem 5.1.2) $p(G) - q(G)$ of these vectors, and they are linearly independent. We will refer to the space that they span as the *Faria space*. It may be that there are eigenvectors corresponding to 1 that are not in the Faria space, as Theorem 5.1.2 is not necessarily sharp.

It will be useful to consider the orbits of the automorphism group. These are a partition of the vertex set of the graph into maximal sets such that given any two vertices i and j in the same part of the partition, there exists an automorphism mapping i to j. We will abuse the language by speaking of "applying an automorphism to an eigenvector", and write $\phi(x)$; by this we mean permuting the values of the coordinates of the eigenvector according to the permutation corresponding to the automorphism.

It may happen that an eigenvector is constant on all the orbits. Thus, by applying automorphisms to this eigenvector, we do not obtain any new eigenvectors. Note that even if an eigenvector is not constant, applying a permutation does yield a "new" eigenvector, but it may not necessarily produce a linearly independent one. As a trivial example, consider the graph P_3 shown in Figure 7.5. There is only one non-trivial automorphism. Two of the eigenvectors are constant on the orbits, one is not, though they are all simple.

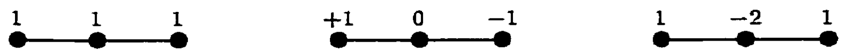


Figure 7.5: eigenvectors for P_3 corresponding to $\lambda_1 = 0, \lambda_2 = 1, \lambda_3 = 3$

We will define the *symmetric* spectrum of a graph as that part of the spectrum with corresponding eigenvectors that are constant on the orbits, and the *alternating* part of the spectrum as that part of the spectrum with corresponding eigenvectors that are not constant on the orbits, both counted according to the number of linearly independent eigenvectors. Note that a (multiple) eigenvalue may belong to both parts; the (total) multiplicity of an eigenvalue is the sum of its multiplicity in the alternating spectrum and its multiplicity in the symmetric spectrum. We observe that if $\Gamma(G)$ is trivial, then the orbits consist of one vertex each, in which case the alternating part of the spectrum is empty; if the graph is vertex-transitive, then there is exactly one orbit, consisting of all the vertices, and the symmetric part of the spectrum consists of the eigenvalue 0 of multiplicity one. So as the graph becomes more "symmetric", the spectrum becomes "less so".

The Faria vectors are never constant on all the orbits, so the dimension of the alternating spectrum is at least $p(G) - q(G)$. It is possible that 1 belongs to the alternating spectrum without originating from a Faria vector, or that 1 belongs to the symmetric spectrum. The examples of C_6 or P_6 shown in Figure 7.6 (the idea extends easily to C_{6k} or P_{6k}, as well as other graphs using Merris's Edge Principle or other techniques). As an example (Figure 7.7), the star graph S_n has as its alternating spectrum 1 of multiplicity $n - 2$, all of which originates in the Faria space, and $0, n$ as its symmetric spectrum. Figure 7.6 and Figure 7.7 also illustrate the following characterisation of the alternating spectrum for trees, given in [19]. The alternating spectrum consists exactly of those eigenvalues for which there exists a nonzero vector x such that for some automorphism ϕ, $\phi(x) = -x$ (see also Theorem 7.6.2).

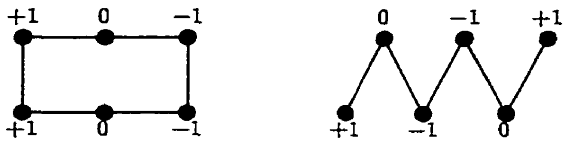


Figure 7.6: eigenvectors for C_6 and P_6 corresponding to 1

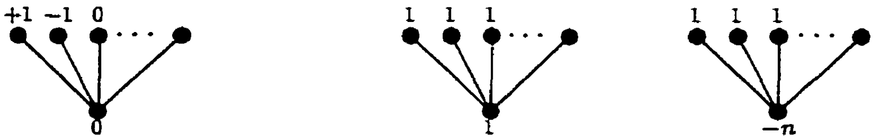


Figure 7.7: a typical eigenvector for the alternating spectrum, and two eigenvectors giving the symmetric spectrum

The number of symmetric eigenvalues (counting multiplicities) is simply the number of orbits of the graph. In fact, we may easily determine the symmetric spectrum as the spectrum of another matrix, in the following way [19]. Partition the matrix L according to the orbits. Let k be the number of orbits, and define $n_i, 1 \leq i \leq k$ to be the number of vertices in the i^{th} orbit. Form the $k \times k$ matrix $\tilde{L}$ by defining $(\tilde{L})_{ij}$ to be the sum of the elements in the ij^{th} block of L divided by $\sqrt{n_i n_j}$. The spectrum of $\tilde{L}$ is exactly the symmetric spectrum of L. Furthermore, there is a one-to-one correspondence between the eigenvectors as follows: $\tilde{x}$ is an eigenvector of $\tilde{L}$ if and only if x is an eigenvector of L, where $x_i\sqrt{n_j} = \tilde{x}_j$ where vertex i is in orbit j. So for the graph in Figure 7.8, we have

$$Lx = \left(\begin{array}{cc|c|c|ccc} 1 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 & 0 & 0 & 0 \\ \hline -1 & -1 & 3 & -1 & 0 & 0 & 0 \\ \hline 0 & 0 & -1 & 4 & -1 & -1 & -1 \\ \hline 0 & 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 1 \end{array}\right) \begin{pmatrix} a \\ a \\ b \\ c \\ d \\ d \\ d \end{pmatrix}$$

$$\tilde{L}\tilde{x} = \begin{pmatrix} 1 & -\sqrt{2} & 0 & 0 \\ -\sqrt{2} & 3 & -1 & 0 \\ 0 & -1 & 4 & -\sqrt{3} \\ 0 & 0 & -\sqrt{3} & 1 \end{pmatrix} \begin{pmatrix} a\sqrt{2} \\ b\sqrt{1} \\ c\sqrt{1} \\ d\sqrt{3} \end{pmatrix}$$

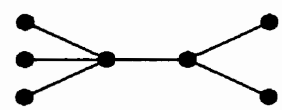


Figure 7.8: a graph with four orbits

In fact, let $u^{(j)}, 1 \leq j \leq k$ be the vector that takes on the value $1/\sqrt{j}$ on those vertices in the j^{th} orbit and zero otherwise. Form any orthonormal matrix U that has as its first k columns the vectors $u^{(j)}$. Then the matrix $U^t L U$ is block diagonal with the upper block being exactly $\tilde{L}$ (giving the symmetric spectrum) and the lower block giving the alternating spectrum.

7.6 Automorphisms on trees

Consider the automorphism group Γ of a tree T. Of course, F is fixed by Γ, and thus if T is of type 1, then the characteristic vertex is a fixed point.

We can characterise whether or not λ_2 is in the alternating spectrum based on the isomorphic branches at the characteristic vertex. It turns out that λ_2 is in the alternating spectrum exactly when there are two nonisomorphic branches at the characteristic vertex. To show this, we will need two lemmas, from [19].

Lemma 7.6.1. *Let T be a tree and v some vertex of T. If there are k isomorphic branches $B_1, B_2, \ldots, B_k$ at v, with λ an eigenvalue of $\hat{L}(B_1)$ with multiplicity m, then λ is an alternating eigenvalue of T with multiplicity at least $m(k-1)$.*

Proof. For each linearly independent eigenvalue x of $\hat{L}(B_1)$, define a vector $y^{(i)}$ that is equal to x on B_1, equal to $-x$ on B_i, and zero elsewhere. This gives a set of $m(k-1)$ linearly independent eigenvectors corresponding to λ, none of which are constant on the orbits. $\square$

Lemma 7.6.2. *Let T be a type 1 tree with centre w, and B one of its branches at w. Define $U_i = B \cap V_i$, where V_i are the orbits of G. If $x \in \xi(T)$, then x is constant on each U_i.*

Proof. The result is obvious for passive branches, so assume B is active. Let v be a vertex in B, and $\phi \in \Gamma(G)$ such that $\phi(v) \in B$. By Theorem 7.1.3, we may assume that both x_v and $x_{\phi(v)}$ are positive. Furthermore, letting $r(B)$ be the vertex of B that is adjacent (in T) to w, we see that $\phi(w) = w$. If $x_v \neq x_{\phi(v)}$, then we can construct (as a linear combination of x and $\phi(x)$) a vector that is zero on w, nonzero on v, yet in $\xi(T)$. By Theorem 7.1.3, this is impossible. Thus $x_v = x_{\phi(v)}$ and the result follows. □

Hence we can now prove [19]

Theorem 7.6.3. *Let T be a type 1 tree with characteristic vertex w. Then λ_2 is in the alternating spectrum if and only if T has two isomorphic active branches at w.*

Proof. If there are two nonisomorphic branches, then Theorem 7.3.1 and Lemma 7.6.1 give that λ_2 is in the alternating spectrum.

If λ_2 is alternating, then there is a $x \in \xi(T)$ and a vertex v such $x_v \neq x_{\phi(v)}$ (obviously v must be in an active branch). So Lemma 7.6.2 gives that v and $\phi(v)$ are in different branches. Since w is a fixed point, we conclude that ϕ permutes the branches, and hence that ϕ is an automorphism that maps the branch containing v to the branch containing $\phi(v)$. □

In [19], the following construction to obtain type 1 trees is given, based on Theorem 7.3.1. Take any two rooted trees, T_1 and T_2 such $\hat{L}(T_1)$ and $\hat{L}(T_2)$ have the same smallest eigenvalue, $\hat{\lambda}$. Form the tree T by taking the disjoint union of T_1 and T_2, and adding a single vertex, w, that is adjacent to both roots. Define a vector x which is zero on the new vertex, the restriction of x to T_1 or T_2 gives an eigenvector corresponding, respectively, to $\hat{L}(T_1)$ or $\hat{L}(T_2)$, and x takes on the values $+1$ and -1, respectively, at the two roots. Following the ideas of Theorem 7.3.1, it may be seen that $\lambda_2(T) = \hat{\lambda}$, with the new vertex being the characteristic vertex of T. Note that in this construction, that $y \in \xi(T)$ forces $y_w = 0$. Now if y is not zero at one of the vertices adjacent to w, then the eigenvalue condition at w forces $y = cx$, where c is some constant. On the other had, Theorem 7.1.3 guarantees that, since $y \neq 0$, it cannot be zero at both vertices adjacent to w.

If T_1 and T_2 are isomorphic branches, then in fact the restrictions of x to T_1 and T_2 respectively will be equal in value but opposite in sign. Thus $\lambda_2(T)$ will be in the alternating spectrum. If T_1 and T_2 are nonisomorphic branches, then by Theorem 7.6.3, λ_2 will not be in the alternating spectrum. Furthermore, by adjoining in the same manner a second copy of T_1 (or T_2), we see that λ_2 can be in both the alternating and symmetric spectra. In fact, we can construct a tree with any prescribed values for the multiplicity of λ_2 as both an alternating and a symmetric eigenvalue.

Chapter 8

Other Matrices

8.1 Other Laplacians

We will specifically mention two other Laplacians; both can be viewed as ways of normalising with respect to the number of vertices.

Chung [7] considers eigenvalues of the matrix $\mathcal{L}$ defined by

$$\mathcal{L}_{ij} = \begin{cases} 1, & \text{if } i = j \text{ and } d_i \neq 0 \\ -1/(d_i d_j), & \text{if } i \sim j \\ 0, & \text{otherwise} \end{cases}$$

Note that if we define D^{-1} to be the inverse of D, the (diagonal) matrix of vertex degrees (with the convention that $(D^{-1})_{ii} = 0$ if $D_{ii} = 0$, then we have

$$\mathcal{L} = D^{-1/2} L D^{-1/2} \tag{8.1}$$

Thus the two matrices are related. In fact, given an eigenvector x of L, the vector $D^{1/2}x$ is an eigenvector of $\mathcal{L}$. In terms of operators, we see that

$$\begin{aligned}(\mathcal{L}y)_j &= y_j - \sum_{i \sim j} \frac{y_i}{\sqrt{d_i d_j}} \\ &= \frac{1}{\sqrt{d_j}} \sum_{i \sim j} \left(\frac{y_i}{\sqrt{d_i}} - \frac{y_j}{\sqrt{d_j}} \right)\end{aligned}$$

Note that in the case of regular graphs, the spectrum is again equivalent to the spectrum of the ordinary adjacency matrix.

In general, one can say that the bounds obtained for $\mathcal{L}$ are "normalised" with respect to n, in some sense. This does not mean that they are obtained by dividing the eigenvalues of L by n. In general, the properties of the two spectra are different, though they share some global similarities. For instance, we still have that the multiplicity of 0 is equal to the number of connected components of the graph. We give here without proof some basic results from [7], using $0 = \tilde{\lambda}_1 \leq \tilde{\lambda}_2 \leq \cdots \leq \tilde{\lambda}_n$ for the eigenvalues of $\mathcal{L}$.

$$\begin{aligned}
&\tilde{\lambda}_2 \leq \frac{n}{n-1} \\
&\tilde{\lambda}_n \geq \frac{n}{n-1} \quad \text{if } G \text{ has no isolated vertices} \\
&\tilde{\lambda}_2 \leq 1 \quad \text{unless } G \text{ is complete} \\
&\tilde{\lambda}_n \leq 2 \\
&\tilde{\lambda}_n = 2 \iff G \text{ has a nontrivial connected bipartite component}
\end{aligned} \tag{8.2}$$

Recall that for bipartite graphs the spectrum of the adjacency matrix is symmetric about zero, and that for trees the spectrum of L is "roughly symmetric about one" (see Proposition 5.1.11 and the remarks following). For $\mathcal{L}$ we have the following result [7].

Theorem 8.1.1. *A graph G is bipartite if and only if the spectrum of $\mathcal{L}(G)$ is symmetric about* 1.

Most of the major results in this paper have analogies for $\mathcal{L}$. Using the alternative definitions of the isoperimetric constants

$$\begin{aligned}
\tilde{h}(G) &= \min_{|X| \leq n/2} \frac{|\partial X|}{\mathrm{vol}(X)} \\
\tilde{h}'(G) &= \min_{|X| \leq n/2} \frac{\mathrm{vol}(\delta X)}{\mathrm{vol}(X)} \\
\text{where } \mathrm{vol}(A) &= \sum_{i \in A} d_i \text{ for } A \subseteq V(G).
\end{aligned} \tag{8.3}$$

Chung obtains analogies for Theorem 2.2.1, Theorem 2.2.2, Theorem 3.2.2, Theorem 3.2.3, and Theorem 4.1.2, among others. It is perhaps worth noting that the relationship between vertex expansion and edge expansion is different. Although we trivially have $h'(G) \leq h(G)$, here we have $\tilde{h}'(G) \geq \tilde{h}(G)$.

Some authors also consider the Laplacian defined by

$$(L'y)_j = y_j - \frac{1}{d_j} \sum_{i \sim j} y_i$$

This matrix is again related to the combinatorial Laplacian, through

$$L' = D^{-1}L$$

Again, for the case of regular graphs, we have nothing that we didn't already know from the spectrum of the ordinary adjacency matrix. In general, however, the spectra of these different Laplacians do not coincide, although analogous results do often hold.

One can, as does Colin de Verdière [8], consider a more general family of operators, such that the corresponding matrix A has

$$A_{ij} = \begin{cases} < 0, & \text{if } i \sim j \\ = 0, & \text{if } i \nsim j \text{ and } i \neq j \end{cases}$$

A Laplacian is such an A with the condition that the row-sums are zero (i.e.: the constant vector is an eigenvector).

8.2 $Q = D + A$

The results of Chapter 2 can be summed up by saying that the connectedness properties can be approximated by the spectrum of a matrix (L) of the graph.

It is interesting in this regard to mention a paper of Desai and Rao [11]. They consider the matrix $Q = D+A$, and specifically, it's smallest eigenvalue. For a set $S \subseteq V(G)$, define $e(S)$ to be the minimum number of edges that need to be removed from the induced subgraph on S so as to make it bipartite. Then define

$$\psi(G) = \min_{\emptyset \neq S \subseteq V(G)} \frac{e(S) + |\partial X|}{|S|}$$

This may be thought of as an analogue to the isoperimetric constant of the graph, except that ψ measures how close G is to being bipartite. Clearly $\psi = 0$ if and only if G is bipartite.

Note that the matrix Q is positive semidefinite. This follows for basically the same reasons as for L, except that here $Q = K_+ {K_+}^t$, where K_+ is the unsigned version of the incidence matrix. Write the eigenvalues of Q as $\gamma_1 \leq \gamma_2 \leq \cdots \leq \gamma_n$. If G is d-regular, then we trivially have that $\gamma_i = 2d - \lambda_i = d + \mu_i$, where μ_i are the eigenvalues of A. Thus we may state for regular graphs, using a well known property of the A-spectrum that

Proposition 8.2.1. *A regular graph G is bipartite if and only if $\gamma_1 = 0$.*

In fact, we can say more [11].

Proposition 8.2.2. *The matrix Q is singular (i.e. $\gamma_1 = 0$) if and only if $\psi = 0$.*

Their main results can be thought of as analogous to Theorem 2.2.1 and Theorem 2.2.2. In fact even the proofs share some of the spirit of the proofs of Theorem 2.2.1 and Theorem 2.2.2.

Theorem 8.2.3. $\gamma_1 \leq 4\psi$

Theorem 8.2.4. $\gamma_1 \geq \frac{\psi^2}{4\Delta}$

Furthermore, define the parameter

$$\psi'(G) = \min_{\emptyset \neq S \subseteq V(G)} \frac{4e(S) + |\partial X|}{|S|}$$

(which also gives a slight variation on Theorem 8.2.3). For any eigenvector x of Q corresponding to γ_1, define $\mathrm{Val}(x) = \{|x_i| \mid x_i \neq 0, 1 \leq i \leq n\}$. They give an alternate lower bound for γ_1,which may sometimes be better than Theorem 8.2.4 as

Theorem 8.2.5. $\gamma_1 \geq \frac{\psi'}{|\mathrm{Val}(x)|}$

Echoing remarks made elsewhere on λ_2 and h, they remark at the end of the paper that computation of ψ is typically difficult and thus that γ_1 provides easily computable bounds on an otherwise hard to compute structural parameter of the graph.

8.3 An "inverse" of L

Obviously, L is singular and has no inverse. However, it turns out that the matrix

$$\Omega = (I + L)^{-1},$$

encapsulates some interesting properties of the graph. We note that $I + L$ is positive definite. Indeed, the eigenvalues of Ω are

$$1 = \frac{1}{1+\lambda_1}, \frac{1}{1+\lambda_2}, \frac{1}{1+\lambda_3}, \dots, \frac{1}{1+\lambda_n}.$$

In fact the eigenvectors of Ω are the same as the eigenvectors of L. Observing that the all-ones vector is an eigenvector of Ω corresponding to 1, we see that Ω has constant row-sum equal to 1. Since it is symmetric, the same can be said for the column-sum, hence Merris refers to Ω as the *doubly stochastic matrix of the graph.*

We have some relations between Ω and the structure of the graph, which we reproduce here without proof.

Proposition 8.3.1. *Let G be a graph, and Ω its doubly stochastic graph matrix. If $d_u = n - 1$ for some vertex u then $\omega_{uu} = 2(n+1)$ and $\omega_{uj} = 1(n+1), j \neq u$. If $d_v = 0$ for some vertex v then $\omega_{vv} = 1$ and $\omega_{vj} = 0, j \neq u$. $\omega_{jj} \geq 2(n+1)$ with equality if and only if $d_j = n - 1$. If $\omega_{ui} = \omega_{uj}$ for all $i \neq u \neq j$ then either $d_u = 0$ or $d_u = n - 1$.*

Proposition 8.3.2. *Let u, v be nonadjacent vertices of a graph G. Let the graph G' be obtained by adding the edge uv to G. Let Ω and Ω' be the doubly stochastic graph matrices of G and G', respectively. Then $\omega_{uu} > \omega'_{uu}$ and $\omega_{vv} > \omega'_{vv}$. Furthermore, $\omega_{ii} \geq \omega'_{ii}$ with equality if and only if $\omega_{iu} = \omega_{iv}$ if and only if $\omega_{ij} = \omega'_{ij}$ for all $j \neq i$*

Define $\rho(i,j) = \omega_{ii} + \omega_{jj} - 2\omega_{ij}$. This behaves like a distance, motivating the definition of the *ρ-diameter* D_ρ to be the maximum of $\rho(i,j)$ over all pairs of vertices i, j.

For each vertex j, define

$$r(j) = \sum_{i \neq j} \rho(i,j).$$

Based on this definition, a vertex j that maximises [minimises] $r(j)$ is said to be a *most remote* [*least remote*] vertex. The following result characterises the most and least remote vertices of the graph.

Theorem 8.3.3. *Let G be a graph and $\Omega = (\omega)_{ij} = (L+I)^{-1}$. Then vertex k is a most remote vertex if and only if ω_{kk} is a maximal main diagonal entry, and a least remote vertex if and only if ω_{kk} is a minimal main diagonal entry.*

Proof. The proof is straightforward. By the definition of $\rho(i,j)$ we have

$$\begin{aligned} r(j) &= \sum_{i \neq j} \rho(i,j) \\ &= \sum_{i \neq j} \omega_{ii} + \omega_{jj} - 2\omega_{ij} \\ &= (n-1)\omega_{jj} + \text{trace}(\Omega) - \omega_{jj} - 2(1 - w_{jj}) \\ &= n\omega_{jj} + \text{trace}(\Omega) - 2 \end{aligned}$$

□

Not surprisingly, we can also relate r back to λ.

Corollary 8.3.4.

$$W_\rho(G) = \frac{1}{2}\sum_{j=1}^{n} r(j) = n\sum_{j=1}^{n-1} \frac{1}{1+\lambda_j}$$

Proof. Following the proof above, we have

$$\begin{aligned} 2W_\rho &= \sum_{j=1}^{n} n\omega_{jj} + \text{trace}(\Omega) - 2 \\ &= n\text{trace}(\Omega) + n\text{trace}(\Omega) - 2n \\ &= 2n\sum_{j=1}^{n} \lambda_j \end{aligned}$$

□

Merris remarks that the quantity W_ρ is analogous to the chemical Weiner Index, thus giving a link between the definition of "remoteness" given above, the Laplacian eigenvalues of the graph, and the chemistry of a molecule based on that graph.

This section is based principally on [43], [40], to which the reader is referred for more details.

8.4 Further directions

We mention here some further reading for more results relating to Laplacian matrices.

The survey papers [46, 48, 36, 37] deal with the Laplacian as we have defined it. The two books [7, 8] deal extensively with different forms of the Laplacian then we consider here.

Graphs with boundary and the Dirichlet problem are considered extensively in [56, 57]. The theory of the Laplacian matrix for graphs is seen in the context of the theory of the Laplacian operator on Riemannian manifolds. Infinite graphs are considered in, for instance, [8].

The Laplacian can be used to partition graphs into sets with minimal overlap. This can be seen partly as a specific consequence of the bounds relating to the isoperimetric constant, among others, but more can be said. The eigenvectors of λ_2 can be used to heuristically divide the graph into two sets with minimal crossover; this is a consequence of the fact that ordering the vertices based on an eigenvector of λ_2 comes close to minimising the bandwidth of L [46, 53].

J Tan has shown that the inequality in Theorem 2.2.2 is in fact strict [55].

Further results on the diameter can be found in [58], and in [52, 54], a more general method is advanced than that seen here.

Graph theory has many applications in chemistry, and in fact the Laplacian spectrum of the underlying graph of certain molecules can be used to predict some of their chemical properties; see [46, 36] and the references therein.

There is much more that could be said about Laplacian spectra. Indeed, a "complete" survey of all the material relating to the Laplacian spectrum is beyond the scope of this paper. Hopefully, this paper has demonstrated some of the important connections that exist between the structure of graphs and their Laplacian spectrum.

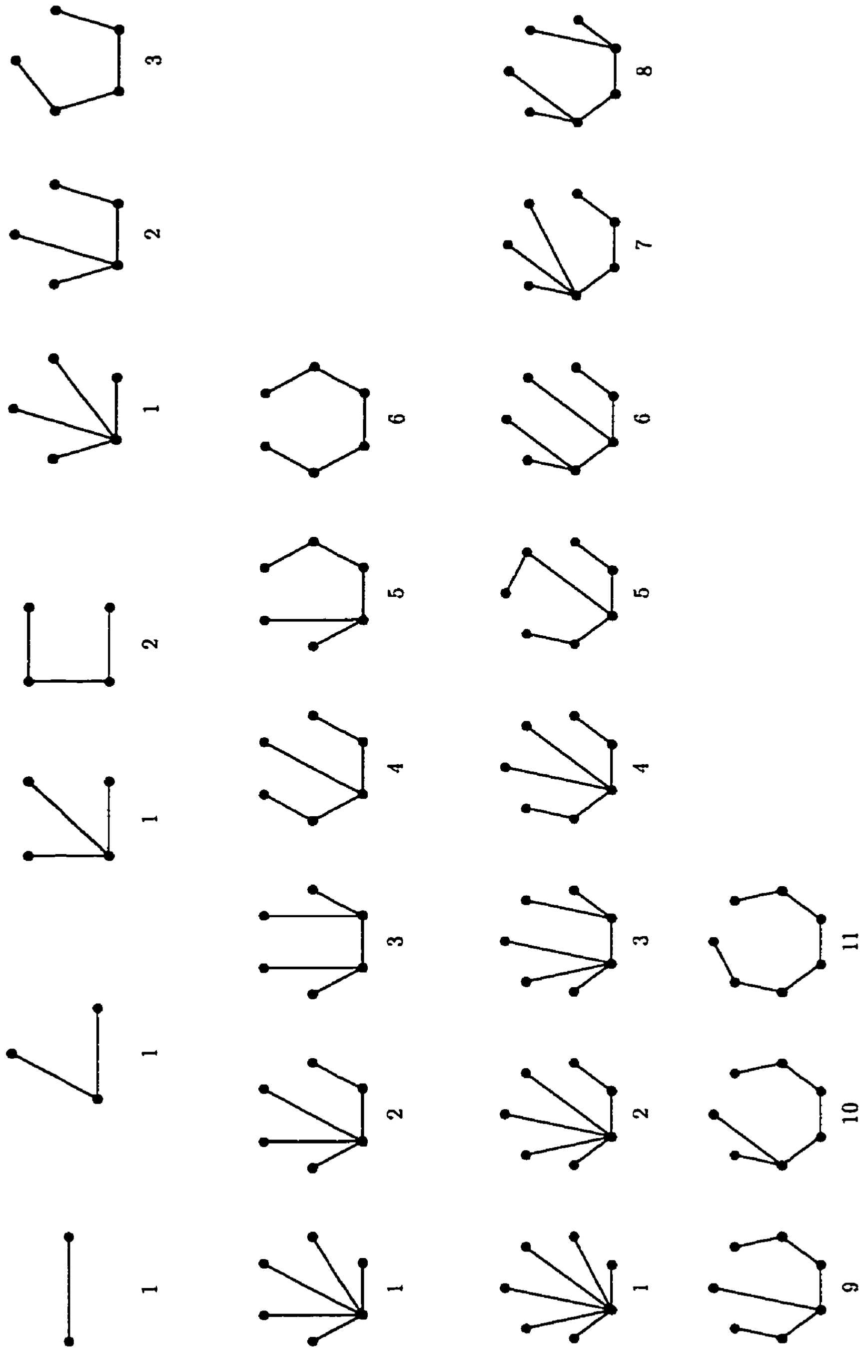
Appendix A

Graph Tables

We give tables of the Laplacian spectrum and characteristic polynomial for trees up to $n = 10$ vertices and connected graphs up to $n = 6$ vertices. They are sorted with λ_2 in nonincreasing order. The eigenvalue $\lambda_1 = 0$ is omitted for brevity, as is the (zero) constant coefficient of the characteristic polynomial. So, for instance, the first tree on four vertices, $K_{1,3}$, has spectrum $\{0, 1, 1, 4\}$ and characteristic polynomial $\det(D - xI) = 4x - 9x^2 + 6x^3 - x^4$. Of course, 4 is exactly the number of vertices multiplied by the number of spanning trees, and 6 is the sum of the degrees, or twice the number of edges, which (for trees) is $2(n - 1)$.

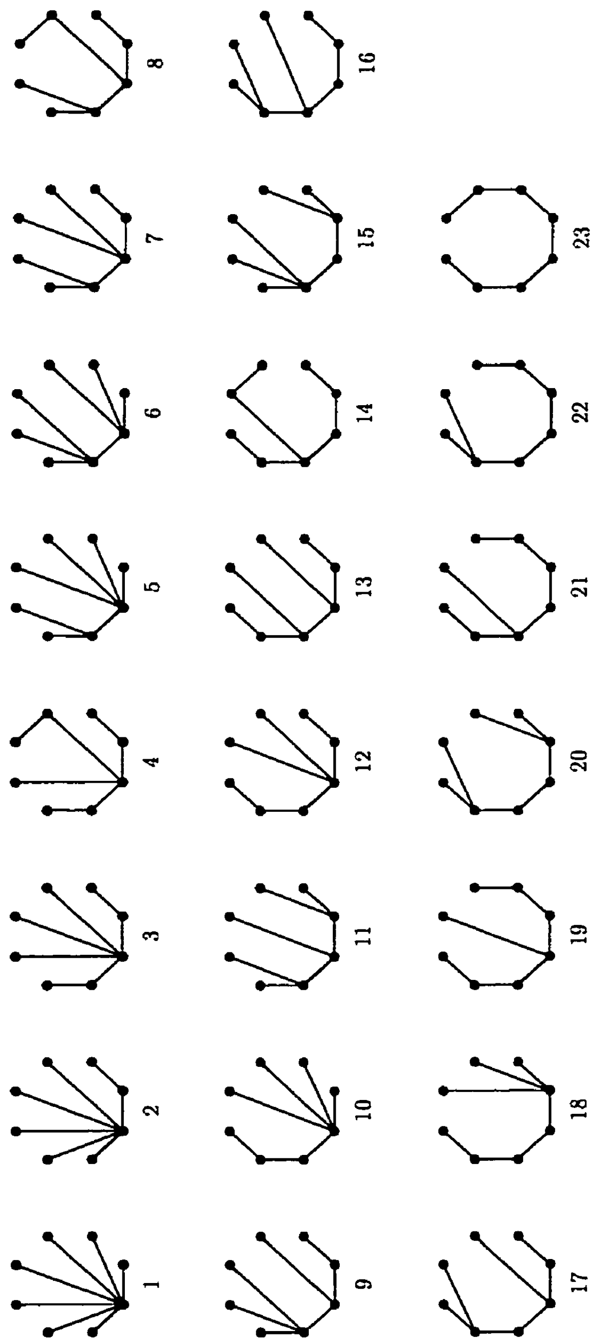
There are two pairs of isospectral graphs within these tables: 79, 80 and 82, 83, both from the table of connected graphs on six vertices. Within each pair, exactly one edge has been moved; between the two pairs, one edge (the "same" one) has been removed/added. Within each pair, the number of edges and diameter are equal. Graphs 79, 80 have the same girth and chromatic number. However, graph 82 has girth 3 and chromatic number 3, while graph 83 is bipartite. The isospectral constants are $\frac{2}{3}, 1, \frac{2}{3}, 1$, respectively.

The graphs were generated using geng, a subset of Brendan McKay's nauty software package, available from `http://cs.anu.edu.au/people/bdm/`. The spectra were calculated using `Maple`® and were then sorted by λ_2. The pictures were generated automatically from the graph files by the author.



Laplacian spectra of trees, $2 \leq n \leq 10$

n	tree	eigenvalues						characteristic polynomial
2	1	2						2, -1
3	1	1	3					3, -4, 1
4	1	1	1	4				4, -9, 6, -1
	2	0.586	2	3.414				4, -10, 6, -1
5	1	1	1	1	5			5, -16, 18, -8, 1
	2	0.519	1	2.311	4.170			5, -18, 20, -8, 1
	3	0.382	1.382	2.618	3.618			5, -20, 21, -8, 1
6	1	1	1	1	1	6		6, -25, 40, -30, 10, -1
	2	0.486	1	1	2.428	5.086		6, -28, 46, -33, 10, -1
	3	0.438	1	1	3	4.562		6, -29, 48, -34, 10, -1
	4	0.382	0.697	2	2.618	4.303		6, -31, 52, -35, 10, -1
	5	0.325	1	1.461	3	4.214		6, -32, 52, -35, 10, -1
	6	0.268	1	2	3	3.732		6, -35, 56, -36, 10, -1
7	1	1	1	1	1	1	7	7, -36, 75, -80, 45, -12, 1
	2	0.466	1	1	1	2.483	6.051	7, -40, 87, -92, 49, -12, 1
	3	0.398	1	1	1	3.340	5.262	7, -42, 93, -98, 51, -12, 1
	4	0.382	0.609	1	2.227	2.618	5.164	7, -44, 100, -104, 52, -12, 1
	5	0.382	0.382	1.586	2.618	2.618	4.414	7, -48, 114, -114, 54, -12, 1
	6	0.322	0.680	1	2.140	3.230	4.629	7, -46, 105, -108, 53, -12, 1
	7	0.296	1	1	1.491	3.117	5.097	7, -46, 102, -104, 52, -12, 1
	8	0.268	1	1	1.586	3.732	4.414	7, -48, 107, -108, 53, -12, 1
	9	0.260	0.626	1.405	2.274	3.100	4.334	7, -50, 115, -114, 54, -12, 1
	10	0.225	1	1	2.186	3.360	4.228	7, -52, 116, -114, 54, -12, 1
	11	0.198	0.753	1.555	2.445	3.247	3.802	7, -56, 126, -120, 55, -12, 1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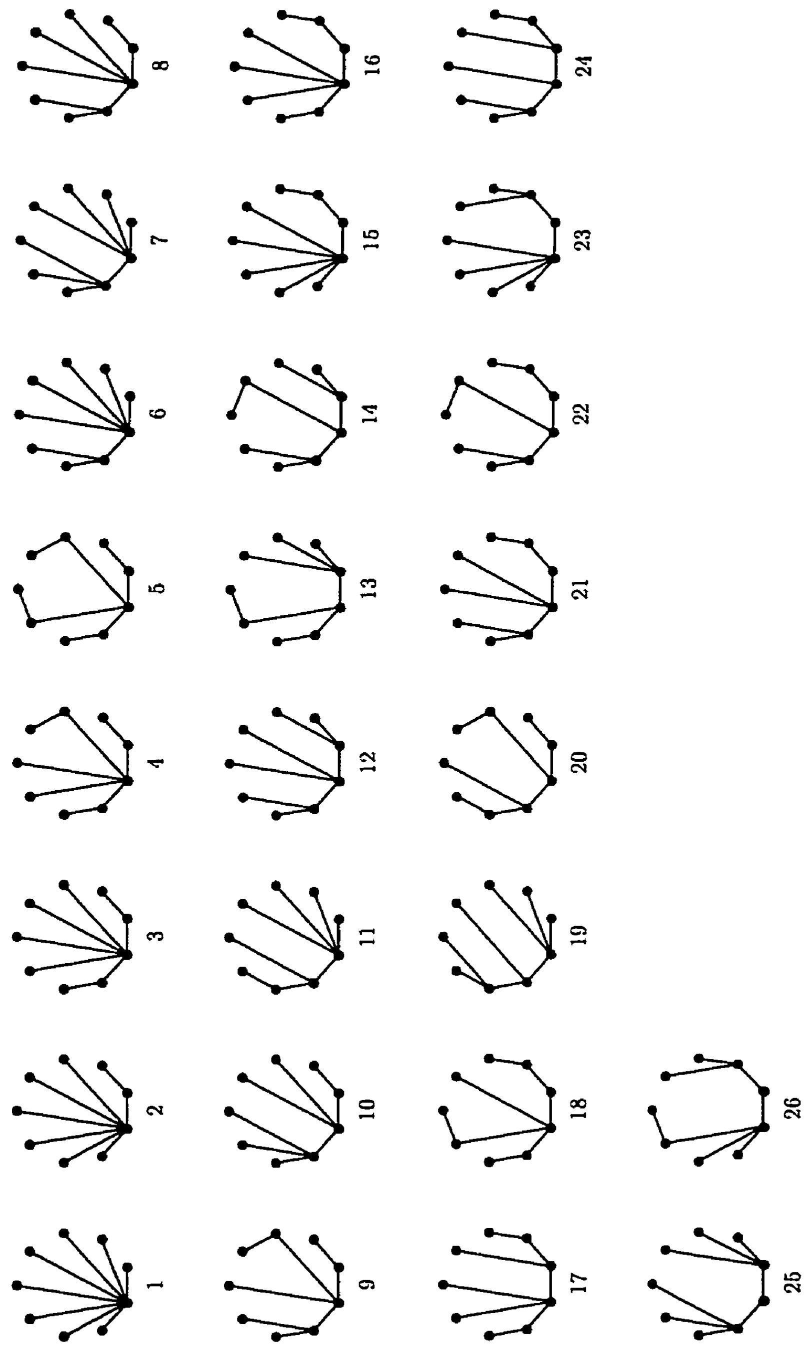
n	tree	eigenvalues							characteristic polynomial
8	1	1	1	1	1	1	1	8	8, -49, 126, -175, 140, -63, 14, -1
	2	0.452	1	1	1	1	2.513	7.034	8, -54, 146, -205, 160, -68, 14, -1
	3	0.382	0.561	1	1	2.339	2.618	6.100	8, -59, 168, -238, 180, -72, 14, -1
	4	0.382	0.382	0.764	2	2.618	2.618	5.236	8, -64, 192, -273, 198, -75, 14, -1
	5	0.374	1	1	1	1	3.485	6.141	8, -57, 158, -223, 172, -71, 14, -1
	6	0.354	1	1	1	1	4	5.646	8, -58, 162, -229, 176, -72, 14, -1
	7	0.319	0.586	1	1	2.358	3.414	5.323	8, -62, 180, -255, 190, -74, 14, -1
	8	0.306	0.382	1	1.670	2.618	3.330	4.694	8, -67, 204, -286, 204, -76, 14, -1
	9	0.289	0.674	1	1	2.169	3.586	5.282	8, -63, 182, -256, 190, -74, 14, -1
	10	0.277	1	1	1	1.507	3.161	6.055	8, -62, 174, -241, 180, -72, 14, -1
	11	0.268	0.657	1	1	2.529	3.732	4.814	8, -65, 190, -267, 196, -75, 14, -1
	12	0.254	0.547	1	1.469	2.407	3.150	5.173	8, -67, 198, -275, 198, -75, 14, -1
	13	0.251	0.586	0.729	2	2.335	3.414	4.686	8, -68, 204, -286, 204, -76, 14, -1
	14	0.243	0.382	1.180	2	2.618	3.139	4.438	8, -72, 224, -307, 212, -77, 14, -1
	15	0.238	1	1	1	1.637	4	5.125	8, -66, 188, -259, 190, -74, 14, -1
	16	0.224	0.586	1	1.411	2.724	3.414	4.641	8, -70, 208, -287, 204, -76, 14, -1
	17	0.214	0.618	1	1.498	2.354	3.841	4.476	8, -71, 210, -288, 204, -76, 14, -1
	18	0.202	1	1	1	2.247	3.453	5.098	8, -71, 204, -277, 198, -75, 14, -1
	19	0.198	0.492	1.320	1.555	2.826	3.247	4.362	8, -75, 228, -308, 212, -77, 14, -1
	20	0.186	1	1	1	2.471	4	4.343	8, -74, 214, -289, 204, -76, 14, -1
	21	0.186	0.586	1	2	2.471	3.414	4.343	8, -76, 228, -308, 212, -77, 14, -1
	22	0.167	0.728	1	1.635	2.673	3.564	4.233	8, -79, 232, -309, 212, -77, 14, -1
	23	0.152	0.586	1.235	2	2.765	3.414	3.848	8, -84, 252, -330, 220, -78, 14, -1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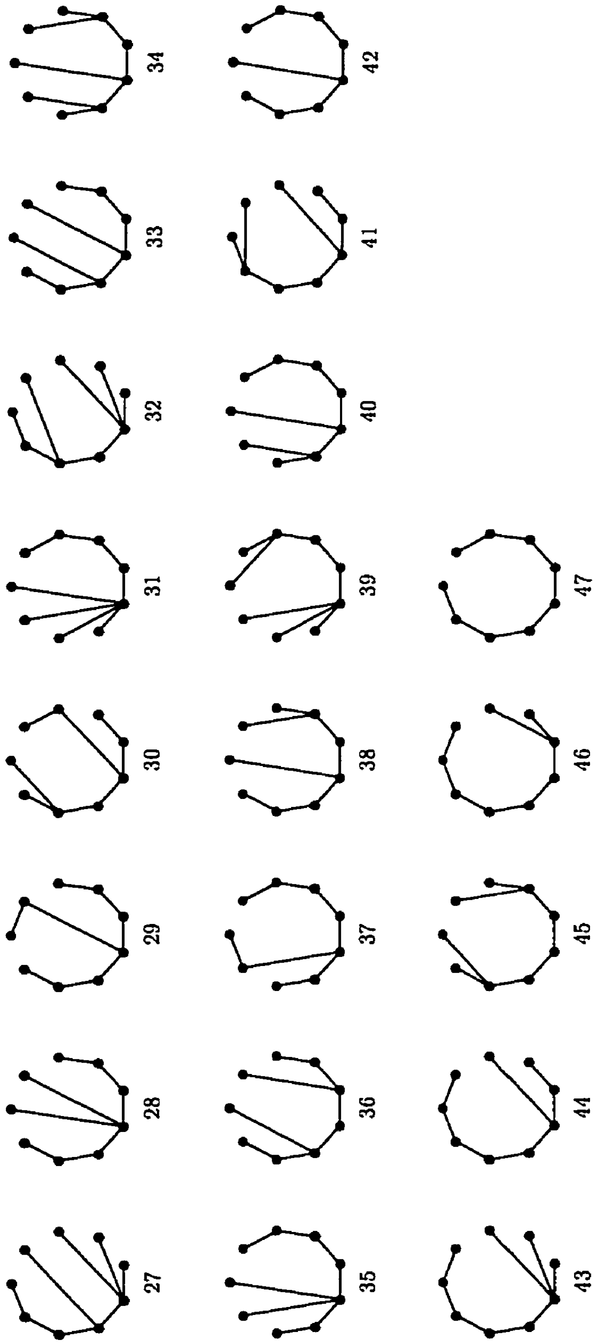
n	tree	eigenvalues								characteristic polynomial
9	1	1	1	1	1	1	1	1	9	9, -64, 196, -336, 350, -224, 84, -16, 1
	2	0.443	1	1	1	1	1	2.533	8.024	9, -70, 226, -396, 410, -254, 90, -16, 1
	3	0.382	0.530	1	1	1	2.403	2.618	7.067	9, -76, 259, -464, 476, -284, 95, -16, 1
	4	0.382	0.382	0.671	1	2.181	2.618	2.618	6.147	9, -82, 295, -540, 546, -312, 99, -16, 1
	5	0.382	0.382	0.382	1.697	2.618	2.618	2.618	5.303	9, -88, 334, -624, 615, -336, 102, -16, 1
	6	0.357	1	1	1	1	1	3.555	7.087	9, -74, 246, -436, 450, -274, 94, -16, 1
	7	0.327	1	1	1	1	1	4.352	6.321	9, -76, 256, -456, 470, -284, 96, -16, 1
	8	0.316	0.536	1	1	1	2.447	3.515	6.186	9, -80, 280, -506, 516, -302, 98, -16, 1
	9	0.305	0.382	0.757	1	2.096	2.618	3.461	5.382	9, -86, 317, -582, 582, -326, 101, -16, 1
	10	0.282	0.578	1	1	1	2.373	4.086	5.679	9, -82, 289, -522, 530, -308, 99, -16, 1
	11	0.268	0.671	1	1	1	2.181	3.732	6.147	9, -82, 286, -512, 518, -302, 98, -16, 1
	12	0.268	0.551	1	1	1	3	3.732	5.449	9, -84, 300, -544, 550, -316, 100, -16, 1
	13	0.268	0.382	1	1	1.697	2.618	3.732	5.303	9, -88, 325, -590, 584, -326, 101, -16, 1
	14	0.268	0.345	1	1	1.789	3	3.732	4.866	9, -90, 338, -616, 606, -334, 102, -16, 1
	15	0.265	1	1	1	1	1.516	3.183	7.035	9, -80, 271, -476, 480, -284, 95, -16, 1
	16	0.248	0.506	1	1	1.495	2.470	3.177	6.104	9, -86, 308, -552, 549, -312, 99, -16, 1
	17	0.243	0.537	0.689	1	2.130	2.417	3.643	5.341	9, -88, 322, -586, 583, -326, 101, -16, 1
	18	0.240	0.382	0.720	1.424	2.203	2.618	3.169	5.244	9, -92, 348, -634, 617, -336, 102, -16, 1
	19	0.238	0.648	1	1	1	2.650	4.132	5.331	9, -86, 306, -550, 552, -316, 100, -16, 1
	20	0.231	0.382	0.642	1.613	2.259	2.618	3.513	4.742	9, -94, 361, -662, 640, -344, 103, -16, 1
	21	0.223	0.492	1	1	1.471	3	3.484	5.330	9, -90, 329, -592, 584, -326, 101, -16, 1
	22	0.222	0.333	1	1.192	2.107	3	3.441	4.705	9, -96, 370, -668, 641, -344, 103, -16, 1
	23	0.220	1	1	1	1	1.663	4.055	6.062	9, -86, 298, -524, 522, -302, 98, -16, 1
	24	0.212	0.555	0.722	1	2.078	2.734	3.853	4.847	9, -92, 340, -616, 606, -334, 102, -16, 1
	25	0.209	1	1	1	1	1.697	4.791	5.303	9, -88, 307, -540, 536, -308, 99, -16, 1
	26	0.204	0.540	1	1	1.599	2.443	4.017	5.197	9, -92, 335, -598, 586, -326, 101, -16, 1



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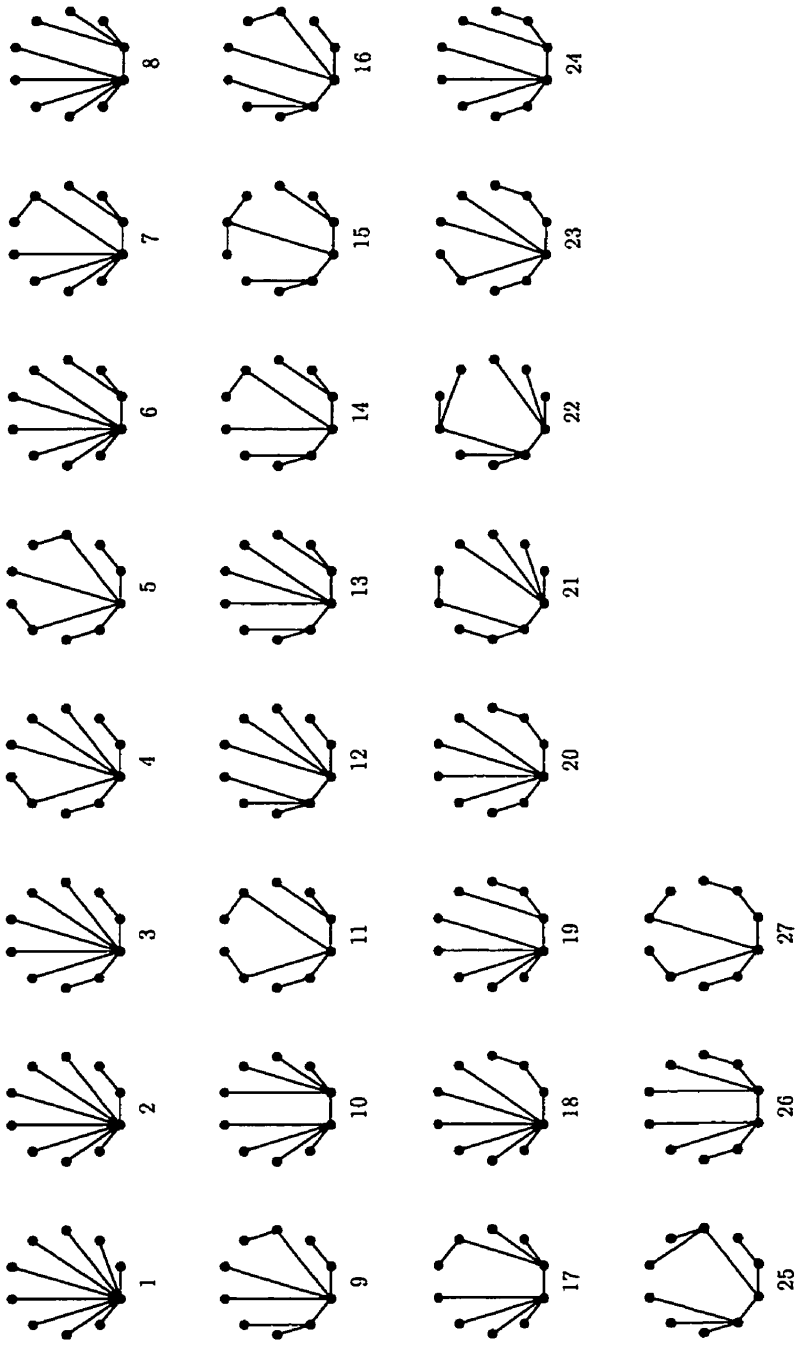
n	tree	eigenvalues								characteristic polynomial
9	27	0.202	0.569	1	1	1.412	2.827	3.705	5.284	9, -92, 334, -596, 585, -326, 101, -16, 1
	28	0.198	0.412	1	1.406	1.555	3	3.247	5.182	9, -96, 361, -644, 619, -336, 102, -16, 1
	29	0.198	0.300	1	1.555	2.239	3	3.247	4.461	9, -102, 405, -724, 677, -354, 104, -16, 1
	30	0.195	0.382	1	1.211	2.145	2.618	3.906	4.543	9, -98, 375, -672, 642, -344, 103, -16, 1
	31	0.188	1	1	1	1	2.275	3.482	6.055	9, -92, 323, -564, 552, -312, 99, -16, 1
	32	0.188	0.614	1	1	1.533	2.380	4.154	5.130	9, -94, 340, -602, 587, -326, 101, -16, 1
	33	0.186	0.482	0.704	1.407	2.134	2.853	3.537	4.696	9, -98, 371, -668, 641, -344, 103, -16, 1
	34	0.183	0.572	1	1	1.509	3	4.044	4.691	9, -96, 352, -626, 608, -334, 102, -16, 1
	35	0.177	0.524	1	1	2.161	2.496	3.467	5.174	9, -98, 363, -644, 619, -336, 102, -16, 1
	36	0.173	0.559	0.662	1.433	2.209	2.485	3.956	4.523	9, -100, 376, -672, 642, -344, 103, -16, 1
	37	0.171	0.382	0.850	1.676	2.416	2.618	3.442	4.444	9, -104, 406, -724, 677, -354, 104, -16, 1
	38	0.166	0.468	1	1.343	1.653	3	3.879	4.491	9, -102, 384, -678, 643, -344, 103, -16, 1
	39	0.165	1	1	1	1	2.568	4.165	5.102	9, -98, 349, -608, 588, -326, 101, -16, 1
	40	0.163	0.532	1	1	2.089	3	3.572	4.644	9, -102, 381, -674, 642, -344, 103, -16, 1
	41	0.154	0.576	1	1	2.113	2.676	4.075	4.406	9, -104, 386, -678, 643, -344, 103, -16, 1
	42	0.151	0.427	1	1.423	2.172	3	3.458	4.370	9, -108, 416, -730, 678, -354, 104, -16, 1
	43	0.149	0.717	1	1	1.663	2.740	3.633	5.098	9, -104, 377, -654, 621, -336, 102, -16, 1
	44	0.140	0.536	0.775	1.580	2.245	2.778	3.599	4.346	9, -110, 417, -730, 678, -354, 104, -16, 1
	45	0.139	0.697	1	1	1.746	3	4.115	4.303	9, -108, 395, -684, 644, -344, 103, -16, 1
	46	0.129	0.554	1	1.261	2.133	3	3.688	4.235	9, -114, 427, -736, 679, -354, 104, -16, 1
	47	0.121	0.468	1	1.653	2.347	3	3.532	3.879	9, -120, 462, -792, 715, -364, 105, -16, 1



n	tree	eigenvalues									characteristic polynomial
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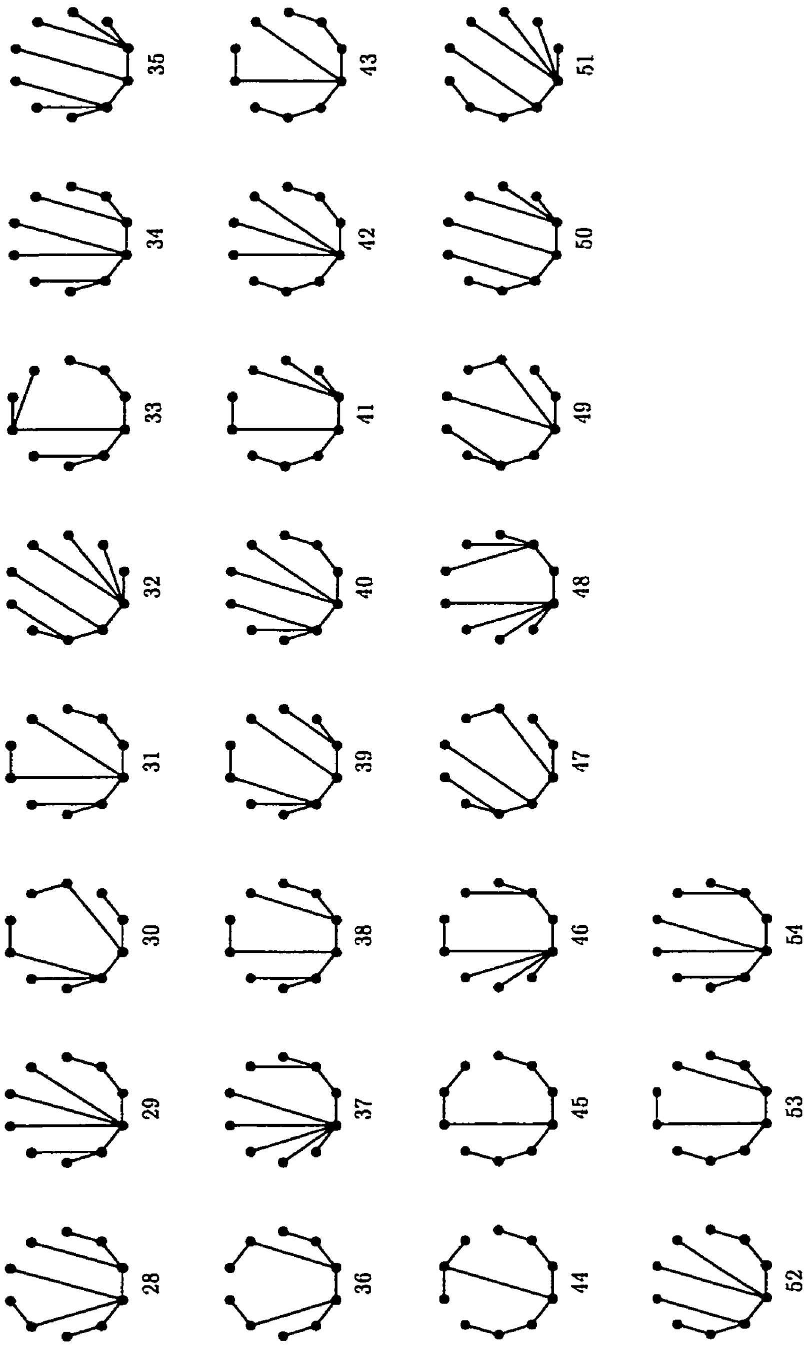
	2	0.435	1	1	1	1	1	1	2.546	9.018	10, -88, 330, -693, 896, -735, 378, -115, 18, -1
	3	0.382	0.509	1	1	1	1	2.443	2.618	8.048	10, -95, 376, -813, 1056, -850, 420, -121, 18, -1
	4	0.382	0.382	0.617	1	1	2.284	2.618	2.618	7.100	10, -102, 426, -949, 1236, -972, 460, -126, 18, -1
	5	0.382	0.382	0.382	0.807	2	2.618	2.618	2.618	6.193	10, -109, 480, -1102, 1434, -1095, 496, -130, 18, -1
	6	0.345	1	1	1	1	1	1	3.596	8.059	10, -93, 360, -768, 996, -810, 408, -120, 18, -1
	7	0.313	0.504	1	1	1	1	2.493	3.571	7.119	10, -100, 408, -895, 1164, -927, 448, -125, 18, -1
	8	0.309	1	1	1	1	1	1	4.511	7.180	10, -96, 378, -813, 1056, -855, 426, -123, 18, -1
	9	0.303	0.382	0.660	1	1	2.270	2.618	3.538	6.229	10, -107, 460, -1037, 1348, -1046, 484, -129, 18, -1
	10	0.298	1	1	1	1	1	1	5	6.702	10, -97, 384, -828, 1076, -870, 432, -124, 18, -1
	11	0.297	0.382	0.382	1	1.771	2.618	2.618	3.494	5.437	10, -114, 516, -1195, 1542, -1158, 514, -132, 18, -1
	12	0.277	0.528	1	1	1	1	2.456	4.383	6.357	10, -103, 426, -939, 1220, -966, 462, -127, 18, -1
	13	0.268	0.492	1	1	1	1	3.244	3.732	6.264	10, -105, 440, -976, 1268, -998, 472, -128, 18, -1
	14	0.268	0.343	0.748	1	1	2.234	3.175	3.732	5.500	10, -112, 494, -1121, 1448, -1107, 502, -131, 18, -1
	15	0.268	0.268	1	1	1	2	3.732	3.732	5	10, -117, 528, -1196, 1524, -1146, 512, -132, 18, -1
	16	0.264	0.382	0.754	1	1	2.116	2.618	4.153	5.713	10, -110, 478, -1077, 1392, -1072, 492, -130, 18, -1
	17	0.259	0.575	1	1	1	1	2.379	4.454	6.333	10, -104, 430, -945, 1224, -967, 462, -127, 18, -1
	18	0.256	1	1	1	1	1	1.523	3.196	8.025	10, -100, 396, -843, 1076, -855, 420, -121, 18, -1
	19	0.254	0.669	1	1	1	1	2.188	3.800	7.090	10, -103, 420, -913, 1176, -930, 448, -125, 18, -1
	20	0.244	0.481	1	1	1	1.509	2.505	3.192	7.069	10, -107, 448, -982, 1256, -976, 460, -126, 18, -1
	21	0.244	0.382	1	1	1	1.710	2.618	3.892	6.154	10, -111, 480, -1069, 1368, -1050, 484, -129, 18, -1
	22	0.237	0.538	1	1	1	1	3.163	4.315	5.748	10, -108, 456, -1011, 1308, -1023, 480, -129, 18, -1
	23	0.237	0.382	0.630	1	1.476	2.320	2.618	3.187	6.150	10, -114, 504, -1137, 1452, -1098, 496, -130, 18, -1
	24	0.236	0.503	0.678	1	1	2.165	2.473	3.754	6.192	10, -110, 472, -1054, 1358, -1048, 484, -129, 18, -1
	25	0.236	0.338	1	1	1	1.827	3.085	4.162	5.353	10, -115, 510, -1147, 1464, -1110, 502, -131, 18, -1
	26	0.233	0.519	0.616	1	1	2.311	2.441	4.170	5.710	10, -111, 480, -1078, 1392, -1072, 492, -130, 18, -1
	27	0.232	0.382	0.382	1.277	2	2.618	2.618	3.182	5.310	10, -121, 564, -1309, 1656, -1212, 526, -133, 18, -1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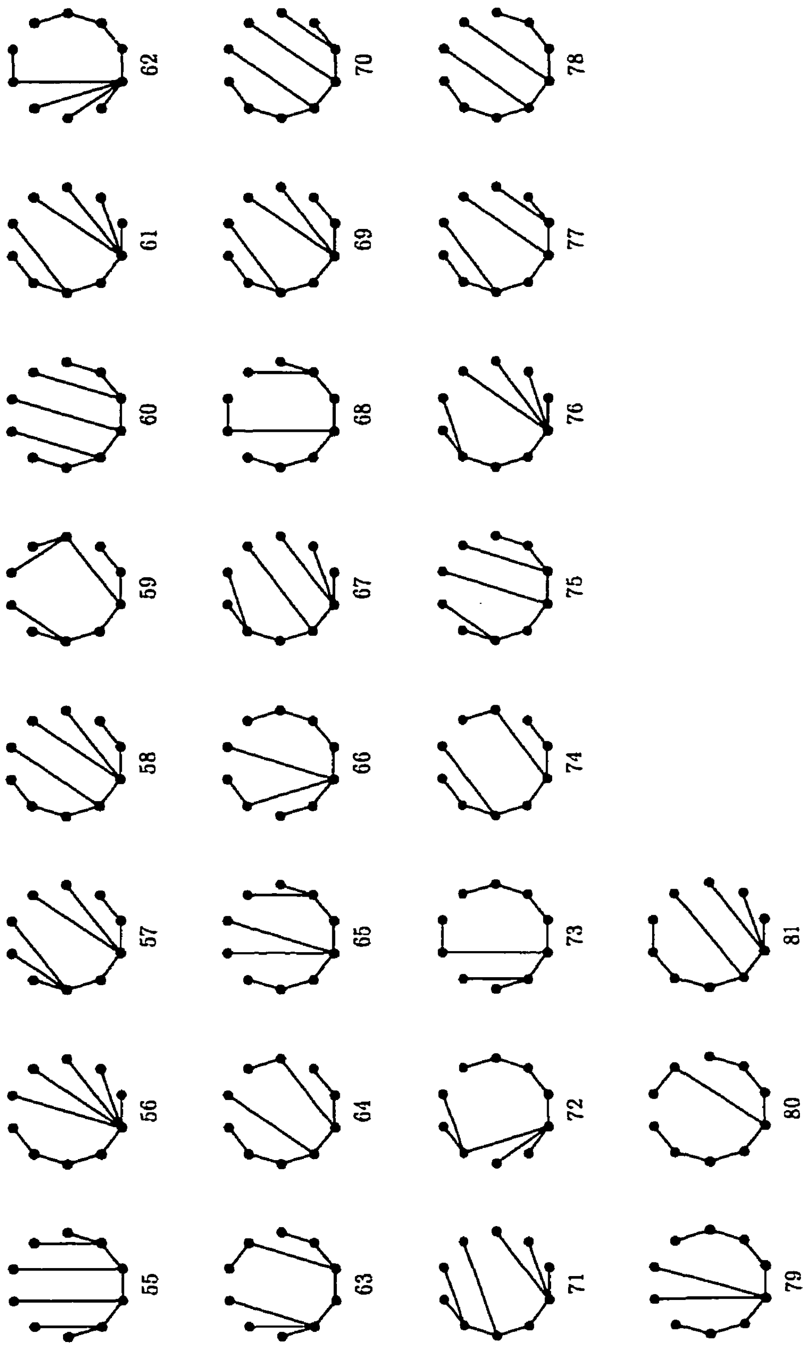
n	tree	eigenvalues									characteristic polynomial
10	28	0.226	0.382	0.627	0.773	2	2.293	2.618	3.684	5.397	10, -117, 528, -1208, 1548, -1159, 514, -132, 18, -1
	29	0.222	0.441	1	1	1	1.496	3.108	3.544	6.189	10, -112, 482, -1069, 1366, -1049, 484, -129, 18, -1
	30	0.221	0.382	0.555	1	1.677	2.401	2.618	3.787	5.359	10, -118, 534, -1219, 1554, -1160, 514, -132, 18, -1
	31	0.221	0.330	0.707	1	1.429	2.327	3.092	3.507	5.388	10, -119, 540, -1226, 1556, -1160, 514, -132, 18, -1
	32	0.218	0.644	1	1	1	1	2.698	4.280	6.159	10, -109, 456, -1000, 1284, -1002, 472, -128, 18, -1
	33	0.215	0.268	1	1	1.206	2.367	3.338	3.732	4.874	10, -124, 576, -1303, 1632, -1199, 524, -133, 18, -1
	34	0.210	0.486	0.687	1	1	2.153	3.137	3.864	5.463	10, -115, 504, -1133, 1454, -1108, 502, -131, 18, -1
	35	0.209	0.639	1	1	1	1	2.833	4.791	5.529	10, -111, 468, -1029, 1320, -1026, 480, -129, 18, -1
	36	0.209	0.382	0.382	1.382	2	2.618	2.618	3.618	4.791	10, -125, 592, -1378, 1730, -1251, 536, -134, 18, -1
	37	0.208	1	1	1	1	1	1.680	4.075	7.038	10, -108, 440, -943, 1196, -935, 448, -125, 18, -1
	38	0.208	0.333	0.639	1	1.705	2.288	3.076	3.855	4.896	10, -122, 562, -1284, 1624, -1198, 524, -133, 18, -1
	39	0.202	0.519	0.672	1	1	2.311	2.742	4.170	5.384	10, -116, 508, -1139, 1458, -1109, 502, -131, 18, -1
	40	0.202	0.470	1	1	1	1.472	3.062	4.112	5.682	10, -115, 498, -1104, 1406, -1074, 492, -130, 18, -1
	41	0.202	0.316	1	1	1.197	2.132	3.046	3.803	5.305	10, -122, 556, -1249, 1568, -1162, 514, -132, 18, -1
	42	0.198	0.368	1	1	1.447	1.555	3.079	3.247	6.107	10, -119, 528, -1171, 1470, -1101, 496, -130, 18, -1
	43	0.198	0.294	0.660	1.343	1.555	2.383	3.069	3.247	5.252	10, -126, 590, -1341, 1670, -1214, 526, -133, 18, -1
	44	0.198	0.237	1	1	1.555	2.563	3.247	3.483	4.716	10, -131, 628, -1419, 1746, -1253, 536, -134, 18, -1
	45	0.198	0.198	0.830	1.555	1.555	2.689	3.247	3.247	4.481	10, -138, 684, -1545, 1866, -1308, 548, -135, 18, -1
	46	0.197	0.501	1	1	1	1.643	2.489	4.060	6.110	10, -115, 494, -1087, 1378, -1052, 484, -129, 18, -1
	47	0.192	0.382	0.605	1	1.625	2.618	2.756	3.941	4.882	10, -123, 564, -1285, 1624, -1198, 524, -133, 18, -1
	48	0.190	1	1	1	1	1	1.729	5	6.081	10, -112, 462, -993, 1256, -975, 462, -127, 18, -1
	49	0.190	0.382	0.715	1	1.527	2.274	2.618	4.030	5.264	10, -122, 552, -1243, 1566, -1162, 514, -132, 18, -1
	50	0.188	0.541	0.720	1	1	2.090	2.880	4.242	5.338	10, -118, 516, -1150, 1464, -1110, 502, -131, 18, -1
	51	0.187	0.560	1	1	1	1.413	2.860	3.832	6.148	10, -116, 496, -1087, 1376, -1051, 484, -129, 18, -1
	52	0.186	0.411	0.682	1	1.470	2.167	3.058	3.678	5.347	10, -122, 550, -1238, 1562, -1161, 514, -132, 18, -1
	53	0.186	0.299	0.633	1.183	2	2.318	3.044	3.586	4.752	10, -129, 612, -1399, 1738, -1252, 536, -134, 18, -1
	54	0.180	0.479	1	1	1	1.605	3.322	4.068	5.346	10, -120, 526, -1165, 1472, -1111, 502, -131, 18, -1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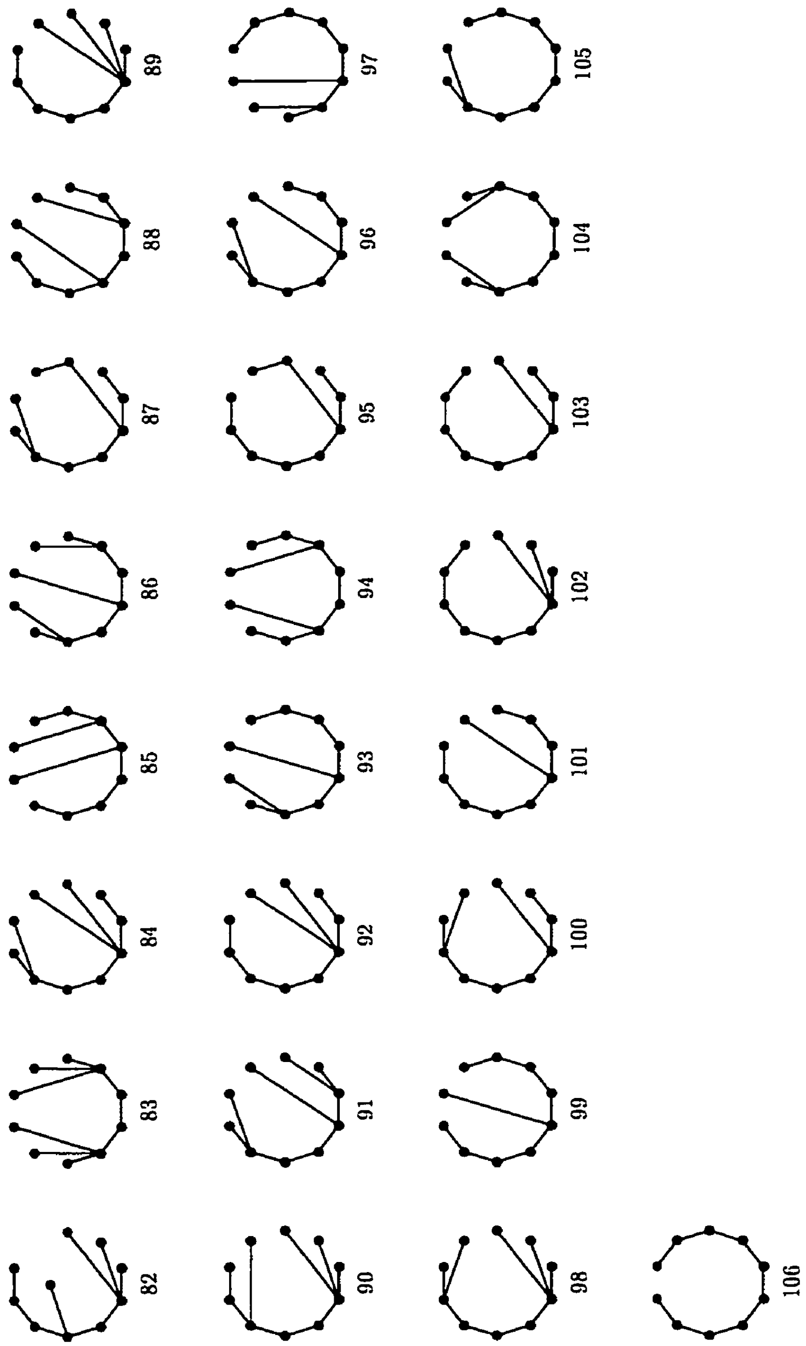
n	tree	eigenvalues									characteristic polynomial
10	55	0.179	0.519	0.714	1	1	2.311	3.159	4.170	4.947	10, -121, 536, -1200, 1524, -1146, 512, -132, 18, -1
	56	0.177	1	1	1	1	1	2.291	3.496	7.036	10, -115, 476, -1018, 1276, -980, 460, -126, 18, -1
	57	0.177	0.538	1	1	1	1.652	2.454	4.839	5.339	10, -119, 514, -1128, 1422, -1078, 492, -130, 18, -1
	58	0.177	0.472	0.629	1	1.411	2.350	2.870	3.749	5.343	10, -123, 552, -1239, 1562, -1161, 514, -132, 18, -1
	59	0.177	0.330	1	1	1.229	2.249	3.217	4.050	4.747	10, -127, 586, -1315, 1638, -1200, 524, -133, 18, -1
	60	0.173	0.475	0.662	0.742	2	2.209	2.906	3.956	4.876	10, -125, 568, -1286, 1624, -1198, 524, -133, 18, -1
	61	0.172	0.613	1	1	1	1.552	2.392	4.209	6.062	10, -119, 508, -1105, 1388, -1054, 484, -129, 18, -1
	62	0.170	0.491	1	1	1	2.229	2.517	3.488	6.104	10, -122, 534, -1174, 1470, -1101, 496, -130, 18, -1
	63	0.170	0.382	1	1	1.223	2.197	2.618	4.276	5.135	10, -126, 570, -1267, 1578, -1164, 514, -132, 18, -1
	64	0.170	0.382	0.508	1.382	1.696	2.618	2.876	3.618	4.750	10, -130, 612, -1399, 1738, -1252, 536, -134, 18, -1
	65	0.165	0.388	1	1	1.436	1.668	3.115	4.023	5.205	10, -127, 574, -1272, 1580, -1164, 514, -132, 18, -1
	66	0.165	0.382	0.681	1	2	2.431	2.618	3.477	5.245	10, -129, 596, -1343, 1670, -1214, 526, -133, 18, -1
	67	0.164	0.553	1	1	1	1.513	3.283	4.197	5.290	10, -123, 536, -1177, 1478, -1112, 502, -131, 18, -1
	68	0.164	0.289	1	1	1.639	2.325	3.098	3.929	4.557	10, -134, 638, -1431, 1752, -1254, 536, -134, 18, -1
	69	0.163	0.519	0.627	1	1.507	2.311	2.503	4.170	5.201	10, -126, 564, -1256, 1572, -1163, 514, -132, 18, -1
	70	0.161	0.444	0.691	1	1.408	2.460	3.083	3.901	4.852	10, -128, 582, -1305, 1632, -1199, 524, -133, 18, -1
	71	0.160	0.567	1	1	1	1.549	3.061	4.518	5.145	10, -124, 540, -1183, 1482, -1113, 502, -131, 18, -1
	72	0.159	0.456	1	1	1	2.212	3.258	3.584	5.331	10, -127, 568, -1258, 1570, -1162, 514, -132, 18, -1
	73	0.157	0.328	0.845	1	1.753	2.452	3.182	3.576	4.707	10, -134, 632, -1420, 1746, -1253, 536, -134, 18, -1
	74	0.156	0.382	0.597	1.186	2	2.454	2.618	4.030	4.577	10, -133, 624, -1412, 1744, -1253, 536, -134, 18, -1
	75	0.154	0.462	0.703	1	1.502	2.159	3.204	4.083	4.735	10, -130, 590, -1316, 1638, -1200, 524, -133, 18, -1
	76	0.151	1	1	1	1	1	2.611	4.182	6.056	10, -124, 524, -1123, 1396, -1055, 484, -129, 18, -1
	77	0.149	0.519	0.650	1	1.440	2.311	3.056	4.170	4.706	10, -131, 592, -1317, 1638, -1200, 524, -133, 18, -1
	78	0.149	0.382	0.650	1.382	1.440	2.618	3.056	3.618	4.706	10, -135, 632, -1420, 1746, -1253, 536, -134, 18, -1
	79	0.149	0.362	1	1	1.475	2.240	3.109	3.482	5.183	10, -134, 620, -1374, 1684, -1216, 526, -133, 18, -1
	80	0.148	0.281	0.787	1.293	2	2.463	3.093	3.469	4.466	10, -141, 688, -1546, 1866, -1308, 548, -135, 18, -1
	81	0.147	0.509	1	1	1	2.105	3.177	3.777	5.284	10, -130, 578, -1270, 1576, -1163, 514, -132, 18, -1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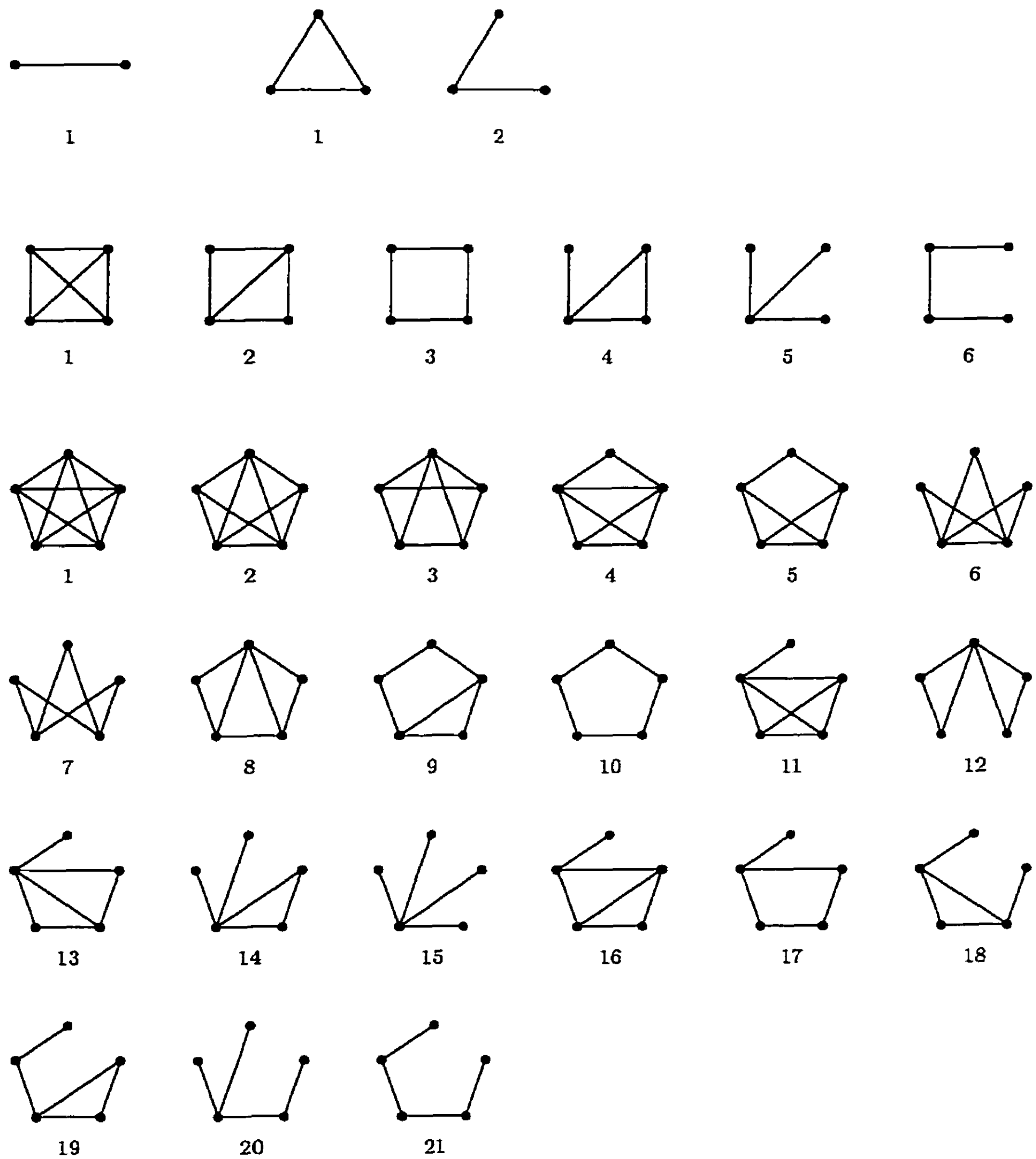
n	tree	eigenvalues									characteristic polynomial
10	82	0.147	0.458	1	1	1.349	1.695	3.025	4.196	5.130	10, -131, 586, -1285, 1586, -1165, 514, -132, 18, -1
	83	0.144	1	1	1	1	1	2.678	5	5.177	10, -127, 540, -1158, 1436, -1080, 492, -130, 18, -1
	84	0.144	0.519	1	1	1	2.311	2.678	4.170	5.177	10, -131, 582, -1276, 1580, -1164, 514, -132, 18, -1
	85	0.140	0.425	0.693	1	2	2.257	3.146	3.641	4.698	10, -137, 636, -1421, 1746, -1253, 536, -134, 18, -1
	86	0.139	0.438	1	1	1.382	1.746	3.618	4.115	4.562	10, -135, 612, -1345, 1652, -1202, 524, -133, 18, -1
	87	0.139	0.382	0.830	1	1.746	2.618	2.689	4.115	4.481	10, -138, 644, -1433, 1752, -1254, 536, -134, 18, -1
	88	0.138	0.426	0.632	1.328	1.582	2.344	3.024	3.992	4.534	10, -138, 642, -1432, 1752, -1254, 536, -134, 18, -1
	89	0.137	0.711	1	1	1	1.676	2.768	3.652	6.055	10, -131, 564, -1210, 1488, -1104, 496, -130, 18, -1
	90	0.135	0.572	1	1	1	2.140	2.755	4.296	5.103	10, -134, 592, -1288, 1586, -1165, 514, -132, 18, -1
	91	0.134	0.519	1	1	1	2.311	3.211	4.170	4.655	10, -136, 610, -1337, 1646, -1201, 524, -133, 18, -1
	92	0.132	0.501	0.737	1	1.642	2.385	2.788	3.641	5.174	10, -138, 626, -1376, 1684, -1216, 526, -133, 18, -1
	93	0.129	0.392	1	1	1.522	2.218	3.344	3.900	4.494	10, -142, 660, -1452, 1760, -1255, 536, -134, 18, -1
	94	0.128	0.519	0.630	1	2	2.311	2.797	4.170	4.446	10, -141, 648, -1434, 1752, -1254, 536, -134, 18, -1
	95	0.128	0.382	0.630	1.382	2	2.618	2.797	3.618	4.446	10, -145, 692, -1547, 1866, -1308, 548, -135, 18, -1
	96	0.126	0.410	1	1	1.429	2.423	3.095	4.093	4.424	10, -143, 662, -1453, 1760, -1255, 536, -134, 18, -1
	97	0.124	0.479	0.772	1	1.590	2.535	3.167	3.688	4.644	10, -143, 656, -1442, 1754, -1254, 536, -134, 18, -1
	98	0.123	0.684	1	1	1	1.785	3.097	4.212	5.099	10, -139, 608, -1306, 1594, -1166, 514, -132, 18, -1
	99	0.121	0.349	1	1	2	2.347	3.274	3.532	4.377	10, -149, 712, -1568, 1874, -1309, 548, -135, 18, -1
	100	0.117	0.519	0.759	1	1.667	2.311	3.085	4.170	4.372	10, -146, 666, -1454, 1760, -1255, 536, -134, 18, -1
	101	0.117	0.382	0.759	1.382	1.667	2.618	3.085	3.618	4.372	10, -150, 712, -1568, 1874, -1309, 548, -135, 18, -1
	102	0.115	0.540	1	1	1.271	2.174	3.064	3.739	5.098	10, -146, 654, -1408, 1698, -1218, 526, -133, 18, -1
	103	0.110	0.462	0.670	1.241	2	2.401	3.058	3.712	4.346	10, -153, 716, -1569, 1874, -1309, 548, -135, 18, -1
	104	0.109	0.519	1	1	1.295	2.311	3.317	4.170	4.278	10, -151, 684, -1474, 1768, -1256, 536, -134, 18, -1
	105	0.103	0.437	1	1	1.725	2.506	3.226	3.768	4.236	10, -158, 736, -1590, 1882, -1310, 548, -135, 18, -1
	106	0.098	0.382	0.824	1.382	2	2.618	3.176	3.618	3.902	10, -165, 792, -1716, 2002, -1365, 560, -136, 18, -1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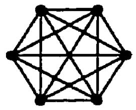
Laplacian spectra of connected graphs, $2 \leq n \leq 6$

n	graph	eigenvalues				characteristic polynomial
2	1	2				2, -1
3	1	3	3			9, -6, 1
	2	1	3			3, -4, 1
4	1	4	4	4		64, -48, 12, -1
	2	2	4	4		32, -32, 10, -1
	3	2	2	4		16, -20, 8, -1
	4	1	3	4		12, -19, 8, -1
	5	1	1	4		4, -9, 6, -1
	6	0.586	2	3.414		4, -10, 6, -1
5	1	5	5	5	5	625, -500, 150, -20, 1
	2	3	5	5	5	375, -350, 120, -18, 1
	3	3	3	5	5	225, -240, 94, -16, 1
	4	2	4	5	5	200, -230, 93, -16, 1
	5	2	3	4	5	120, -154, 71, -14, 1
	6	2	2	5	5	100, -140, 69, -14, 1
	7	2	2	3	5	60, -92, 51, -12, 1
	8	1.586	3	4.414	5	105, -146, 70, -14, 1
	9	1.382	2.382	3.618	4.618	55, -90, 51, -12, 1
	10	1.382	1.382	3.618	3.618	25, -50, 35, -10, 1
	11	1	4	4	5	80, -136, 69, -14, 1
	12	1	3	3	5	45, -84, 50, -12, 1
	13	1	2	4	5	40, -78, 49, -12, 1
	14	1	1	3	5	15, -38, 32, -10, 1
	15	1	1	1	5	5, -16, 18, -8, 1
	16	0.830	2.689	4	4.481	40, -82, 50, -12, 1
	17	0.830	2	2.689	4.481	20, -46, 34, -10, 1
	18	0.697	1.382	3.618	4.303	15, -40, 33, -10, 1
	19	0.519	2.311	3	4.170	15, -44, 34, -10, 1
	20	0.519	1	2.311	4.170	5, -18, 20, -8, 1
	21	0.382	1.382	2.618	3.618	5, -20, 21, -8, 1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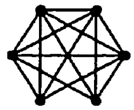
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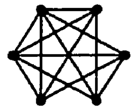
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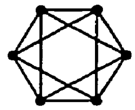
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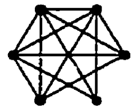
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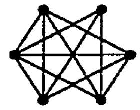
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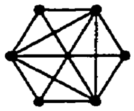
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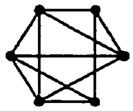
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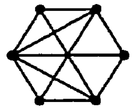
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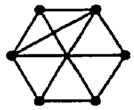
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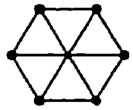
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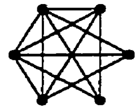
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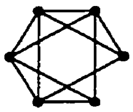
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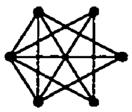
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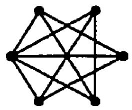
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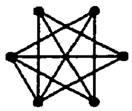
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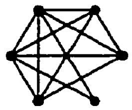
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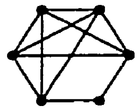
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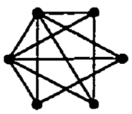
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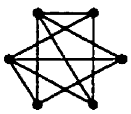
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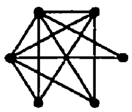
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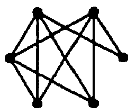
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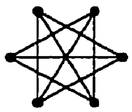
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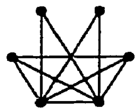
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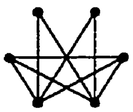
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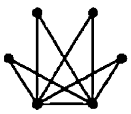
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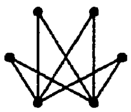
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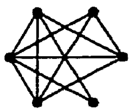
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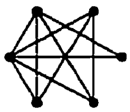
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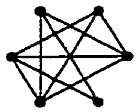
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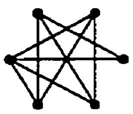
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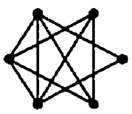
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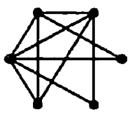
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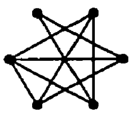
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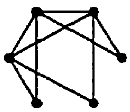
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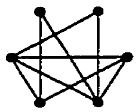
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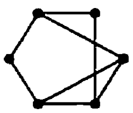
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n	graph	eigenvalues					characteristic polynomial
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	3	4	4	6	6	6	3456, -3456, 1368, -268, 26, -1
	4	4	4	4	6	6	2304, -2496, 1072, -228, 24, -1
	5	3	5	6	6	6	3240, -3348, 1350, -267, 26, -1
	6	3	4	5	6	6	2160, -2412, 1056, -227, 24, -1
	7	3	3	6	6	6	1944, -2268, 1026, -225, 24, -1
	8	3	3	5	5	6	1350, -1665, 804, -190, 22, -1
	9	3	3	4	6	6	1296, -1620, 792, -189, 22, -1
	10	3	3	3	5	6	810, -1107, 594, -156, 20, -1
	11	3	3	3	3	6	486, -729, 432, -126, 18, -1
	12	2.586	4	5.414	6	6	2016, -2328, 1040, -226, 24, -1
	13	2.586	4	4	5.414	6	1344, -1664, 804, -190, 22, -1
	14	2.382	3.382	4.618	5.618	6	1254, -1601, 790, -189, 22, -1
	15	2.382	2.382	4.618	4.618	6	726, -1045, 580, -155, 20, -1
	16	2.268	3	4	5	5.732	780, -1091, 592, -156, 20, -1
	17	2	5	5	6	6	1800, -2220, 1022, -225, 24, -1
	18	2	4	5	5	6	1200, -1580, 788, -189, 22, -1
	19	2	4	4	6	6	1152, -1536, 776, -188, 22, -1
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	22	2	3	4	5	6	720, -1044, 580, -155, 20, -1
	23	2	3	3	5	5	450, -705, 428, -126, 18, -1
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	25	2	2	4	4	6	384, -640, 408, -124, 18, -1
	26	2	2	2	6	6	288, -528, 368, -120, 18, -1
	27	2	2	2	4	6	192, -368, 272, -96, 16, -1
	28	1.830	3.689	5	5.481	6	1110, -1517, 774, -188, 22, -1
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	31	1.786	3	3	4.539	5.675	414, -672, 418, -125, 18, -1
	32	1.697	3.382	4	5.303	5.618	684, -1027, 578, -155, 20, -1
	33	1.697	2.382	4.618	5.303	6	594, -939, 554, -153, 20, -1
	34	1.697	2.382	4	4.618	5.303	396, -659, 416, -125, 18, -1
	35	1.697	1.697	4	5.303	5.303	324, -585, 394, -123, 18, -1
	36	1.607	2.302	3.641	4.863	5.587	366, -628, 406, -124, 18, -1
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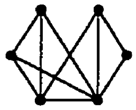
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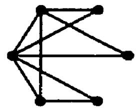
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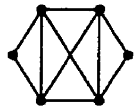
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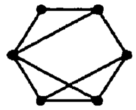
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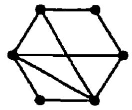
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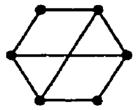
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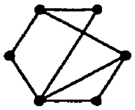
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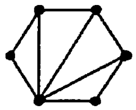
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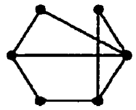
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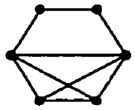
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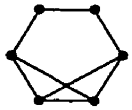
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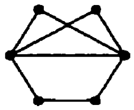
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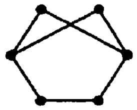
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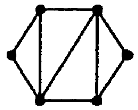
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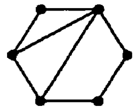
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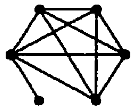
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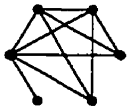
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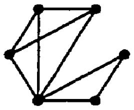
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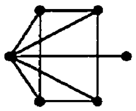
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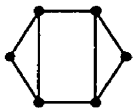
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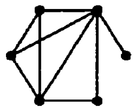
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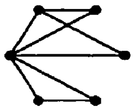
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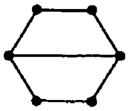
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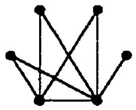
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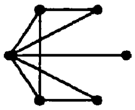
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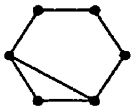
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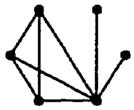
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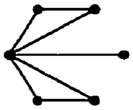
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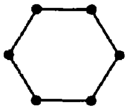
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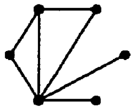
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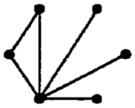
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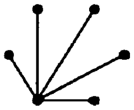
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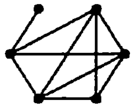
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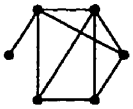
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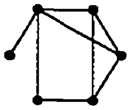
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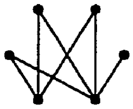
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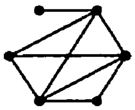
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	46	1.382	1.697	3.618	4	5.303	180, -365, 276, -97, 16, -1
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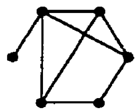
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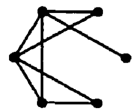
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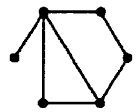
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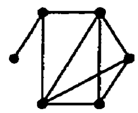
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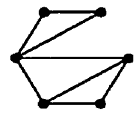
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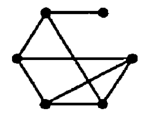
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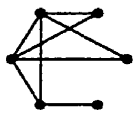
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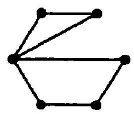
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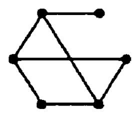
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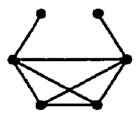
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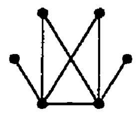
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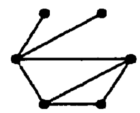
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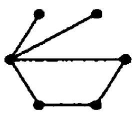
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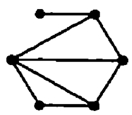
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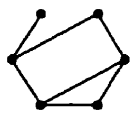
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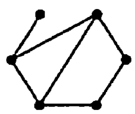
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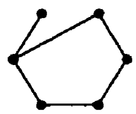
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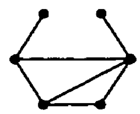
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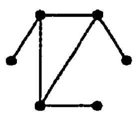
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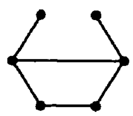
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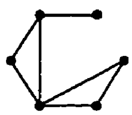
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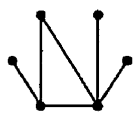
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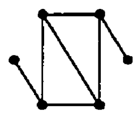
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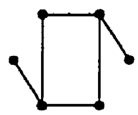
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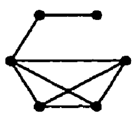
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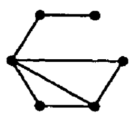
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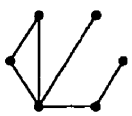
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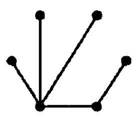
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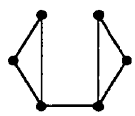
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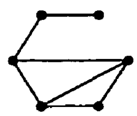
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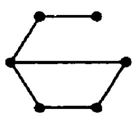
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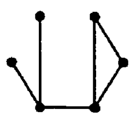
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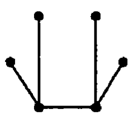
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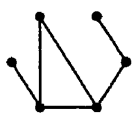
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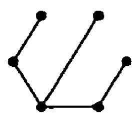
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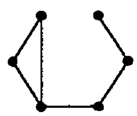
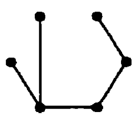
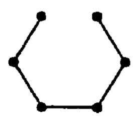

110

111

112

n	graph	eigenvalues					characteristic polynomial
6	75	0.893	2.212	3	4.526	5.369	144, -333, 266, -96, 16, -1
	76	0.885	1.697	3.254	4.861	5.303	126, -305, 256, -95, 16, -1
	77	0.882	1.451	2.534	3.865	5.269	66, -176, 168, -72, 14, -1
	78	0.764	3	4	5	5.236	240, -548, 390, -123, 18, -1
	79	0.764	3	3	4	5.236	144, -348, 274, -97, 16, -1
	80	0.764	3	3	4	5.236	144, -348, 274, -97, 16, -1
	81	0.764	2	3	5	5.236	120, -304, 256, -95, 16, -1
	82	0.764	2	3	3	5.236	72, -192, 176, -73, 14, -1
	83	0.764	2	3	3	5.236	72, -192, 176, -73, 14, -1
	84	0.764	1.268	4	4.732	5.236	96, -264, 244, -94, 16, -1
	85	0.764	1.268	2	4.732	5.236	48, -144, 152, -70, 14, -1
	86	0.764	1	3	4	5.236	48, -148, 158, -71, 14, -1
	87	0.764	1	2	3	5.236	24, -80, 96, -51, 12, -1
	88	0.731	2.135	3.466	4.549	5.118	126, -320, 264, -96, 16, -1
	89	0.722	1.683	3	3.705	4.891	66, -184, 174, -73, 14, -1
	90	0.697	2	2.382	4.303	4.618	66, -185, 174, -73, 14, -1
	91	0.697	1.382	2	3.618	4.303	30, -95, 106, -53, 12, -1
	92	0.697	1.139	2.746	4.303	5.115	48, -149, 158, -71, 14, -1
	93	0.697	0.697	2	4.303	4.303	18, -69, 92, -51, 12, -1
	94	0.657	1	2.529	3	4.814	24, -83, 100, -52, 12, -1
	95	0.631	1.474	3	3.788	5.107	54, -165, 166, -72, 14, -1
	96	0.631	1	1.474	3.788	5.107	18, -67, 88, -50, 12, -1
	97	0.586	1.268	3.414	4	4.732	48, -156, 164, -72, 14, -1
	98	0.586	1.268	2	3.414	4.732	24, -84, 100, -52, 12, -1
	99	0.486	2.428	4	4	5.086	96, -304, 262, -96, 16, -1
	100	0.486	2	2.428	4	5.086	48, -164, 166, -72, 14, -1
	101	0.486	1	2.428	3	5.086	18, -72, 94, -51, 12, -1
	102	0.486	1	1	2.428	5.086	6, -28, 46, -33, 10, -1
	103	0.438	3	3	3	4.562	54, -189, 180, -74, 14, -1
	104	0.438	2	3	4	4.562	48, -172, 172, -73, 14, -1
	105	0.438	2	2	3	4.562	24, -92, 106, -53, 12, -1
	106	0.438	1	3	3	4.562	18, -75, 98, -52, 12, -1
	107	0.438	1	1	3	4.562	6, -29, 48, -34, 10, -1
	108	0.413	1.137	2.359	3.698	4.393	18, -76, 98, -52, 12, -1
	109	0.382	0.697	2	2.618	4.303	6, -31, 52, -35, 10, -1
	110	0.325	1.461	3	3	4.214	18, -84, 104, -53, 12, -1
	111	0.325	1	1.461	3	4.214	6, -32, 52, -35, 10, -1
	112	0.268	1	2	3	3.732	6, -35, 56, -36, 10, -1

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