GRAPH SPECTRA IN COMPUTER SCIENCE

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A paper with the same title is being prepared jointly with S. Simić and D. Stevanović

I am not giving a survey
on applications of matrices in computer science, or
on applications of graphs in computer science

the subject of the talk :
Applications of the *theory of graph spectra* (or of *spectral graph theory*) in computer science

Spectral graph theory is a mathematical theory where linear algebra and graph theory meet together

A spectral graph theory is a theory in which graphs are studied by means of eigenvalues of a matrix M which is in a prescribed way defined for any graph.

This theory is called *M–theory*.

Frequently used graph matrices:
A adjacency matrix
D diagonal matrix of vertex degrees
$L = D - A$ Laplacian
$Q = D + A$ signless Laplacian

The spectral graph theory is the union of all these particular theories + interactions

For example, the adjacency matrix of the graph shown in Fig. 1

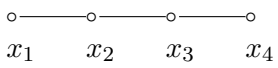


Fig.1

is given by $A = \begin{Vmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{Vmatrix}$.

For the graph G on Fig.1 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 $1.6180,\ 0.6180,\ -0.6180,\ -1.6180$ or

$$\frac{1+\sqrt{5}}{2},\ \frac{-1+\sqrt{5}}{2},\ \frac{1-\sqrt{5}}{2},\ \frac{-1-\sqrt{5}}{2}$$

Adjacency matrix - characteristic features

A *walk of length* k in a graph (or digraph) is a sequence of (not necessarily different) vertices $x_1, x_2, \ldots, x_k, x_{k+1}$ such that for each $i = 1, 2, \ldots, k$ there is an edge (or arc) from x_i to x_{i+1}. The walk is *closed* if $x_{k+1} = x_1$.

Counting walks in a graph (or digraph) is related to graph spectra by the following well-known result.

Theorem. If A is the adjacency matrix of a graph, then the (i, j)-entry $a_{ij}^{(k)}$ of the matrix A^k is equal to the number of walks of length k that originate at vertex i and terminate at vertex j.

Thus, for example, the number of closed walks of length k is equal to the k-th spectral moment, since $\Sigma_{i=1}^{n} a_{ii}^{(k)} = \mathrm{tr}(A^k) = \Sigma_{i=1}^{n} \lambda_i^k$.

Laplacian matrix - characteristic features

Let G be a connected graph on n vertices. Eigenvalues in non-decreasing order and corresponding orthonormal eigenvectors of the Laplacian $L = D - A$ of G are denoted by $\nu_1 = 0, \nu_2, \ldots, \nu_n$ and $u_1, u_2, \ldots, u_n$, respectively.

Note that if $\mathbf{x}^T = (x_1, x_2, \ldots, x_n)$, then

$$\mathbf{x}^T L \mathbf{x} = \sum_{i \sim j,\ i<j} (x_i - x_j)^2.$$

We also have

$$\nu = \sum_{i \sim j,\ i<j} (x_i - x_j)^2$$

if $\mathbf{x}$ is a normalized eigenvector belonging to eigenvalue ν of L.

Biggs N.L., *Algebraic Graph Theory*, Cambridge University Press, Cambridge, 1993.

Chung F., *Spectral Graph Theory*, American Mathematical Society, Providence, Rhode Island, 1997.

Cvetković D., Doob M., Sachs H., *Spectra of Graphs, Theory and Application*, 3rd edition, Johann Ambrosius Barth Verlag, Heidelberg–Leipzig, 1995.

Cvetković D., Rowlinson P., Simić S. K., *An Introduction to the Theory of Graph Spectra*, Cambridge University Press, Cambridge, 2009.

Typical research subjects in mathematical theory:

– characterizations of graphs by their spectra,

– inequalities for eigenvalues,

– extremal problems with eigenvalues,

– graph energy (the sum of the absolute values of eigenvalues).

1 A survey of applications

1.1 Expanders and combinatorial optimization

1.2 Complex networks

1.3 Data mining

1.4 Computer vision and pattern recognition

1.5 Internet search

1.6 Load balancing and multiprocessor interconnection networks

1.7 Anti-virus protection versus spread of knowledge

1.8 Statistical databases and social networks

1.9 Quantum computing

Expanders and combinatorial optimization

One of the oldest applications (from 1970's) of graph eigenvalues in Computer Science is related to graphs called *expanders*.

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*) 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*.

Expanders are related to some problems of combinatorial optimization. More generally, several algorithms of combinatorial optimization are considered as part of computer science.

Numerous relations between eigenvalues of graphs and *combinatorial optimization* have been known for last twenty years. The section titles of an excellent expository article

Mohar B., Poljak S., *Eigenvalues in combinatorial optimization*, in: *Combinatorial and Graph-Theoretical Problems in Linear Algebra*, (ed. R. Brualdi, S. Friedland, V. Klee), Springer-Verlag, New York, 1993, 107–151.

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. Cut-width, 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;

Note that one of early heuristics for graph bisection uses the *Fiedler vector*, ie. the eigenvector belonging to the second smallest eigenvalue of the graph Laplacian. This eigenvalue is called *algebraic connectivity* of the graph and was introduced by M. Fiedler in the paper

Algebraic connectivity of graphs, Czech. J. Math., 23(98)(1973), 298-305.

The algebraic connectivity has been used in

D. Cvetković, M. Čangalović and V. Kovačević-Vujčić, Semidefinite programming methods for the symmetric traveling salesman problem, *Integer Programming and Combinatorial Optimization, Proc. 7th Internat. IPCO Conf.*, Graz, Austria, June 1999, Lecture Notes Comp. Sci. 1610, Springer, Berlin, 1999, 126-136.

to formulate the following discrete semidefinite programming model of the symmetric *travelling salesman problem* (STSP):

STSP:

minimize $F(X) = \Sigma_{i=1}^{n} \Sigma_{j=1}^{n} \left(-\frac{1}{2} d_{ij}\right) x_{ij} + \frac{\alpha}{2} \Sigma_{i=1}^{n} \Sigma_{j=1}^{n} d_{ij}$

subject to

$x_{ii} = 2 + \alpha - \beta \quad (i = 1, \ldots, n),$

$\Sigma_{j=1}^{n} x_{ij} = n\alpha - \beta, \quad (i = 1, \ldots, n),$

$x_{ij} \in \{\alpha - 1, \alpha\} \quad (j = 1, \ldots, n : \ i < j), \qquad X \geq 0$

Here $X \geq 0$ means that the matrix X is symmetric and positive semidefinite, while α and β are chosen so that $\alpha > h_n/n$ and $0 < \beta \leq h_n$ with $h_n = 2 - 2\cos(2\pi/n)$ being the algebraic connectivity of the cycle C_n.

Complex networks

Complex networks is a common name for various real networks which are presented by graphs with an enormously great number of vertices. Here belong Internet graphs, phone graphs, e-mail graphs, social networks and many other. In spite of their diversity such networks show some common properties.

Several models of random graphs have been used to describe complex networks including the classical Erdös-Rényi model where we have a constant probability for the existence of each edge. There are models where given degree distribution is realized.

Main characteristic of complex networks is the degree and eigenvalue distribution. Both distributions obey a *power low* of the form $x^{-\beta}$ for a positive β.

In particular, if n_k denotes the number of vertices of degree k, then asymptotically $n_k = ak^{-\beta}$ for some constant a.

It was conjectured in

Faloutsos M., Faloutsos P., Faloutsos C., *On power-low relationships of the Internet topology*, Proc. ACM SIGCOMM '99, ACM Press, New York, 1999, 251-262.

that in networks with degree power law the largest eigenvalues of the adjacency matrix have also a power law distribution. That was proved under some conditions in

Mihail M. Papadimitrou C.H., *On the eigenvalue power-low*, RANDOM 2002, LNCS 2483, Springer, Berlin, 2002, 254-262.

The power law for eigenvalues can be formulated in the following way. Let $\lambda_1, \lambda_2, \ldots$ be non-increasing sequence of eigenvalues of the adjacency matrix, then asymptotically $\lambda_i = ai^{-\gamma}$ for some constant a and positive γ.

The following book is devoted to complex networks.

Chung F., Lu L., *Complex Graphs and Networks*, American Mathematical Society, Providence, Rhode Island, 2006.

There are two chapters which describe spectral properties of such networks.

Note that most of the papers on complex networks appear in scientific journals in the area of Physics.

Empirical studies of the Internet topology have been conducted in many papers using the normalized Laplacian matrix

$$\hat{L} = D^{-\frac{1}{2}}(D - A)D^{-\frac{1}{2}} = D^{-\frac{1}{2}}LD^{-\frac{1}{2}}.$$

This matrix has 1's on the diagonal, and at an off-diagonal position (i, j) the entry is equal to 0 for non-adjacent and $-\frac{1}{\sqrt{d_i d_j}}$ for adjacent vertices i, j of degrees d_i, d_j. The spectrum of $\hat{L}$ belongs to the interval $[0, 2]$ independently of the number of vertices. The book

Chung F., *Spectral Graph Theory*, American Mathematical Society, Providence, Rhode Island, 1997.

is devoted to the normalized Laplacian.

The eigenvalues $\gamma_i;\ i = 1, 2, \ldots, n$ of $\hat{L}$ in non-decreasing order can be represented by points $(\frac{i-1}{n-1}, \gamma_i)$ in the region $[0, 1] \times [0, 2]$ and can be approximated by a continuous curve. It was noticed in

Vukadinović D., Huang P., Erlebach T., *A spectral analysis of the Internet topology*, 2001

that this curve is practically the same during the time for several networks in spite of the increasing number of vertices and edges of the corresponding graph. Therefore the authors consider the spectrum of $\hat{L}$ as a *fingerprint* of the corresponding network topology.

Data mining

Data mining discovers interesting and unknown relationships and patterns in huge data sets. Such hidden information could contribute very much to many domains such as image processing, web searching, computer security and many others including those outside computer science.

Among many tools used in data mining, spectral techniques play an important role

Sawilla R., *A survey of data mining of graphs using spectral graph theory*, Defence R&D Canada ' Ottawa, Technical Memorandum TM 2008-317, Ottawa, 2008.

Here belong, in particular, clustering and ranking the vertices of a graph. While ranking will be treated later, here we consider the clustering.

A description of *spectral clustering* methods is given in the tutorial

Luxburg U. von, *A tutorial on spectral clustering*, Stat. Comput. 17(2007), 395-416.

We shall present an algorithm for graph clustering which is based on the Laplacian matrix of a graph.

Let G be a connected graph on n vertices. Eigenvalues in non-decreasing order and corresponding orthonormal eigenvectors of the Laplacian $L = D - A$ of G are denoted by $\nu_1 = 0, \nu_2, \ldots, \nu_n$ and $u_1, u_2, \ldots, u_n$, respectively.

In order to construct k clusters in a graph we form an $n \times k$ matrix U containing the vectors $u_1, u_2, \ldots, u_k$ as columns. We have a geometric representation $\mathcal{G}$ of G in the k-dimensional space R^k: we just take rows of U as point coordinates representing the vertices of G. Edges are straight line segments between the corresponding points. Now classical clustering methods (say k-means algorithm) should be applied to this new graph presentation.

The following well-known inequality for the Rayleigh quotient

$$\nu_1 \leq \frac{\mathbf{x}^T L \mathbf{x}}{\mathbf{x}^T \mathbf{x}} \leq \nu_n$$

holds for any non-zero vector $\mathbf{x}$ of the corresponding dimension. Equality holds for relevant eigenvectors.

More generally, the eigenvalue ν_i is the minimal value of the Rayleigh quotient of L over the orthogonal complement of the subspace generated by eigenvectors $u_1, u_2, \ldots, u_{i-1}$.

Note that if $\mathbf{x}^T = (x_1, x_2, \ldots, x_n)$, then

$$\mathbf{x}^T L \mathbf{x} = \sum_{i \sim j,\ i<j} (x_i - x_j)^2.$$

We also have

$$\nu = \sum_{i \sim j,\ i<j} (x_i - x_j)^2$$

if $\mathbf{x}$ is a normalized eigenvector belonging to eigenvalue ν of L.

The sum of squares of lengths of all edges in the representation $\mathcal{G}$ of G is equal to $\nu_1 + \nu_2 + \ldots + \nu_k$. This is the minimal value over all representations obtained via matrix U with orthonormal columns.

Such an extremal graph representation must have remarkable properties. It enhances the cluster-properties of the original data and clusters can now be easily detected.

In regular graphs we can use the adjacency matrix A instead of the Laplacian L. We have $L = rI - A$ for a regular graph of degree r and $\lambda_i = r - \nu_i$ for $i = 1, 2, \ldots, n$.

Eigenvectors of L are also eigenvectors of A for the corresponding eigenvalues.

Instead of first k smallest eigenvalues we have to consider now k largest eigenvalues.

Example. Consider the adjacency matrix A of a cycle of C_n length n. It is well known that the eigenvalues λ_j of the matrix A are given by $\lambda_j = 2\cos(2\pi j/n)$ $(j = 1, \ldots, n)$.

For $j = 1$ and $j = n - 1$ we get the second largest eigenvalue $2\cos(2\pi/n)$ which corresponds to the second smallest eigenvalue $2 - 2\cos(2\pi/n)$ of the Laplacian.

Two independent eigenvectors x, y are given by coordinates
$x_l = \cos(2\pi l/n)$ $(l = 1, \ldots, n)$, $y_l = \sin(2\pi l/n)$ $(l = 1, \ldots, n)$.

If we represent vertices by points (x_i, y_i), the picture of the graph is a regular n-gon. ■

Graph representation obtained by the Laplacian matrix has been used in graph drawings:

Koren Y., *Drawing graphs by eigenvectors: theory and practice*, Comput. Math. appl., 49(2005), 1867-1888.

Tutte W.T., *How to draw a graph*, Proc. London Math. Soc., 13(1963),743-768.

Example. In our context interesting are also *fullerene graphs* corresponding to carbon compounds called *fullerenes*. Fullerene graphs are planar regular graphs of degree 3 having as faces only pentagons and hexagons. The Euler theorem for planar graphs yields that the number of pentagons is exactly 12. Although being planar, fullerene graphs are represented (and this really corresponds to actual positions of carbon atoms in a fullerene) in 3-space with its vertices embedded in a quasi-spherical surface.

A typical fullerene is C_{60}. It can be described also as a truncated icosahedron and has the shape of a football.

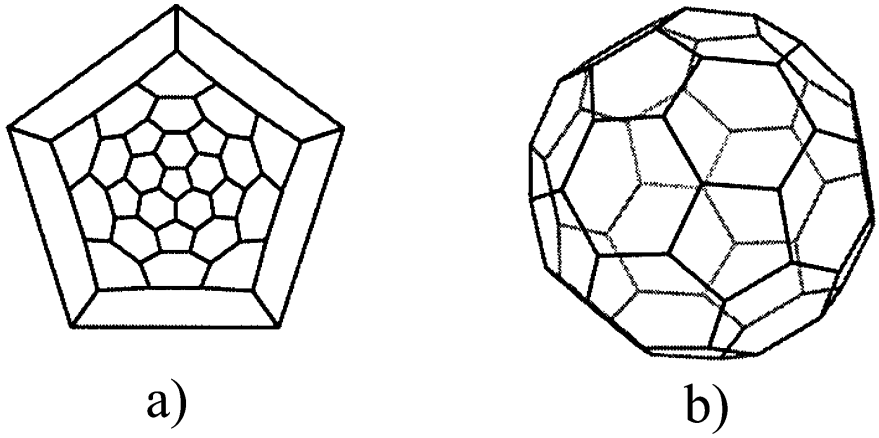


Figure 1: a) Planar and b) 3D visualization of the icosahedral fullerene C_{60}

Fullerene graphs have a nice 3D-representation in which the coordinates of the positions of vertices can be calculated from three eigenvectors of the adjacency matrix (the so called *topological coordinates* which were also used in producing the atlas

P. W. Fowler and D. E. Manolopoulos, *An Atlas of Fullerenes*, Clarendon Press, Oxford, 1995.). ■

Together with the Laplacian L and the normalized Laplacian $\hat{L}$ also the matrix $D^{-1}L$ has been used in clustering algorithms. According to

Luxburg U. von, *A tutorial on spectral clustering*, Stat. Comput. 17(2007), 395-416.

the last matrix performs best.

Computer vision and pattern recognition

Spectral graph theory has been widely applied in computer vision and pattern recognition. Examples include image segmentation, routing, image classification, etc. These methods use the spectrum, i.e. eigenvalues and eigenvectors, of the adjacency or Laplacian matrix of a graph.

The basic idea is to represent an image by a weighted graph with a vertex for each pixel and the edges between the neighbouring pixels with weight depending on how similar the pixels are.

A more sophisticated idea is to represent an image's content by a graph with specially selected points as vertices. The interesting points are points in an image which have a well-defined position and can be robustly detected.

Several other graphs are used.

Shi J., Malik J., Normalized cuts and image segmentation, Proc. IEEE Conf. Computer Vision and Pattern Recognition, 1997, 731-737; IEEE Trans. Pattern Analysis Machine Intell., 28(2000), 888-905.

It is shown how the Fiedler vector (i.e. the eigenvector associated to the second smallest eigenvalue of the Laplacian matrix) can be used to separate the foreground from the background structure in images. The original procedure has been improved by using the normalized Laplacian matrix (so as to maximize the normalized graph cut).

More generally, image segmentation is an important procedure in computer vision and pattern recognition. The problem is to divide the image into regions according to some criteria. Very frequently the image segmentation is obtained using eigenvectors of some graph matrices.

Internet search

Web search engines are based on eigenvectors of the adjacency and some related graph matrices:

PageRank (used in Google)

Brin S., Page L., *The Anatomy of Large-Scale Hypertextual Web Search Engine*, Proc. 7th International WWW Conference, 1998.

and Hyperlinked Induced Topics Search (HITS)

Kleinberg J., *Authoratitive sources in a hyperlinked environment*, J. ACM, 48 (1999), 604-632.

Internet is represented by a digraph G, web pages – vertices, links – arcs.

HITS exploits eigenvectors belonging to the largest eigenvalues of the matrices AA^T and A^TA where A is the adjacency matrix of a subgraph of G induced by the set of web pages obtained from search key words by some heuristics. Eigenvectors define ordering of selected web pages.

PageRank uses random walks. Adjacency matrix of G is normalized so that the sum of entries in each row is equal to 1. This matrix P is the transition matrix of a Markov chain and the normalized eigenvector of the largest eigenvalue of P^T defines the equilibrium state of the chain. Pages are ranked by the coordinates of this eigenvector.

Expository paper

Langville A.N., Meyer C.D., *A survey of eigenvector methods for Web information retrieval*, SIAM Rev., 47(2005), No. 1, 135-161.

contains a survey of both techniques.

From the mathematical point of view, the subject of ranking individuals or objects by eigenvectors of suitably chosen graph matrices is very old. One of the basic references is the thesis

Wei T.H., The algebraic foundations of ranking theory, Thesis, Cambridge, 1952.

In particular, the ranking of the participants of a round-robin tournament can be carried out in that way (see, for example, *Spectra of Graphs, Theory and Application*, , p. 226).

These methods have been used in the sociology for a long time as well; see, for example,

Bonacich P. Power and centrality: A family of measures, Amer. J. Soc., 92(1987), 1170-1182.

We reproduce here a relevant result. The following theorem of T.H. Wei (1952) is noted in *Eigenspaces of Graphs*, p. 26:

Theorem. *Let $N_k(i)$ be the number of walks of length k starting at vertex i of a non-bipartite connected graph G with vertices $1, 2, \ldots, n$. Let*

$$s_k(i) = \frac{N_k(i)}{\Sigma_{j=1}^{n} N_k(j)}.$$

Then, for $k \to \infty$, the vector $(s_k(1), s_k(2), \ldots, s_k(n))^T$ tends towards the eigenvector corresponding to the index of G.

Load balancing and multiprocessor interconnection networks

The job which has to be executed by a multiprocessor system is divided into parts (elementary jobs or items) that are given to particular processors. Elementary jobs distribution among processors can be represented by a vector x whose coordinates are non-negative integers associated to graph vertices and indicate how many elementary jobs are given to corresponding processors.

The load balancing problem requires creation of algorithms for moving elementary jobs among processors in order to achieve the uniform distribution, i.e., that the vector x is an integer multiple of the vector j whose all coordinates are equal to 1.

Let G be a connected graph on n vertices. Eigenvalues and corresponding orthonormal eigenvectors of the Laplacian $L = D - A$ of G are denoted by $\nu_1, \nu_2, \ldots, \nu_n = 0$ and $u_1, u_2, \ldots, u_n$, respectively. Any vector x from R^n can be represented as a linear combination of the form $x = \alpha_1 u_1 + \alpha_2 u_2 + \cdots + \alpha_n u_n$.

Suppose now that G has distinct Laplacian eigenvalues $\mu_1, \mu_2, \ldots, \mu_m = 0$ with multiplicities $k_1, k_2, \ldots, k_m = 1$, respectively. Vector x can now be represented in the form $x = y_1 + y_2 + \cdots + y_m$ where y_i belongs to the eigenspace of μ_i for $i = 1, 2, \ldots, m$. We also have $y_m = \beta j$ for some β.

Since $Lx = L(y_1+y_2+\cdots+y_m) = \mu_1 y_1+\mu_2 y_2+\cdots+\mu_m y_m$, we have $x^{(1)} = x-\frac{1}{\mu_1}Lx = (I-\frac{1}{\mu_1}L)x = (1-\frac{\mu_2}{\mu_1})y_2+\cdots+\beta j$. We see that the component of x in the eigenspace of μ_1 has been cancelled by the transformation by the matrix $I-\frac{1}{\mu_1}L$ while the component in the eigenspace of μ_m remains unchanged. The transformation $I-\frac{1}{\mu_2}L$ will cause that the component of $x^{(2)} = (I-\frac{1}{\mu_2}L)x^{(1)}$ in the eigenspace of μ_2 disappears. Continuing in this way

$$x^{(k)} = (I-\frac{1}{\mu_k}L)x^{(k-1)}, \quad k = 1, 2, \ldots, m-1 \tag{1}$$

we shall obtain $x^{(m-1)} = \beta j$.

We have seen how a vector x can be transformed to a multiple of j using the iteration process (1) which involves the Laplacian matrix of the multiprocessor graph G.

Let vector $x^{(k)}$ have coordinates $x_1^{(k)}, x_2^{(k)}, \ldots, x_n^{(k)}$. Relations (1) can be rewritten in the form

$$x_i^{(k)} = x_i^{(k-1)} - \frac{1}{\mu_k} \sum_{i*j} (d_i x_i^{(k-1)} - x_j^{(k-1)}) \tag{2}$$

where d_i is the degree of vertex i. This means that the current load at vertex i is changed in such a way that vertex (processor) i sends $\frac{1}{\mu_k}$-th part of its load to each of its d_i neighbors and, because this holds for every vertex, also receives $\frac{1}{\mu_k}$-th part of the load from each of its d_i neighbors.

We have a load flow on the edge set of G. If $x_i^{(k-1)}$ is negative, then vertex i, in fact, receives the corresponding amount. For each edge ij we have two parts of the flow: the part which is sent (or received) by i and the part which is sent (or received) by j. Adding algebraically we get final value of the flow through edge ij. This flow at the end has a non-negative value which is sent either from i to j or vice versa.

The number of iterations in (1) is equal to the number m of non-zero distinct Laplacian eigenvalues of the underlying graph. The maximum vertex degree Δ of G also affects computation of the balancing flow. The complexity of the balancing flow calculations essentially depends on the product $m\Delta$ and that is why this quantity was proposed in

R. Elsässer, R. Královič, B. Monien, *Sparse topologies with small spectrum size*, Theor. Comput. Sci. 307:549–565, 2003.

as a parameter relevant for the choice and the design of multiprocessor interconnection networks.

The following definitions of four kinds of graph *tightness* have been introduced and used in Cvetković D., Davidović D., 2008, 2009.

First type mixed tightness $t_1(G)$ of a graph G is defined as the product of the number of distinct eigenvalues m and the maximum vertex degree Δ of G, i.e., $t_1(G) = m\Delta$.

Structural tightness $stt(G)$ is the product $(D+1)\Delta$ where D is diameter and Δ is the maximum vertex degree of a graph G.

Spectral tightness $spt(G)$ is the product of the number of distinct eigenvalues m and the largest eigenvalue λ_1 of a graph G.

Second type mixed tightness $t_2(G)$ is defined as a function of the diameter D of G and the largest eigenvalue λ_1, i.e., $t_2(G) = (D+1)\lambda_1$.

Several arguments were given which support the claim that graphs with small tightness t_2 are well suited for multiprocessor interconnection networks.

It was proved that the number of connected graphs with a bounded tightness is finite and graphs with tightness values not exceeding 9 are determined explicitly. There are 69 such graphs and they contain up to 10 vertices. In addition, graphs with minimal tightness values when the number of vertices is $n = 2, \ldots, 10$ are identified.

Anti-virus protection versus spread of knowledge

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

Wang Y., Chakrabarti D., Wang C., Faloutsos C., *Epidemic spreading in real networks: An eigenvalue viewpoint*, 22nd Symp. Reliable Distributed Computing, Florence, Italy, Oct. 6–8, 2003.

that the epidemic threshold in spreading viruses is proportional to $1/\lambda_1$. Another model of virus propagation in computer networks has been developed in

Van Mieghem P., Omić J., Kooij R., *Virus spread in networks*,

with the same conclusion concerning $1/\lambda_1$.

Research and development networks (R&D networks) are studied using the largest eigenvalue of the adjacency matrix in

König, M. D., Battiston S., Napoletano M., Schweityer F., *The efficiency and evolution of R&D networks*, Working Paper 08/95, Economics Working Paper Series, Eidgenössische Technische Hochschule Zürich, Zŕich, 2008.

König, M. D., Battiston S., Napoletano M., Schweityer F., *On algebraic graph theory and the dynamics of innovation networks*, Networks and Heterogenous Media, 3 (2008), No. 2, 201–219.

In such networks it is desirable that the knowledge is spread through network as much as possible. Therefore the tendency is to achieve high values of the largest eigenvalue, just opposite to considerations of virus propagation.

An intuitive explanation of both phenomena, advantage to have minimal index for virus protection and maximal index for knowledge spread, can be obtained by the fact that the number of walks of length k in a connected graph behaves asymptotically as $c\lambda_1^k$ for a constant $c > 0$. The greater the number of walks the more intensive is the spread of the mowing substance, does not matter whether this is the virus or the knowledge.

The virus propagation model of Wang Y. et al. is a discrete time model. It uses the vector $\mathbf{P}_t = (p_{1,t}, p_{2,t}, \ldots, p_{n,t})^T$ where $p_{i,t}$ is the probability that the vertex i is infected at time t. The basic relation is

$$p_{i,t} = (1 - \delta)p_{i,t-1} + \beta \sum_{i \sim j} p_{j,t-1},$$

where β is the virus birth rate on an edge connected to an infected vertex and δ the virus curing rate on an infected vertex. The corresponding matrix relation is

$$\mathbf{P}_t = ((1 - \delta)I + \beta A)\mathbf{P}_{t-1},$$

where A is the adjacency matrix of the graph representing the network.

Further we have $\mathbf{P}_t = S^t\mathbf{P}_0$ for $t = 0, 1, 2, \ldots$ where $S = (1-\delta)I + \beta A$. We see that the the vector $\mathbf{P}_t$ will tend to a zero-vector for $t \to \infty$ if and only if all eigenvalues of the matrix S are smaller than 1 in modulus. This would mean that virus epidemic has died and will happen if $1 - \delta + \beta\lambda_1 < 1$, i.e.

$$\frac{\beta}{\delta} < \frac{1}{\lambda_1}.$$

Given β and δ, we see that the network is as safer as the smaller is λ_1. We can denote the quantity $\tau = \frac{1}{\lambda_1}$ as the epidemic threshold in spreading viruses. Hence if $\frac{\beta}{\delta} < \tau$ the network is safe and in the opposite case the network will be conquered by viruses.

There are numerous mathematical investigations in both directions: to find graphs in particular classes of graphs which have minimal or maximal largest eigenvalue. We mention a few results and references.

We need the following definition.

Definition. A graph G with the edge set E_G is called a *nested split graph* if its vertices can be ordered so that $jq \in E_G$ implies $ip \in E_G$ whenever $i \leq j$ and $p \leq q$.

This definition is used in

Cvetković D., Rowlinson P., Simić S. K., *Eigenspaces of Graphs*, Cambridge University Press, Cambridge, 1997,

where the graphs in question were called graphs with a *stepwise* adjacency matrix. Some other definitions and terms are used in the literature, e.g. degree maximal graphs, threshold graphs. Note that graphs with a stepwise adjacency matrix are exactly the nested split graphs. We also have

Proposition. *A graph is a nested split graph if and only if it does not contain as an induced subgraph any of the graphs* $P_4, 2K_2, C_4$.

It is well-known that in connected graphs with the given numbers of vertices and edges the graph with maximal largest eigenvalue is a nested split graph.

There are less results concerning minimal values of the largest eigenvalue. The paper

Simić S., On the largest eigenvalue of bicyclic graphs, Publ. Inst. Math.(Beograd), 46(60)(1989), 1-6.

solves the problem for bicyclic graphs.

Motivated by this fact, the authors of

van Dam E. R., Kooij R. E., *The minimal spectral radius of graphs with a given diameter*, Linear Alg. Appl. 423 (2007), 408–419.

determine graphs with minimal λ_1 among graphs with given numbers of vertices and edges, and having a given diameter.

Statistical databases and social networks

Statistical databases allow only statistical access to their records. Individual values are 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 looking for the sum of values, minimum or maximum value of some parameters, 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

Branković L., *Usability of secure statistical data bases*, PhD Thesis, Newcastle, Australia, 1998.

Branković L., Miller M., Širáň J., *Graphs, (0,1)-matrices and usability of statistical data bases*, Congressus Numerantium, 120 (1996), 186–192.

show an amazing connection between compromise-free query collections and graphs with least eigenvalue -2. This connection was recognized in the paper

Branković Lj., Cvetković D., *The eigenspace of the eigenvalue -2 in generalized line graphs and a problem in security of statistical data bases*, Univ. Beograd, Publ. Elektrotehn. Fak., Ser. Mat., 14 (2003), 37–48.

The problem of protecting the privacy appears also in social networks at the Internet (for example, FaceBook). To protect the privacy of personal data the network is randomized 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) as described in the paper

Ying X., Wu X., *Randomizing social networks: a spectrum preserving approach*, Proc. SIAM Internat. Conf. Data Mining, SDM2008, April 24–26, 2008, Atlanta, Georgia, USA, SIAM, 2008, 739–750.

Quantum computing

Quantum computation is a model of computation based on the principles of quantum mechanics although the corresponding computers have not yet been realized. In spite of the non-existence of actual machines, the theory of quantum computing is very much developed.

For a general overview on Quantum Information Technology see, for example, special issue of the journal

NEC Research & Developments, 44(2003), No. 3.

A graph is called *integral* if its spectrum consists entirely of integers.

It has been discovered recently in

Christandl M., Datta N., Ekert A., Landahl A.J., *Perfect state transfer in quantum spin networks*, Phys. Rev. Lett., 92(2004),187902.

that integral graphs can play a role in the so called perfect state transfer in quantum spin networks.

According to definition in Physics, there is perfect state transfer between two vertices of a graph if a single excitation can travel with fidelity one between the corresponding sites of a spin system modelled by the graph.

Mathematically, let G be a graph with adjacency matrix A and consider the matrix $H(t) = e^{iAt}$ where t is a real variable and $i^2 = -1$. According to

Godsil C., *Periodic graphs*, arXiv:0806.2704 [math.CO].

perfect state transfer occurs between vertices u and v of G if there is a value of t such that $|H(t)_{u,v}| = 1$.

This can happen in integral graphs but not always.

There are exactly 13 connected, cubic, integral graphs

Bussemaker F. C., Cvetković D., *There are exactly 13 connected, cubic, integral graphs*, Univ. Beograd, Publ. Elektrotehn. Fak., Ser. Mat. Fiz., No. 544 - No. 576(1976), 43-48.

Among them are, for example, the 3-cube and the Petersen graph.

The 3-cube is the only connected cubic integral graph with perfect state transfer

Severini, S., The 3-dimensional cube is the only connected cubic graph with perfect state transfer, to appear.

Comments and suggestions

After completing our survey of applications of graph spectra to several branches in computer science, we have some observations and comments including some new results.

Our general suggestion is that mathematicians should react on the explosion of the number of papers in computer science which use graph spectra by selecting for their own research some subjects from or inspired by such applications.

We have a number of detailed comments.

Computer networks resistent to the spread of viruses.

We have some results on graphs with a minimal value of the largest eigenvalue. As we know, such graphs are models of computer networks resistent to the spread of viruses.

Graphs with a minimal value of the largest eigenvalue in a set of graphs will be called *minimal* graphs.

Let $\deg(v)$ be the degree of the vertex v. An *internal path* in some graph is a path $v_0, v_1, \ldots, v_{k+1}$ for which $\deg(v_0), \deg(v_{k+1}) \geq 3$ and $\deg(v_1) = \cdots = \deg(v_k) = 2$ (here $k \geq 0$, or $k \geq 2$ whenever $v_{k+1} = v_0$).

Consider connected graphs with fixed numbers of vertices and edges.

A minimal graph cannot contain vertices of degree 1 because deleting a vertex of degree 1 and a simultaneous insertion of a vertex of degree 2 in the middle of an edge on an internal path would diminish the largest eigenvalue λ_1 (by a result from

Hoffman A.J., Smith J.H., *On the spectral radii of topologically equivalent graphs*, Recent Advances in Graph Theory, ed. M. Fiedler, Academia Praha, 1975, 273-281.)

As a consequence, all edges belong to internal paths. Subdividing edges in such graphs we can further diminish λ_1. However, we have $\lambda_1 \geq \Delta/\sqrt{\Delta - 1}$, where Δ is the maximum vertex degree (as follows form a result from the same paper). Therefore it is reasonable to choose Δ as small as possible. Obviously we should accept $\Delta = 3$ since graphs with $\Delta < 3$ are not of much interest in this context.

Let H be a connected graph with q edges and with vertex degrees at least 3. For each $i = 1, 2, \ldots, q$ we want to subdivide edge i by inserting l_i vertices of degree 2. Suppose that $\Sigma_{i=1}^{q} l_i = e$ is fixed. In this way we obtain a graph G. An explicit relation between the largest eigenvalue of G and quantities $l_1, l_2, \ldots, l_q$ can be found. A standard procedure with Lagrange's multipliers for finding the minimum of an implicit function leads to the conclusion that under some reasonable additional assumptions the quantities l_i should be almost equal (equal if possible). Such a subdivision of a graph is called *balanced* subdivision.

Details will appear in the paper

Belardo F., Li Marzi E.M., Simić S.K., *Connected graphs of fixed order and size with minimal index*, to appear.

Indeed many of the examples of minimal graphs found by computer have this property.

Earlier results on the subject are special cases of this result. It started with a conjecture that a balanced subdivision minimizes the largest eigenvalue in a cycle with an additional edge. The problem was solved in a generalized form. There are results for broken wheels and for trees.

The above presented procedure enables explicit construction of minimal tricyclic graphs. Previous result for bicyclic graphs has been proved in a shorter way.

Our conclusion is that balanced subdivisions of cubic graphs should be considered as good models of virus resistent computer networks.

Signless Laplacian could be useful

We suggest to try to create models for virus propagation and the spread of knowledge in which the adjacency matrix would be replaced by the signless Laplacian. In such models desirable graphs for anti-virus protection would be those with small q_1 and for R&D networks those with large q_1.

We believe that there are situations in which viruses or knowledge move along lazy random walks rather than along standard random walks. This can be expected in situations when the vertices when receiving something from their neighbours are likely to respond back with some action.

Integral graphs in load balancing

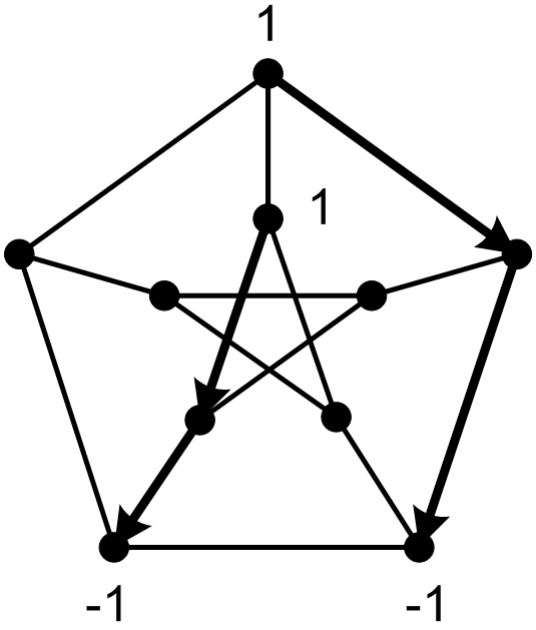
As defined, a graph is called *integral* if its spectrum consists entirely of integers. Each eigenvalue has integral eigenvectors and each eigenspace has a basis consisting of such eigenvectors.

In integral graphs load balancing algorithms, which use eigenvalues and eigenvectors, can be executed in integer arithmetics as noted in the paper

Cvetković D., Davidović T., *Multiprocessor interconnection networks with small tightness*, Internat. J. Foundations Computer Sci., 20(2009), No. 5, 941-963.

The further study of integral graphs in connection to multiprocessor topologies seems to be a promising subject for future research.

Recall that $3, 1^5, (-2)^4$ is the spectrum of the Petersen graph.



An eigenvector for eigenvalue 1 and a load balancing flow

Thank you for your attention