1
Introduction

In order to make the reading of this book easier, in Section 1.1 we give a survey of the main graph-theoretic terminology and notation. Section 1.2 deals with matrix theory and graph spectra. In Section 1.3 we emphasize some more specific results of the theory of graph spectra that will frequently be used. Once we have fixed the notation and given all the necessary results, in Section 1.4 we say more about the applications of the theory of graph spectra and give some details related to the content of the book.

1.1 Graph-theoretic notions

Let G be a finite undirected graph without loops or multiple edges on n vertices labelled $1,2,\dots,n$. We denote the set of vertices of G by V (or $V(G)$). We say that two vertices i and j are *adjacent* (or *neighbours*) if they are joined by an edge and we write $i \sim j$. We denote the set of edges of G by E (or $E(G)$), where an edge ij belongs to E if and only if $i \sim j$. In this case we say that the edge ij is incident with vertices i and j. A graph consisting of a single vertex is called the *trivial graph*. Two edges are said to be *adjacent* if they are incident with a common vertex. Non-adjacent edges are said to be mutually *independent*. The number of vertices n and edges m in a graph are called the *order* and *size*, respectively.

Two graphs G and H are said to be *isomorphic* if there is a bijection between $V(G)$ and $V(H)$ which preserves the adjacency of their vertices. The fact that G and H are isomorphic we denote by $G \cong H$, but we also use the simple notation $G = H$. A graph is *asymmetric* if the only permutation of its vertices which preserves their adjacency is the identity mapping.

We say that G is the unique graph satisfying given properties if and only if any other graph with the same properties is isomorphic to G.

A graph H obtained from a given graph G by deleting some vertices (together with their edges incident) is called an *induced subgraph* of G. In this case, we also say that H is induced in G, and that G is a *supergraph* of H. We say that a graph G is *H-free* if it does not contain H as an induced subgraph. A *subgraph* of G is any graph H satisfying $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$. If $V(H) = V(G)$, H is called a *spanning subgraph* of G.

If $U \subset V(G)$, then we write $G[U]$ to denote the induced subgraph of G with vertex set U and two vertices being adjacent if and only if they are adjacent in G. Similarly, an induced subgraph of G obtained by deleting a set of vertices $V' \subseteq V(G)$ is denoted by $G - V'$ (rather than $G[V(G)\backslash V']$). If V' consists of a single vertex v, we simply write $G - v$ (instead of $G - \{v\}$). Similarly, $G - E'$ and $G - e$ designate the deletion of a subset of edges E' and a single edge e, respectively. By $G + e$ we denote a graph obtained from G by inserting a single edge. If V_1 and V_2 are disjoint subsets of $V(G)$, then $m(V_1)$ and $m(V_1, V_2)$ stand for the number of edges in $G[V_1]$ and the number of edges with one end in V_1 and the other in V_2, respectively.

The *degree* d_u of a vertex u (in a graph G) is the number of edges incident with it. In particular, the minimal and the maximal vertex degrees are denoted by δ and Δ, respectively. We say that a graph G is *regular* of degree r (or r_G) if all its vertices have degree r. If so, then we usually say that G is r-regular. The *complete graph* on n vertices, K_n, is a graph whose every pair of vertices is joined by an edge. A regular graph of degree 3 is called a *cubic graph*. The unique $(2n-2)$-regular graph on $2n$ $(n \geq 1)$ vertices is called a *cocktail party*, and is denoted by $CP(n)$. Obviously, it is an $(n-1)$-regular graph. A *bidegreed graph* has exactly two distinct vertex degrees. The *edge degree* of an edge uv is defined as $d_u + d_v - 2$ (i.e., it is the number of edges that have a common vertex with uv).

The set of neighbours (or the open neighbourhood) of a vertex u is denoted by $N(u)$. The closed neighbourhood of u is denoted by $N[u]$ $(= \{u\} \cup N(u))$. The average degree of vertices in $N(u)$ is denoted by m_u, and it is also called the *average 2-degree* of u.

A graph is said to be properly coloured if each vertex is coloured so that adjacent vertices have different colours. G is *k-colourable* if it can be properly coloured by k colours. The *chromatic number* χ is k if G is k-colourable and not $(k-1)$-colourable. G is called *bipartite* if its chromatic number is 1 or 2. The vertex set of a bipartite graph can be partitioned into two parts (or colour classes) X and Y such that every edge of G joins a vertex in X with a vertex in Y. A graph is called *complete bipartite* if every vertex in one part is adjacent to every vertex in the other part. If $|X| = n_1$ and $|Y| = n_2$, the complete bipartite

graph is denoted by K_{n_1,n_2}. In particular, if $n_1 = 1$, it is called a *star*. More generally, a *k-partite graph* is a graph whose set of vertices is discomposed into k disjoint sets such that no two vertices within the same set are adjacent. If there are $n_1, n_2, \ldots, n_k$ vertices in the k sets, and if each two vertices which belong to different sets are adjacent, the graph is called *complete k-partite* (or simply *complete multipartite*) and denoted by $K_{n_1,n_2,\ldots,n_k}$.

A graph is called *semiregular bipartite* if it is bipartite and the vertices belonging to the same part have equal degree. If the corresponding vertex degrees are, say, r and s, the graph is referred to as (r,s)-semiregular bipartite.

A vertex of degree 1 (in a graph G) is called an *endvertex* or *pendant vertex*. The edge incident with such a vertex is a *pendant edge*.

A *k-walk* (or simply *walk*) in a graph G is an alternative sequence of vertices and edges $v_1, e_1, v_2, e_2, \ldots, e_{k-1}, v_k$ such that each edge e_i is incident with v_i and v_{i+1} $(1 \leq i \leq k-1)$. The walk is closed if v_1 coincides with v_k. The number of k-walks is denoted by w_k. Similarly, the number of k-walks starting with u (resp. starting with u and ending with v) is denoted by $w_k(u)$ (resp. $w_k(u,v)$).

If all vertices of a walk are distinct, it is called a *path*. A graph which is itself a path on n vertices is denoted by P_n. An endvertex of P_n is often called an *end* of P_n. By joining the ends of P_n by an edge we get a *cycle* C_n. In particular, C_3 is called a *triangle* and C_4 is called a *quadrangle*. The number of triangles in a graph G is denoted by $t(G)$. The *length* of a path P_n or a cycle C_n is equal to the number of edges contained in it. A graph is *Hamiltonian* if it contains a spanning subgraph which is a cycle, while any such cycle is referred to as a *Hamiltonian cycle*.

We say that a graph G is *connected* if every two distinct vertices are the ends of at least one path in G. Otherwise, G is *disconnected* and its maximal connected induced subgraphs are called the *components* of G. A component consisting of a single vertex is called an *isolated vertex* (or *trivial component*) of G. A graph is *totally disconnected* if it consists entirely of isolated vertices. If G has exactly one non-trivial component, this component is called the *dominant component*.

The *distance* $d(u,v)$ between the vertices u and v is the length of the shortest path between u and v, and the *girth* $\mathrm{gr}(G)$ is the length of the shortest cycle induced in G. The *diameter* D of a graph G is the longest distance between two vertices of G. A shortest path between any pair of vertices u and v such that $d(u,v) = D$ is called a *diametral path*.

A connected graph G whose number of edges m equals $n-1$ is called a *tree*. Furthermore, if $m = n - 1 + k$ $(k \geq 1)$, G is said to be *k-cyclic*.

For $k = 1$, the corresponding graph is called *unicyclic*; for $k = 2$, it is called

bicyclic. Clearly, any unicyclic graph contains a unique cycle as an induced subgraph. If this cycle has odd length then the graph is said to be *odd unicyclic*.

Any complete induced subgraph of a graph G is called a *clique*. The *clique number* ω is the number of vertices in the largest clique of G. Similarly, any totally disconnected induced subgraph is called a *co-clique*. The vertices of a co-clique make an *independent set* of vertices of G, and the number of vertices in the largest independent set is called the *independence number*, denoted by α.

A *matching* in G is a set of edges without common vertices. A matching is *perfect* if each vertex of G is incident with an edge from the matching. The *matching number* μ is the maximal size of a matching in G.

A *vertex* (resp. *edge*) cover of a graph G is a set of vertices (resp. edges) such that each edge (resp. vertex) of G is incident with at least one vertex (resp. edge) of the set. The *vertex* (resp. *edge*) *cover number* of G, denoted by β (resp. β'), is the minimum of the cardinalities of all vertex (resp. edge) covers.

A *dominating set* for a graph G is a subset D of $V(G)$ such that every vertex not in D is adjacent to at least one vertex in D. The *domination number* φ is the number of vertices in a smallest dominating set for G.

A *cut vertex* (resp. *cut edge*) of a connected graph is any vertex (resp. edge) whose removal yields a disconnected graph. The *vertex* (resp. *edge*) *connectivity*, denoted by c_v (resp. c_e), of a connected graph is the minimal number of vertices (resp. edges) whose removal gives a disconnected graph.

A *rooted graph* is a graph in which one vertex has been distinguished as the *root*. A pendant vertex of a rooted tree is often called a *terminal vertex*.

For two graphs G and H we define $G \cup H$ to be their disjoint union.[1] In addition, we use kG to denote the disjoint union of k copies of G. The *join* $G \nabla H$ is the graph obtained by joining every vertex of G with every vertex of H. In particular, $K_1 \nabla G$ is called the *cone* over G.

The *complement* of a graph G is a graph $\overline{G}$ with the same vertex set as G, in which any two distinct vertices are adjacent if and only if they are non-adjacent in G.

[1] With no confusion, we use the same symbol to denote the union of two sets. In addition, $\sqcup$ will stand for the union of disjoint sets.

1.1.1 Some graphs

The vertex with maximal degree in the star $K_{1,n}$ is called the *centre* of the star. The *double star* $DS(n_1,n_2)$ is a graph obtained from the stars K_{1,n_1-1} and K_{1,n_2-1} by inserting an edge between their centres.

A *starlike tree* $S_{i_1,i_2,\dots,i_k}$ is a tree with exactly one vertex of degree greater than two such that the removal of this vertex gives rise to paths $P_{i_1}, P_{i_2}, \dots, P_{i_k}$. For $k=3$, the corresponding starlike tree is often called a *T-shape tree*.

A *caterpillar* is a tree in which the removal of all pendant vertices gives a path. Let the vertices of a path P_k $(k \geq 3)$ be labelled $1,2,\dots,k$ (in natural order), then $T(m_2,m_3,\dots,m_{k-1})$ denotes the caterpillar obtained by attaching m_i pendant vertices at the ith vertex of P_k $(2 \leq i \leq k-1)$. If a caterpillar is obtained by attaching just a few pendant vertices at the same path, we use the shorter notation $T_n^{i_1,i_2,\dots,i_l}$, where n denotes the order and i_j $(1 \leq j \leq l)$ indicates attaching a pendant vertex at the vertex labelled i_j $(2 \leq i_j \leq k-1)$. A *closed caterpillar* is a unicyclic graph in which the removal of all pendant vertices gives a cycle.

An *open quipu* is a tree with maximal vertex degree 3 such that all vertices of degree 3 lie on a path. A *closed quipu* is a unicyclic graph with maximal vertex degree 3 such that all vertices of degree 3 lie on a cycle.

A *cactus* is a connected graph G such that any two cycles induced in G have at most one common vertex.

The *comet* $C(k,l)$ is a tree obtained by attaching k pendant vertices at one end of the path P_l. The *double comet* $DC(k,l)$ is a tree obtained by attaching k pendant vertices at one end of the path P_l and another k pendant vertices at the other end of the same path.

The *kite* $K(k,l)$ is a graph obtained by identifying one end of the path P_{l+1} with a vertex of the complete graph K_k. The *double kite* $DK(k,l)$ is a graph obtained by identifying one end of the path P_{l+2} with a vertex of the complete graph K_k and the other end of the same path with a vertex of another complete graph K_k.

The *pineapple* $P(k,l)$ is a graph obtained by attaching l pendant vertices at a vertex of K_k.

$C(k,l)$, $K(k,l)$, and $P(k,l)$ have $k+l$ vertices, while $DC(k,l)$ and $DK(k,l)$ have $2k+l$ vertices.

Let $G^D = G^D(n_1,n_2,\dots,n_{D+1})$ denote the graph defined as follows: $V(G^D) = \bigcup_{i=1}^{D+1} V_i$, where $G^D[V_i] \cong K_{n_i}$ $(1 \leq i \leq D+1)$ and

$$G^D[V_i \cup V_j] \cong \begin{cases} K_{n_i+n_j}, & \text{if } |i-j|=1, \\ K_{n_i} \cup K_{n_j}, & \text{otherwise.} \end{cases}$$

The graph G^D consists of a chain of $D+1$ cliques $K_{n_1}, K_{n_2}, \ldots, K_{n_{D+1}}$, where neighbouring cliques are fully interconnected (i.e., each vertex in one is adjacent to all vertices in the other). According to this, we name this graph the *clique chain graph*. Its order is $n = \sum_{i=1}^{D+1} n_i$.

Similarly, let $G_*^D = G_*^D(n_1, n_2, \ldots, n_{D+1})$ denote the graph of the same order defined as follows: $V(G_*^D) = \bigcup_{i=1}^{D+1} V_i$, where $G_*^D[V_i] \cong n_i K_1$ $(1 \leq i \leq D+1)$ and

$$G_*^D[V_i \cup V_j] \cong \begin{cases} K_{n_i,n_j}, & \text{if } |i-j|=1, \\ (n_i+n_j)K_1, & \text{otherwise.} \end{cases}$$

This graph consists of a chain of $D+1$ co-cliques $n_1K_1, n_2K_1, \ldots, n_{D+1}K_1$, where neighbouring co-cliques are fully interconnected. We name it the *co-clique chain graph*. Observe that G_*^D is bipartite.

Recall that a *multigraph* includes the possible existence of multiple edges between any two vertices or loops (i.e. edges with both endvertices identical). We say that a *petal* is added to a graph when we add a pendant vertex and then duplicate the edge incident with it.

The *line graph*[2] $\mathrm{Line}(G)$ of a multigraph G is the graph whose vertices are the edges of G, with two vertices adjacent whenever the corresponding edges have exactly one common vertex.

Let G be a graph with vertex set $V = \{v_1, v_2, \ldots, v_n\}$, and let $a_1, a_2, \ldots, a_n$ be non-negative integers. The *generalized line graph* $\mathrm{Line}(G; a_1, a_2, \ldots, a_n)$ is the graph $\mathrm{Line}(\widehat{G})$, where $\widehat{G}$ is the multigraph $G(a_1, a_2, \ldots, a_n)$ obtained from G by adding a_i petals at vertex v_i $(1 \leq i \leq n)$.

We introduce two classes of graphs called nested split graphs and double nested graphs. For these two classes of graphs we use the common name *nested graphs*.

A *nested split graph* (NSG for short) is a graph which does not contain any of the graphs P_4, C_4 or $2K_2$ as an induced subgraph. This name is derived from its structure; it is also called a *threshold graph* (for more details, see [409]). We describe the structure of connected NSGs. The vertex set of any such graph consists of a co-clique and a clique, where both the co-clique and the clique are partitioned into h cells $U_1, U_2, \ldots, U_h$ and $V_1, V_2, \ldots, V_h$, respectively. Then

[2] The line graph is often denoted by $L(G)$, but in this book $L(G)$ is reserved for the Laplacian matrix (see Section 1.2).

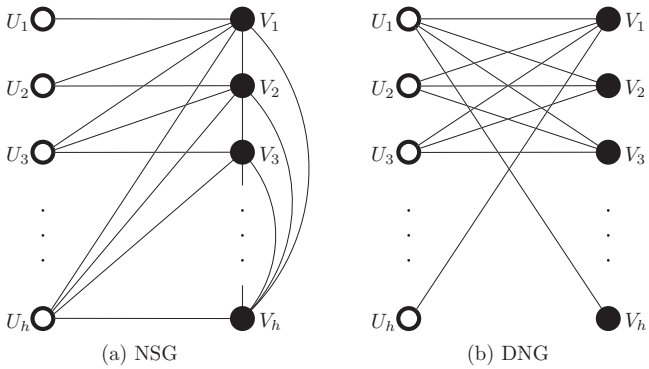

Figure 1.1 The structure of nested graphs.

all vertices in the co-clique U_i $(1 \le i \le h)$ are joined to all vertices in $V_1 \cup V_2 \cup \cdots \cup V_i$, so if $u \in U_i$ and $v \in U_{i+1}$ then $N(u) \subset N(v)$, which explains the nesting property.

A *double nested graph* (DNG for short) is a bipartite graph which does not contain any of the graphs P_4, C_4 or $2K_2$ as an induced subgraph (in [42] these graphs are called *chain graphs*). The nesting property of connected DNGs can be described in a similar way: the vertices of two parts are partitioned into the same h cells as above, and all vertices in U_i $(1 \le i \le h)$ are joined by cross edges to all vertices in $V_1 \cup V_2 \cup \cdots \cup V_{h+1-i}$.

The structure of nested graphs is illustrated in Fig. 1.1. In both cases let $m_i = |U_i|$ and $n_i = |V_i|$ $(1 \le i \le h)$, then any nested graph is determined by the following $2h$ parameters:

$$(m_1, m_2, \ldots, m_h; n_1, n_2, \ldots, n_h).$$

If we denote

$$M_s = \sum_{i=1}^{s} m_i, \quad N_t = \sum_{i=1}^{t} n_i \quad (1 \le s,t \le h),$$

we can easily see that the order of a nested graph is $n = M_h + N_h$ and the size of an NSG (resp. DNG) is $m = \sum_{i=1}^{h} m_i N_i + \binom{N_h}{2}$ (resp. $m = \sum_{i=1}^{h} m_i N_{h+1-i}$). For an NSG, the degree of a vertex $u \in U_i$ is equal to N_i and the degree of a vertex $v \in V_i$ is equal to $n - 1 - M_{i-1}$. For a DNG, these degrees are equal to N_{h+1-i} and M_{h+i-1}, respectively.

1.2 Spectra of graphs

In this section we introduce three matrices associated with graphs (the adjacency matrix, the Laplacian matrix, and the signless Laplacian matrix) and give some basic results related to their spectra. Another three matrices are considered later in Chapter 9.

We start with a small portion of the matrix theory. Let M be an $n \times n$ real matrix. If the eigenvalues of M are real (which, e.g., occurs if M is symmetric), they can be given in non-increasing order as

$$\nu_1\ (=\nu_1(M)) \geq \nu_2\ (=\nu_2(M)) \geq \cdots \geq \nu_n\ (=\nu_n(M)).$$

Here are some results that come from the Perron–Frobenius theory of non-negative matrices (for more details, see [317, Chapter 8]).

A symmetric matrix M is *reducible* if there exists a permutation matrix P such that $P^{-1}MP = \begin{pmatrix} B_1 & 0 \\ 0 & B_2 \end{pmatrix}$, where B_1 and B_2 are square matrices. Otherwise, M is called *irreducible*.

Theorem 1.1 ([98, Theorem 0.6] or [102, Theorem 1.3.6]) *Let M be a real irreducible symmetric matrix with non-negative entries. Then its largest eigenvalue ν_1 is simple, while the coordinates of any eigenvector of ν_1 are non-zero and of the same sign. In addition, $|\nu| \leq \nu_1$ for all eigenvalues ν of M.*

Moreover, the largest eigenvalue of any principal submatrix of M is less than ν_1.

Theorem 1.2 (cf. [317, p. 668]) *For any real symmetric matrix $M = (m_{ij})$ with non-negative entries,*

$$\min_{1\leq i\leq n} \sum_{j=1}^{n} m_{ij} \leq \nu_1(M) \leq \max_{1\leq i\leq n} \sum_{j=1}^{n} m_{ij}.$$

If M is irreducible then each inequality holds if and only if all row sums in M are equal.

Following [102, pp. 11–12], we give a technique which is frequently used for bounding graph eigenvalues. The *Rayleigh quotient* for a real symmetric matrix M is a scalar

$$\frac{\mathbf{y}^T M \mathbf{y}}{\mathbf{y}^T \mathbf{y}}, \tag{1.1}$$

where $\mathbf{y}$ is a non-zero vector in $\mathbb{R}^n$. The supremum of such scalars is the largest eigenvalue of M, and the infimum is the least eigenvalue of M. In other words,

$$\nu_1 = \sup\{\mathbf{y}^T A\mathbf{y} \ : \ \mathbf{y} \in \mathbb{R}^n, ||\mathbf{y}|| = 1\}, \tag{1.2}$$

$$\nu_n = \inf\{\mathbf{y}^T A\mathbf{y} \ : \ \mathbf{y} \in \mathbb{R}^n, ||\mathbf{y}|| = 1\}. \tag{1.3}$$

The *Rayleigh principle* can be stated as follows. If $\{\mathbf{x_1}, \mathbf{x_2}, \dots, \mathbf{x_n}\}$ is an orthonormal basis of the eigenvectors of M and if a non-zero vector $\mathbf{y}$ is spanned by $\{\mathbf{x_i}, \mathbf{x_{i+1}}, \dots, \mathbf{x_n}\}$, then

$$\nu_i \geq \frac{\mathbf{y}^T M\mathbf{y}}{\mathbf{y}^T\mathbf{y}},$$

with equality if and only if $M\mathbf{y} = \nu_i\mathbf{y}$; if a non-zero vector $\mathbf{y}$ is spanned by $\{\mathbf{x_1}, \mathbf{x_2}, \dots, \mathbf{x_i}\}$, then

$$\nu_i \leq \frac{\mathbf{y}^T M\mathbf{y}}{\mathbf{y}^T\mathbf{y}},$$

with equality if and only if $M\mathbf{y} = \nu_i\mathbf{y}$.

We establish some inequalities with wide application in the theory of graph spectra.

Theorem 1.3 (Courant–Weyl Inequalities, cf. [102, Theorem 1.3.15]) *Let M and N be $n \times n$ real symmetric matrices. Then*

$$\nu_i(M+N) \leq \nu_j(M) + \nu_{i-j+1}(N) \ \ (n \geq i \geq j \geq 1),$$

$$\nu_i(M+N) \geq \nu_j(M) + \nu_{i-j+n}(N) \ \ (1 \leq i \leq j \leq n).$$

We use I, J, and O to denote a unit, all-1, and all-0 matrix, respectively. Somewhere, the size of any of these matrices will be given in subscript. The $n \times 1$ all-1 vector is denoted $\mathbf{j}$.

If a graph G has n vertices and m edges, then the *vertex–edge incidence matrix* $R\ (= R(G))$ is an $n \times m$ matrix whose rows and columns are indexed by the vertices and edges of G, that is, the (i,e)-entry is

$$r_{i,e} = \begin{cases} 1, & \text{if } i \text{ is incident with } e, \\ 0, & \text{otherwise.} \end{cases}$$

We are now in a position to consider the above introduced matrices as they are associated with graphs.

1.2.1 Spectrum of a graph

The *adjacency matrix* A (or $A(G)$) of G is defined as $A = (a_{i,j})$, where

$$a_{i,j} = \begin{cases} 1, & \text{if } i \sim j, \\ 0, & \text{otherwise.} \end{cases}$$

The characteristic polynomial of A, $P_G = \det(xI - A)$, is also called the *characteristic polynomial* of G, while its roots are just the *eigenvalues* of G. The collection of eigenvalues of G (with repetition) is called the *spectrum* of G. We denote the eigenvalues of G by

$$\lambda_1\ (=\lambda_1(G)), \lambda_2\ (=\lambda_2(G)), \ldots, \lambda_n\ (=\lambda_n(G)),$$

and we assume that $\lambda_i \geq \lambda_j$ whenever $i < j$. According to this, the spectrum of G may be denoted $[\lambda_1'^{i_1}, \lambda_2'^{i_2}, \ldots, \lambda_k'^{i_k}]$, where $\lambda_1', \lambda_2', \ldots, \lambda_k'$ are the distinct eigenvalues while the exponents stand for their multiplicities.

The largest eigenvalue λ_1 is called the *spectral radius* or the *index* of G. For any non-negative integer k, the kth *spectral moment* of G is $M_k = \sum_{i=1}^{n} \lambda_i^k$. Note that M_k is equal to the trace $\mathrm{tr}(A^k)$.

The *spectral spread* σ of a graph G is the difference between its largest and least eigenvalue, that is, $\sigma = \lambda_1 - \lambda_n$. Similarly, the *spectral gap* η is the difference between the two largest eigenvalues, $\eta = \lambda_1 - \lambda_2$.

Any eigenvalue λ of G satisfies

$$A\mathbf{x} = \lambda\mathbf{x}, \tag{1.4}$$

for some non-zero vector $\mathbf{x} \in \mathbb{R}^n$. Each vector that satisfies (1.4) is called an *eigenvector* of G, and for $\mathbf{x} = (x_1, x_2, \ldots, x_n)^T$ it is usually assumed that the coordinate x_i (which is also called the weight) corresponds to the vertex i ($1 \leq i \leq n$). The *eigenvalue equation* of G follows from (1.4) and reads

$$\lambda x_i = \sum_{j \sim i} x_j \quad (1 \leq i \leq n).$$

If $\mathbf{x_1}, \mathbf{x_2}, \ldots, \mathbf{x_n}$ is a complete system of mutually orthogonal normalized eigenvectors of A belonging to the spectrum $[\lambda_1, \lambda_2, \ldots, \lambda_n]$, $X = (\mathbf{x_1}, \mathbf{x_2}, \ldots, \mathbf{x_n})$,