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APPLICATIONS OF GRAPH SPECTRA: AN INTRODUCTION TO THE LITERATURE

Abstract. We give basic definitions and some results related to the theory of graph spectra. We present a short survey of applications of this theory. In addition, selected bibliographies on applications to particular branches of science are given.

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Contents

This is an introductory chapter to our book. We start with basic definitions and present some results from the theory of graph spectra. A short survey of applications of this theory is presented. Selected bibliographies on applications to particular branches of science are given in the sequel.

The plan of the chapter is as follows.

Section 1 presents basic definitions related to the theory of graph spectra. Some selected results, which will bi used in other chapters, are given in Section 2. A short survey of applications of graph eigenvalues is contained in Section 3. Section 4 contains selected bibliographies of books and papers which are related to applications of the theory of graph spectra in Chemistry, Physics, Computer Science, Engineering, Biology and Economics.

1. Basic notions

A graph $G = (V, E)$ consists of a finite non-empty set V (the vertex set of G), and a set E (of two elements subsets of V, the edge set of G). We also write $V(G)$ ($E(G)$) for the vertex (resp. edge) set of G. The number of elements in $V(G)$, denoted by n ($= |V(G)|$), is called the *order* of G. Usually, we shall assume that $V(G) = \{1, 2, \ldots, n\}$.

Let e_{ij} be the edge connecting vertices i and j. The set $\{e_{i_1 j_1}, e_{i_2 j_2}, \ldots, e_{i_k j_k}\}$ of distinct edges, such that $i = i_1, j_1 = i_2, j_2 = i_3, \ldots, j_k = j$, is called *path* (of *length* k) connecting vertices i and j. The length of the shortest path connecting i and j is called the *distance* between these two vertices. The maximum distance between any two vertices in G is called the *diameter* of G, and it is denoted by D. If there exists a path between any two vertices in G, then G is *connected*; otherwise it is *disconnected*.

Two vertices are called *adjacent* (or *neighbors*) if they are connected by an edge; the corresponding relation between vertices is called the *adjacency relation*. The number of neighbors of a vertex i, denoted by d_i, is its *vertex degree*. The maximum vertex degree (of G) is denoted by Δ. A graph in which all vertex degrees are equal to r is *regular* of degree r (or r-*regular*, or just *regular* if r is unimportant).

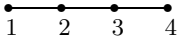
The *adjacency matrix* A is used to represent the adjacency relation, and so the graph G itself. The element a_{ij} of the adjacency matrix A is equal to 1 if vertices i and j are adjacent, and 0 otherwise.

The characteristic polynomial $\det(xI - A)$ of the adjacency matrix A (of G) is called the *characteristic polynomial of* G, and is denoted by $P_G(x)$. The eigenvalues of A (i.e., the zeros of $\det(xI - A)$), and the spectrum of A (which consists of the n eigenvalues) are also called the *eigenvalues* and the *spectrum* of G, respectively. The eigenvalues of G are usually denoted by $\lambda_1, \lambda_2, \ldots, \lambda_n$; they are real because A is symmetric. Unless we indicate otherwise, we shall assume that $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$. We also use the notation $\lambda_i = \lambda_i(G)$ for $i = 1, 2, \ldots, n$. The largest eigenvalue, i.e., λ_1, is called the *index* of G.

If λ is an eigenvalue of G, then a non-zero vector $\mathbf{x} \in \mathbb{R}^n$, satisfying $A\mathbf{x} = \lambda\mathbf{x}$, is called an *eigenvector* of A (or of the labeled graph G) for λ; it is also called a λ-*eigenvector*. The relation $A\mathbf{x} = \lambda\mathbf{x}$ can be interpreted in the following way: if $\mathbf{x} = (x_1, x_2, \ldots, x_n)^T$, then for any vertex u we have $\lambda x_u = \sum_{v \sim u} x_v$, where the summation is over all neighbours v of u. If λ is an eigenvalue of G, then the set $\{\mathbf{x} \in \mathbb{R}^n : A\mathbf{x} = \lambda\mathbf{x}\}$ is a subspace of $\mathbb{R}^n$, called the *eigenspace* of G for λ; it is denoted by $\mathcal{E}(\lambda)$. Such eigenspaces are called *eigenspaces* of G.

For the index of G, since A is non-negative, there exists an eigenvector whose all entries are non-negative.

Example. Let G be the graph shown in Fig. 1 together with its adjacency matrix.



$$A = \begin{vmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{vmatrix}$$

FIGURE 1. An example

For G we have

$$P_G(\lambda) = \begin{vmatrix} \lambda & -1 & 0 & 0 \\ -1 & \lambda & -1 & 0 \\ 0 & -1 & \lambda & -1 \\ 0 & 0 & -1 & \lambda \end{vmatrix} = \lambda^4 - 3\lambda^2 + 1\,.$$

Eigenvalues of G are

$$\frac{1+\sqrt{5}}{2} \approx 1.6180, \qquad \frac{-1+\sqrt{5}}{2} \approx 0.6180,$$
$$\frac{1-\sqrt{5}}{2} \approx -0.6180, \qquad \frac{-1-\sqrt{5}}{2} \approx -1.6180.$$

The following vector $\mathbf{x} = (1, \lambda, \lambda^2 - 1, \lambda^3 - 2\lambda)^T$ is a λ-eigenvector of G. □

Besides the spectrum of the adjacency matrix of a graph G we shall consider the spectrum of another matrix associated with G. The matrix $L = D - A$, where $D = \mathrm{diag}(d_1, d_2, \ldots, d_n)$ is the diagonal matrix of vertex degrees, is known as the *Laplacian* of G. The matrix L is positive semi-definite, and therefore its eigenvalues are non-negative. The least eigenvalue is always equal to 0; the second least eigenvalue is also called the *algebraic connectivity* of of G [Fie].

The basic reference for the theory of graph spectra is the book [CvDSa]. Other books on graph spectra include [CvDGT], [CvRS1], [CvRS3], [CvRS4]. For any notion, not defined here, the reader is referred to [CvRS4] or [CvDSa].

As usual, K_n, C_n, S_n and P_n denote respectively the *complete graph*, the *cycle*, the *star* and the *path* on n vertices; K_{n_1,n_2} denotes the *complete bipartite* graph on $n_1 + n_2$ vertices.

A *tree* is a connected graph without cycles. A connected graph with n vertices and n edges is a *unicyclic graph*. It is called *even* (*odd*) if its unique cycle is even (resp. odd). A *dumbbell* is the graph obtained from two disjoint cycles by joining them by a path.

The *complement* of a graph G is denoted by $\overline{G}$, while mG denotes the union of m disjoint copies of G.

For $v \in V(G)$, $G - v$ denotes the graph obtained from G by deleting v, and all edges incident with it. More generally, for $U \subseteq V(G)$, $G - U$ is the subgraph of G obtained from G by deleting all vertices from U and edges incident to at least one vertex of U; we also say that G_U is induced by the vertex set $V(G) \setminus U$.

The *join* $G \nabla H$ of (disjoint) graphs G and H is the graph obtained from G and H by joining each vertex of G with each vertex of H. For any graph G, the *cone* over G is the graph $K_1 \nabla G$.

The *line graph* $L(H)$ of any graph H is defined as follows. The vertices of $L(H)$ are the edges of H and two vertices of $L(H)$ are adjacent whenever the corresponding edges of H have a vertex of H in common.

A set of disjoint edges in a graph G is called a *matching*. A set of disjoint edges which cover all vertices of the graph is called an 1-*factor* of G.

2. Some results

We present here some known results from the theory of graph spectra that will be used in other chapters.

In graph theory and in the theory of graph spectra, some special types of graphs are studied in detail and their characteristics are well known and summarized in the literature (see, for example, [CvDSa]). Here, we will survey some of them.

Recall, K_n is a complete graph, i.e., a graph with each two vertices connected by an edge (so, the number of edges is equal to $\binom{n}{2}$). The spectrum of K_n consists of $m = 2$ distinct eigenvalues: $\lambda_1 = n - 1$ which is a simple eigenvalue, and $\lambda_i = -1$ for $i = 2, \ldots, n$.

A *path* P_n is a tree on n vertices (and $n - 1$ edges) without vertices of degree greater than two. Two "ending" vertices (for $n \geqslant 2$) have degree one, while the rest

of them (the internal vertices) have degree two. A spectral characteristic of paths is that they have all distinct eigenvalues. In fact, the spectrum of P_n consists of the following eigenvalues: $2\cos\frac{\pi}{n+1}i,\ \ i=1,2,\ldots,n$.

The C_n is a 2-regular connected graph. It contains the following eigenvalues: $2\cos\frac{2\pi}{n}i,\ \ i=0,1,\ldots,n-1$. It has $m=\lfloor\frac{n}{2}\rfloor+1$ distinct eigenvalues. Here $\lfloor x\rfloor$ denotes the largest integer smaller than or equal to x.

The star S_n is a tree having a vertex (central vertex) which is adjacent to all remaining vertices (all of them being of degree one). Each star on $n\geqslant 3$ vertices has $m=3$ distinct eigenvalues. It contains the following eigenvalues: $\pm\sqrt{n-1}$ which are both simple, and $\lambda_i=-1$ for $i=2,\ldots,n-1$.

A complete bipartite graph K_{n_1,n_2} consists of n_1+n_2 vertices divided into two sets of the cardinalities n_1 and n_2 with the edges connecting each vertex from one set to all the vertices in the other set. This means that the number of edges is n_1n_2. In particular, $S_n=K_{1,n-1}$. More generally, *bipartite* graphs consist of two sets of vertices with the edges connecting a vertex from one set to a vertex in the other set. The spectrum of K_{n_1,n_2} (for $n_1+n_2\geqslant 3$) also consists of $m=3$ distinct eigenvalues (simple eigenvalues $\pm\sqrt{n_1n_2}$, and 0 of multiplicity n_1+n_2-2).

In the theory of graph spectra an important role play the graphs with $\lambda_1=2$, known as Smith graphs. They are well studied, and all of them are given in [CvDSa], on Fig. 2.4, p. 79. There are 6 types of Smith graphs (namely, C_n ($n\geqslant 3$), W_n ($n\geqslant 6$), S_5 H_7, H_8 and H_9 – see also Fig. 2). Four of them are concrete graphs S_5, H_7, H_8 and H_9, while the remaining two types (cycles C_n and *double-head snakes* W_n, of order n, can have an arbitrary number of vertices); in Fig. 2 we reproduce those which are not cycles C_n, nor the star $S_5=K_{1,4}$.

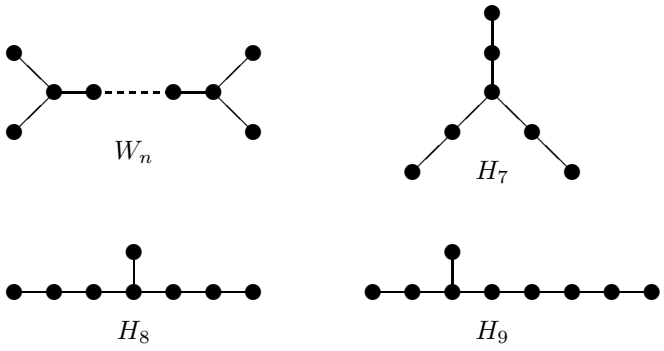


FIGURE 2. Some Smith graphs

In our study we need also graphs with $\lambda_1<2$. To obtain such graphs, it is enough to study (connected) subgraphs of Smith graphs. By removing vertices out of Smith graphs, we obtain paths P_n, $n=2,3,\ldots$; *single-head snakes* Z_n, $n=4,5,\ldots$, given in the upper row of Fig. 3 up to $n=7$; and the three other graphs given in the second row of Fig. 3 and denoted by E_6, E_7 and E_8. It is enough to consider only one vertex removal; removing further vertices leads to the graph already obtained in another way.

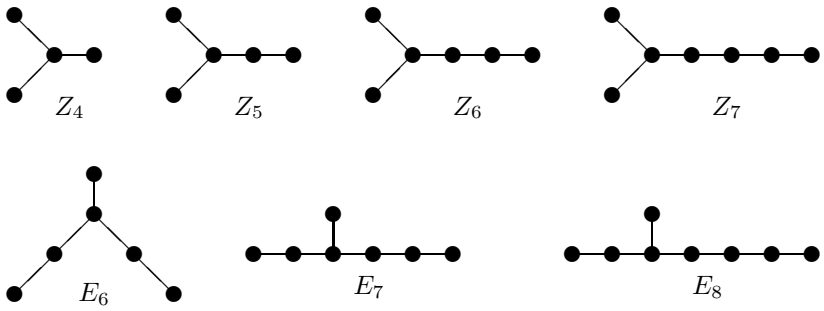


FIGURE 3. Subgraphs of some Smith graphs

By Theorem 3.13. from [CvDSa] for the diameter D of a graph G we have

$$D \leqslant m - 1, \tag{1}$$

where m is the number of distinct eigenvalues.

The largest eigenvalue λ_1 of G and the maximum vertex degree Δ are related in the following way (cf. [CvDSa, p. 112 and p. 85]):

$$\sqrt{\Delta} \leqslant \lambda_1 \leqslant \Delta. \tag{2}$$

A graph is called *strongly regular* with parameters (n, r, e, f) if it has n vertices and is r-regular, and if any two adjacent (non-adjacent) vertices have exactly e (resp. f) common neighbors [CvDSa]. One can show that the number n of vertices of a strongly regular graph is determined by the remaining three parameters. Note that a complement of a strongly regular graph is also a strongly regular graph. Usually, strongly regular graphs which are disconnected, or whose complements are disconnected are excluded from considerations (trivial cases). Under this assumption, the diameter of a strongly regular graph is always equal to 2, and also it has 3 distinct eigenvalues.

A graph is called *integral* if its spectrum consists entirely of integers. Each eigenvalue has integral eigenvectors and each eigenspace has a basis consisting of such eigenvectors.

Graphs with a small number of distinct eigenvalues have attracted much attention in the research community.

The number of distinct eigenvalues of a graph is correlated with its symmetry property [CvDSa]: the graphs with a small number of distinct eigenvalues are (very frequently) highly symmetric. They also have a small diameter, what follows from (1). Let m be the number of distinct eigenvalues of a graph G. Trivial cases are $m = 1$ and $m = 2$. If $m = 1$, all eigenvalues are equal to 0 and G consists of isolated vertices. In the case $m = 2$ G consists of, say $k \geqslant 1$ copies of complete graphs on $s \geqslant 2$ vertices (so the distinct eigenvalues are $s - 1$ (of multiplicity k) and -1 (of multiplicity $k(s - 1)$)).

Further, we shall consider only connected graphs. If $m = 3$ and G is regular, then G is strongly regular (cf. [CvDSa, p. 108]). For example, the well known

Petersen graph (see Fig. 4) is strongly regular with distinct eigenvalues $3, 1, -2$ of multiplicities $1, 5, 4$, respectively.

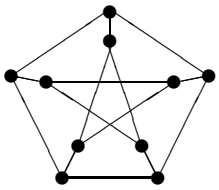


FIGURE 4. The Petersen graph

It is difficult to construct families of strongly regular graphs which contain graphs for any number of vertices. It could be rather expected that one can find sporadic examples with nice properties like it appears in the Petersen graph.

There are also some non-regular graphs with three distinct eigenvalues [Dam]. Such graphs usually have a vertex adjacent to all other vertices (like in stars), i.e., they are cones over some other graphs.

Several classes of regular graphs with four distinct eigenvalues are described in [Dam], but the whole set has not been described yet.

3. A survey of applications

In this section we shall give a short survey of applications of the theory of graph spectra.

The applications are numerous so that we cannot give a comprehensive survey in limited space that we have at the disposal. We shall rather limit ourselves to review representative examples of applications so that the reader can get an impression on the situation but also to become able to use the literature.

The books [CvDSa], [CvDGT] contain each a chapter on applications of graph eigenvalues.

The book [CvRS4] also contains a chapter on applications . There are sections on Physics, Chemistry, Computer Sciences and Mathematics itself.

We shall first mention applications to Chemistry, Physics, Computer Sciences and Mathematics itself (we devote a subsection of this section to each). Graph spectra are used in many other branches of science including Biology, Geography, Economics and Social Sciences and the fifth subsection contains some information about that. In all fields we are forced to give only examples of applications.

3.1. Chemistry. Motivation for founding the theory of graph spectra has come from applications in Chemistry and Physics.

The paper [Huc] is considered as the first paper where graph spectra appear though in an implicit form. The first mathematical paper on graph spectra [CoSi] was motivated by the membrane vibration problem i.e., by approximative solving of partial differential equations.

One of the main applications of graph spectra to Chemistry is the application in a theory of unsaturated conjugated hydrocarbons known as the *Hückel molecular*

orbital theory. Some basic facts of this theory are given at the beginning of the chapter "Selected Topics from the Theory of Graph Energy" in this book.

More detail on the Hückel molecular orbital theory the interested reader can find, for example, in books [CvDSa], [Bal], [CoLM], [Dia], [GrGT], [Gut], [GuTr], [Tri]. For more references to the Hückel theory as well as to other chemical applications see Section 4.

Three separate chapters of this book are devoted to applications in Chemistry.

3.2. Physics. Treating the membrane vibration problem by approximative solving of the corresponding partial differential equation leads to consideration of eigenvalues of a graph which is a discrete model of the membrane (see [CvDSa, Chapter 8]).

The spectra of graphs, or the spectra of certain matrices which are closely related to adjacency matrices appear in a number of problems in statistical physics (see, for example, [Kas], [Mon], [Per]). We shall mention the so-called *dimer problem*.

The dimer problem is related to the investigation of the thermodynamic properties of a system of diatomic molecules ("dimers") adsorbed on the surface of a crystal. The most favorable points for the adsorption of atoms on such a surface form a two-dimensional lattice, and a dimer can occupy two neighboring points. It is necessary to count all ways in which dimers can be arranged on the lattice without overlapping each other, so that every lattice point is occupied.

The dimer problem on a square lattice is equivalent to the problem of enumerating all ways in which a chess-board of dimension $n \times n$ (n being even) can be covered by $\frac{1}{2}n^2$ dominoes, so that each domino covers two adjacent squares of the chess-board and that all squares are so covered.

A graph can be associated with a given adsorption surface. The vertices of the graph represent the points which are the most favorable for adsorption. Two vertices are adjacent if and only if the corresponding points can be occupied by a dimer. In this manner an arrangement of dimers on the surface determines a 1-factor in the corresponding graph, and vice versa. Thus, the dimer problem is reduced to the task of determining the number of 1-factors in a graph. Enumeration of 1-factors involves consideration of walks in corresponding graphs and graph eigenvalues (see [CvDSa, Chapter 8]).

Not only the dimer problem but also some other problems can be reduced to the enumeration of 1-factors (i.e. dimer arrangements). The best known is the famous *Ising problem* arising in the theory of ferromagnetism (see, for example, [Kas], [Mon]).

The graph-walk problem is of interest in physics not only because of the 1-factor enumeration problem. The numbers of walks of various kinds in a lattice graph appear in several other problems: the random-walk and self-avoiding-walk problems (see [Kas], [Mon]) are just two examples.

See also Chapter *Applications of Graph Spectra in Quantum Physics*.

3.3. Computer science. It was recognized in about last ten years that graph spectra have several important applications in computer science. Graph spectra appear in internet technologies, pattern recognition, computer vision and in many other areas. Here we mention applications in treating some of these and other problems.

(See Chapter *Multiprocessor Interconnection Networks* for applications in designing multiprocessor interconnection topologies and Chapter *Spectral Techniques in Complex Networks* for applications on Internet).

One of the oldest applications (from 1970's) of graph eigenvalues in Computer Science is related to graphs called *expanders*. Avoiding a formal definition, we shall say that a graph has good *expanding properties* if each subset of the vertex set of small cardinality has a set of neighbors of large cardinality. Expanders and some related graphs (called *enlargers, magnifiers, concentrators* and *superconcentrators*, just to mention some specific terms) appear in treatment of several problems in Computer Science (for example, communication networks, error-correcting codes, optimizing memory space, computing functions, sorting algorithms, etc.). Expanders can be constructed from graphs with a small second largest eigenvalue in modulus. Such class of graphs includes the so called *Ramanujan graphs*. For an introduction to this type of applications see [CvSi1] and references cited therein. Paper [LuPS] is one of the most important papers concerning Ramanujan graphs.

Referring to the book [CvDSa] as "the current standard work on algebraic graph theory", Van Mieghem gave in his book [Van] a twenty page appendix on graph spectra, thus pointing out the importance of this subject for communications networks and systems.

The paper [Spi] is a tutorial on the basic facts of the theory of graph spectra and its applications in computer science delivered at the 48th Annual IEEE Symposium on Foundations of Computer Science.

The largest eigenvalue λ_1 plays an important role in modelling virus propagation in computer networks. The smaller the largest eigenvalue, the larger the robustness of a network against the spread of viruses. In fact, it was shown in [WaCWF] that the epidemic threshold in spreading viruses is proportional to $1/\lambda_1$. Motivated by this fact, the authors of [DaKo] determine graphs with minimal λ_1 among graphs with given numbers of vertices and edges, and having a given diameter.

Some data on using graph eigenvalues in studying Internet topology can be found in [ChTr] and in the references cited therein.

Web search engines are based on eigenvectors of the adjacency and some related graph matrices [BrPa, Kle].

The indexing structure of object appearing in computer vision (and in a wide range of other domains such as linguistics and computational biology) may take the form of a tree. An indexing mechanism that maps the structure of a tree into a low-dimensional vector space using graph eigenvalues is developed in [ShDSZ].

Statistical databases are those that allow only statistical access to their records. Individual values are typically deemed confidential and are not to be disclosed, either directly or indirectly. Thus, users of a statistical database are restricted to statistical types of queries, such as SUM, MIN, MAX, etc. Moreover, no sequence of answered queries should enable a user to obtain any of the confidential individual values. However, if a user is able to reveal a confidential individual value, the database is said to be *compromised*. Statistical databases that cannot be compromised are called *secure*.

One can consider a restricted case where the query collection can be described as a graph. Surprisingly, the results from [Bra, BrMS] show an amazing connection between compromise-free query collections and graphs with least eigenvalue -2. This connection was recognized in the paper [BraCv].

It is interesting to note that original Doob's description [Doo] in 1973 of the eigenspace of -2 in line graphs in terms of even cycles and odd dumbbells has been extended to generalized line graphs by Cvetković, Doob and Simić [CvDS] in 1981 in terms of the chain groups, not explicitly dealing with cycles and dumbbells. The independent discovery of Branković, Miller and Širáň [BrMS] in 1996 put implicitly some light on the description of the eigenspace in generalized line graphs a bit before Cvetković, Rowlinson and Simić in 2001 (the paper [CvRS2] was submitted in 1998), using the star complement technique and without being aware of [BrMS], gave the entire description of the eigenspace.

Another way to protect the privacy of personal data in databases is to randomize the network representing relations between individuals by deleting some actual edges and by adding some false edges in such a way that global characteristics of the network are unchanged. This is achieved using eigenvalues of the adjacency matrix (in particular, the largest one) and of the Laplacian (algebraic connectivity) [YiWu].

Additional information on applications of graph spectra to Computer Science can be found in [CvSi2]. These applications are classified there in the following way:

1. Expanders and combinatorial optimization,
2. Complex networks and the Internet,
3. Data mining,
4. Computer vision and pattern recognition,
5. Internet search,
6. Load balancing and multiprocessor interconnection networks,
7. Anti-virus protection versus spread of knowledge,
8. Statistical databases and social networks,
9. Quantum computing.

3.4. Mathematics. There are many interactions between the theory of graph spectra and other branches of mathematics. This applies, by definition, to linear algebra. Another field which has much to do with graph spectra is combinatorial optimization.

Combinatorial matrix theory studies matrices by the use of and together with several digraphs which can be associated to matrices. Many results and techniques from the theory of graph spectra can be applied for the foundations and development of matrix theory. A combinatorial approach to the matrix theory is given in the book [BrCv]. Particular topics, described in the book, include determinants, systems of linear algebraic equations, sparse matrices, the Perron–Frobenius theory of non-negative matrices, Markov chains and many others.

Relations between eigenvalues of graphs and *combinatorial optimization* have been known for last twenty years. The section titles of an excellent expository article [MoPo] show that many problems in combinatorial optimization can be treated using eigenvalues: 1. Introduction, 1.1. Matrices and eigenvalues of graphs; 2. Partition problems; 2.1 Graph bisection, 2.2. Connectivity and separation, 2.3. Isoperimetric numbers, 2.4. The maximum cut problem, 2.5. Clustering, 2.6. Graph partition; 3. Ordering, 3.1. Bandwidth and min-p-sum problems, 3.2. Cutwidth, 3.3 Ranking, 3.4. Scaling, 3.5. The quadratic assignment problem; 4. Stable sets and coloring, 4.1. Chromatic number, 4.2. Lower bounds on stable sets, 4.3. Upper bounds on stable sets, 4.4. k-colorable subgraphs; 5. Routing problems, 5.1. Diameter and the mean distance, 5.2. Routing, 5.3. Random walks; 6. Embedding problems; A. Appendix: Computational aspects; B. Appendix: Eigenvalues of random graphs. The paper [MoPo] contains a list of 135 references.

See [CvDSa], third edition, pp. 417–418, for further data and references.

The *travelling salesman problem* (TSP) is one of the best-known NP-hard combinatorial optimization problems, and there is an extensive literature on both its theoretical and practical aspects. The most important theoretical results on TSP can be found in [LaLRS], [GuPu] (see also [CvDM]). Many algorithms and heuristics for TSP have been proposed. In the *symmetric* travelling salesman problem (STSP), it is assumed that the cost of travelling between two points is the same in both directions.

We shall mention here only one approach, which uses semi-definite programming (SDP) to establish a lower bound on the length of an optimal tour. This bound is obtained by relaxing the STSP and can be used in an algorithm of branch-and-bound type. The semi-definite relaxations of the STSP developed in [CvCK1] are based on a result of M. Fiedler [Fie] related to the Laplacian of graphs and algebraic connectivity (the second smallest eigenvalue of the Laplacian).

A semi-definite programming model for the travelling salesman problem was also obtained by Cvetković et al. [CvCK2, CvCK3].

The largest eigenvalue of a minimal spanning tree of the complete weighted graphs, with distances between cities serving as weights, can be used as a complexity index for the travelling salesman problem [CvDM].

3.5. Other sciences. Networks appearing in biology have been analyzed by spectra of normalized graph Laplacian in [Ban], [BaJo].

Research and development networks (R&D networks) are studied by the largest eigenvalue of the adjacency matrix in [KoBNS1], [KoBNS2].

Some older references on applications of graph spectra to Geography and social Sciences can be found in [CvDGT, Section 5.17].

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4. Selected bibliographies on applications of the theory of graph spectra

Subsections contain bibliographies related to Chemistry, Physics, Computer Science, Engineering, Biology and Economics.

4.1. Chemistry. In this bibliography are included books and expository articles that are either completely or to a significant extent concerned with some aspect(s) of chemical applications of graph spectral theory. Some books and expository articles in which graph–spectrum–related topics are mentioned only marginally (not necessarily in an explicit manner) are also included; these are marked by [XX].

Original research papers concerned with chemical applications of graph spectral theory are to numerous to be covered by this bibliography. Some of these papers, of exceptional (mainly historical) relevance, are nevertheless included; these are marked by [OR].

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