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Laplace eigenvalues of graphs—a survey

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Abstract

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Several applications of Laplace eigenvalues of graphs in graph theory and combinatorial optimization are outlined.

1. Introduction

There are several important results in combinatorics whose proofs use linear algebra although the results as such have no direct connection with algebra. One of the early results of this type is the well-known Fischer's inequality [36] which imposes a simple nontrivial condition on the parameters of a design. A similar result is the theorem of Feit and Higman [30]. There are several other results, using linear algebra in their proofs, about non-existence of several combinatorial objects, such as designs, codes, or graphs with certain properties. Let us refer to [8, 26, 27, 53]. The adjacency matrix of a graph and its eigenvalues are closely related to the generating function of the number of walks on graphs. This relationship was particularly useful in the theory of distance-regular graphs, cf. [8, 14]. Lovász [54] used linear algebra in the problem of determining the Shannon capacity of graphs. Finally, let us mention the explicit construction of expanders [55, 56] which were previously known to exist only by probabilistic methods. The proof that the constructed 'Ramanujan graphs' give rise to very good expanders relies on the estimates of eigenvalues of these graphs. Cf. also [5, 60].

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In this paper we survey several applications of eigenvalues of Laplace matrices of graphs, in graph theory and in combinatorial optimization. We refer to the survey paper [60] for a detailed introduction to the Laplace spectrum of graphs. The reason for another survey on a similar topic lies in the fact that since 1988 when [60] was prepared, many new applications of Laplace eigenvalues were discovered. Here we shall shortly discuss the following topics: edge density in cuts, partition of vertices using eigenvectors, an extension to hypergraphs, hamiltonicity, ζ-functions on graphs and some related problems. Several other applications are described in [60]. The main intention of the paper is more in motivating some further research in the outlined areas than presenting new results.

Given a graph G of order n, let $A = A(G)$ be its adjacency matrix. It will be assumed that rows and columns of graph matrices are indexed by $V = V(G)$. The same holds for vectors $x \in \ell^2(V)$ on which such matrices act by matrix multiplication. The entry a_{uv} of $A(G)$ is equal to the number of edges between vertices u and v. If $D = D(G)$ is the diagonal matrix with vertex degrees on the diagonal then the matrix $L(G) := D - A$ is the so-called *Laplacian matrix* of the graph G. The matrix $L(G)$ which will be our main concern, is positive semidefinite and symmetric. Its smallest eigenvalue is $\lambda_1 = 0$. Denote by $\lambda_k = \lambda_k(G)$ the kth smallest eigenvalue of $L(G)$, respecting the multiplicities, $k = 1, 2, \ldots, n$. In particular, λ_n is the maximal eigenvalue of $L(G)$. Cf. [60] for more details.

Let us mention that most of the results presented in this paper hold for general weighted graphs where one has to change the definitions accordingly. Almost all of the proofs and ideas follow the same lines in this general setting. Of course, the adjacency matrix is replaced by the weighted adjacency matrix, the degree of a vertex by the sum of the weights of the edges incident to the vertex, etc.

2. Edge density in cuts

A set of edges $F \subseteq E(G)$ in a graph G is a *cut* (sometimes also called *edge-cut*) if there is a set $X \subseteq V(G)$ of vertices of G such that F consists of precisely those edges of G which have one end in X and the other end in $V(G)\backslash X$. We also write $F = \delta X = \delta(V(G)\backslash X)$. Given X, the corresponding cut δX is also called the *coboundary* of X. A cut F is *nontrivial* if $F = \delta X$ for some $X \subset V(G)$, $X \neq \emptyset$. The *edge-density* of such a cut δX is defined as

$$\rho(X) := \frac{|\delta X|}{|X|\,|V(G)\backslash X|} \tag{2.1}$$

and it represents the density of the edges between the set X and its complement. Notice that in a connected graph G, $\rho(X)$ depends on the cut only, but in general it also depends on the choice of X corresponding to the cut.

It is very important that the eigenvalue $\lambda_2 = \lambda_2(G)$ imposes a nontrivial lower bound on edge-densities in cuts.

Proposition 2.1. *Let G be a graph of order n. For any nontrivial subset X of vertices of G, $X \neq \emptyset$, $X \neq V(G)$, the edge-density is uniformly bounded below and above as*

$$\frac{\lambda_2(G)}{|V(G)|} \leq \rho(X) \leq \frac{\lambda_n(G)}{|V(G)|}. \tag{2.2}$$

The proof of Proposition 2.1 is 'standard': If $x \in \ell^2(V)$ is a vector with entries $x_v = 1/|X|$ for $v \in X$, and $x_v = -1/|V \setminus X|$ for $v \notin X$, then x is orthogonal to the eigenvector $(1, 1, \ldots, 1)^t$ of the smallest Laplacian eigenvalue $\lambda_1 = 0$ of G. Therefore, by the well-known Courant–Fischer's principle,

$$\lambda_2(G) \leq \frac{(L(G)x, x)}{(x, x)} \leq \lambda_n(G).$$

Finally, $(L(G)x, x)/(x, x)$ turns out to be equal to $|\delta X| \cdot |V(G)|/(|X| \cdot |V \setminus X|)$, which in turn implies the bounds of (2.2).

Let us mention that the above proof and (2.2) remain valid also in the case when the graph G is weighted. In this case $|\delta X|$ means the weighted cardinality, i.e., the sum of the weights in the coboundary of X.

There is another upper bound on the minimal density of cuts in terms of $\lambda_2(G)$.

Proposition 2.2. *If $G \neq K_2$ is a nontrivial graph then*

$$\min\{\rho(X) \mid X \subset V(G), X \neq 0\} \leq \frac{2}{|V(G)|} \sqrt{\lambda_2(G) \cdot [2\Delta(G) - \lambda_2(G)]}$$

where $\Delta(G)$ is the maximal vertex degree in G.

Proof. If $G = K_3$, the result obviously holds. Otherwise, let X be a subset of $V(G)$ containing at most half of the vertices such that the ratio $|\delta X|/|X|$ is as minimal as possible. It is shown in [61, Theorem 4.2] that $|\delta X|/|X| \leq \sqrt{\lambda_2(2\Delta - \lambda_2)}$. Since $|X| \leq \frac{1}{2}|V(G)|$, $\rho(X) \leq (2/|V(G)|)(|\delta X|/|X|)$ which implies our inequality. □

Inequalities of the above type are discrete versions of the well-known Cheeger's inequality from differential geometry [16]. Such a bound appeared in [4] and later as an improved edge version in [61].

3. Partitioning with eigenvectors

An eigenvector $x^{(2)}$ corresponding to $\lambda_2(G)$ provides a very good heuristic for partitioning the vertices of a graph into two parts with small interference

(relatively few edges between the two parts). Partitions $V(G) = A \cup B$ with δA relatively small in size can be obtained as follows. Order the vertices of G according to the increase of their coordinates in $x^{(2)}$, if i.e., $u \leq v$ then $x_u^{(2)} \leq x_v^{(2)}$. Let $A_u := \{v \in V(G) \mid v \geq u\}$ and let $B_u := V(G) \setminus A_u$ for $u \in V(G)$. Depending on the problem where we need the partition we choose a vertex u such that the partition $A_u \cup B_u$ is as good as possible. Usually one wants the sets A, B of the partition to be of equal cardinality (within one element).

The reason why such partitions give satisfactory results is simple. Eigenvectors $x^{(2)}$ of λ_2 are the vectors for which the minimum of the quadratic form $(L(G)x, x)$, where $(x, x) = 1$ and $(x, \mathbf{1}) = 0$ where $\mathbf{1} = (1, 1, \ldots, 1)^t$. By using the Lagrange identity

$$n(x, x) - (x, \mathbf{1})^2 = \frac{1}{2} \sum_{u \in V} \sum_{v \in V} (x_u - x_v)^2 \tag{3.1}$$

where $n = (\mathbf{1}, \mathbf{1}) = |V|$, and the well-known expression for $(L(G)x, x)$:

$$(L(G)x, x) = \sum_{uv \in E(G)} (x_u - x_v)^2, \tag{3.2}$$

one immediately has that among all vectors x orthogonal to $\mathbf{1}$, the eigenvectors of λ_2 attain the minimum of

$$\sigma(x) := \frac{\sum_{uv \in E(G)} (x_u - x_v)^2}{\sum_{u \in V} \sum_{v \in V} (x_u - x_v)^2}. \tag{3.3}$$

But $\sigma(x)$ is invariant for adding a constant multiple of $\mathbf{1}$ to x, so these eigenvectors also give the minimum of $\sigma(x)$ on $\ell^2(V)$ without the constant vectors. This means (heuristically) that most of the edges of G will join vertices which are not too far w.r.t. our ordering $\leq$.

It was mentioned in [60] that this strategy based on eigenvectors of λ_2 is a good general heuristic for all problems of 'divide and conquer' type, and it was later applied by Pothen et al. [67] on the problem of partitioning sparse matrices into an 'almost block diagonal' structure. Similar heuristic was also investigated by Juvan and the author [49, 50] on some problems using linear labellings of graphs (bandwidth, cutwidth, the min-sum problem, etc.).

Juhász and Mályusz [48, 46] considered the question of finding a vertex set X which minimizes a quantity similar to $\rho(X)$. They used the eigenvalue approach as well but with a different matrix—$PA(G)P$ where P is the projection to the orthogonal complement of $(1, 1, \ldots, 1)^t$. Juhász [46, 47] and Bolla [9] further analyse eigenvalue approach for partitioning the vertices of a graph into two or more clusters. Further progress in this direction was made by Boppana [10].

A similar idea is used in connection to the max-cut problem by Poljak et al. [28, 64].

We shall do the basic analysis of the proposed partitioning algorithm. We start with some results about trees which show that the heuristic is good but also

'arbitrarily bad' in some degenerate cases. Let $S_{d,k}$ be the tree obtained from d copies of the path P_k by identifying an end-vertex of each of the paths to obtain a vertex in $S_{d,k}$ of degree d. It is easy to see, using the symmetries of $S_{d,k}$, that there exist eigenvectors of $\lambda_2(S_{d,k})$ which have values 0 on all except on two of the original paths. In this case, without an extreme care how to separate vertices with $x_v^{(2)} = 0$, the obtained separations may be far from the optimum. It should be mentioned that this example is degenerate in a sense that it is very unlikely that a numerical algorithm would produce the above eigenvector since λ_2 has large multiplicity in $S_{d,k}$.

By a result of Fiedler [32], every eigenvector x of $\lambda_2(T)$ of a tree T has either

(a) all values x_v different from 0. In this case T contains exactly one edge uw such that $x_u < 0$ and $x_w > 0$. The values x_v along any path in $T - uw$ starting at u decrease, and along the paths starting at w increase.

(b) or $N := \{v \in V(T) \mid x_v = 0\} \neq \emptyset$. Then the subgraph of T induced on N is connected, and there is exactly one vertex $w \in N$ which has neighbours not belonging to N. The x-values along paths in T starting from w either increase, decrease, or are equal to zero.

In [32] there is also a generalization of the above result to the sign structure of $x^{(2)}$ with respect to the block structure of the graph.

Fiedler's results show that the separation of vertices in a tree based on the sign of $x_v^{(2)}$ is heuristically good. A heuristic argument for a general graph is as follows. Eigenvectors of $\lambda_2(G)$ minimize the quadratic form (3.2) subject to $\|x\| = 1$ and $(x, \mathbf{1}) = 0$. Let $x = x^{(2)}$ and let $A = \{v \mid x_v < r\}$, $B = \{v \mid x_v \geq r\}$, for some chosen r, be our vertex partition. Then it is very likely that this partition is a local optimum with respect to exchange of a vertex in A with a vertex in B. The reason is simple: suppose we exchange $v \in A$ with $u \in B$. Define $x' \in \ell^2(V)$ by setting $x'_v = x_u$, $x'_u = x_v$, and $x'_w = x_w$ for other vertices w. Then $\|x'\| = 1$ and $(x', \mathbf{1}) = 0$. The quadratic form (3.2) will not decrease if we take x' instead of x since x determines its minimum. This means that it is very likely that $|\delta A|$ and $\rho(A)$ will increase as well. The reader is referred to [49] and [67] for some additional analysis. Further results can be found in [68].

4. Laplacian on hypergraphs

I was asked several times how could one extend the graph eigenvalue results to hypergraphs. Here we point out one possibility.

Bolla [9] defines the 'Laplacian' matrix $L_2(H)$ of a hypergraph $H = (V, E)$ in the following way. Let $D = D(H)$ be the diagonal matrix of size $|V|$ with vertex degrees on the diagonal, and let $D' = D'(H)$ be the diagonal matrix indexed by E and with edge cardinalities on the diagonal. If $Q = Q(H)$ is the $V \times E$ (unoriented) incidence matrix of H then

$$L_2(H) := D - QD'^{-1}Q^{\mathrm{T}}.$$

It is easily seen that

$$L_2(H) = L(G) \tag{4.1}$$

where $G = (V, E')$ is the weighted graph on the same vertex set V as H, obtained by replacing each edge e of H by a clique on the set of vertices of e, and with edge-weights in this clique equal to $1/|e|$. Of course, if a pair of vertices belongs to more than one edge of H then the weight of the corresponding edge in G is equal to the sum of the contributions $1/|e|$ for all such edges e.

It should be mentioned that there are other possibilities how to assign a graph G to a hypergraph H. For example, the edges in the cliques in the above case may be assigned some other weights. The choice depends on the problem where we try to apply algebraic methods on the graph G to obtain results for H.

Let us mention that the Laplacian of a block design as introduced above can also be used in statistical design [17, 23–25].

A different and slightly less obvious approach to the eigenvalues of hypergraphs was introduced by Friedman and Wigderson [38]. Having a 3-uniform hypergraph H, they look at the norm of the natural trilinear form associated to H, and define $\lambda_2(H)$ as the absolute difference to the norm of the trilinear form obtained from the original one by subtracting a multiple of the trilinear form with all coefficients equal to 1. However, their 'eigenvalues' are not eigenvalues in any classical sense.

Another possibility is presented in [74, 76, 77].

5. Hamiltonicity

The problem to determine whether the given graph G contains a hamilton cycle is extremely difficult. If G is hamiltonian then one may be lucky by guessing a solution, but proving that a graph is not hamiltonian is a hopeless task since this problem is co-NP-complete. Let us present a surprising eigenvalue based criterion for non-hamiltonicity which is proved in [62].

Theorem 5.1. *Let G be a cubic graph of order n, and let $0 = \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$ be its Laplace eigenvalues. If there is an index k such that either*

(i) $\lambda_k > 4 - 2\cos((2\pi/n)\lfloor k/2 \rfloor)$, *or*

(ii) $n/2 < k \leq n$ *and* $\lambda_k < 4 - 2\cos((2\pi/n)\lfloor (5n + 2 - 2k)/4 \rfloor)$

then G does not contain a hamilton cycle.

The Petersen's graph is an example of a graph whose eigenvalue distribution implies on the basis of Theorem 5.1 that it is not hamiltonian. Unfortunately, it seems that Theorem 5.1 can not be applied on very large graphs. But already the fact that algebraic properties may affect hamiltonicity is important since it provides us with a hope that some graphs with 'unusual' eigenvalue properties may be non-hamiltonian. Based on this observation there is an ongoing research

about hamiltonicity of certain Cayley graphs of some simple groups which are known to have strange eigenvalue distribution.

Finally let us mention another algebraic sufficient condition for non-hamiltonicity. Heilmann and Lieb [44] proved that all the zeros of the matching polynomial of a hamiltonian graph must be simple. Therefore multiple zeros indicate non-hamiltonicity. So far, the presented results are the only 'useful' results in this direction known to the author.

6. ζ-Functions on graphs

The Riemann zeta function is defined as

$$\zeta(s) := 1 + 1^{-s} + 2^{-s} + 3^{-s} + \cdots . \tag{6.1}$$

It is naturally connected to the Laplace differential operator on the 1-sphere whose nth eigenvalue is $\lambda_n = n^2$, $n = 0, 1, 2, \ldots$, and thus

$$\zeta(2s) = 1 + \sum_{n=1}^{\infty} \lambda_n^{-s}. \tag{6.2}$$

In analogy to this expression, every Laplacian operator determines the corresponding ζ-function. So, if G is a connected graph with Laplace eigenvalues $0 = \lambda_1 < \lambda_2 \leq \lambda_3 \leq \cdots \leq \lambda_n$, then the ζ-function of G is

$$\zeta(G; 2s) := 1 + \sum_{i=2}^{n} \lambda_i^{-s}, \quad s \in \mathbb{C}. \tag{6.3}$$

Some known results can be formulated in terms of the ζ-function.

Theorem 6.1 (McKay). *If G is a tree of order n then*

$$\zeta(G; 2) = \frac{n-1}{2} \cdot \bar{\rho}(G) + 1$$

where $\bar{\rho}(G)$ is the mean distance of G.

The proof of this result can be found for example in [63], or in [57]. Another result is just the reformulation of the well-known Matrix Tree Theorem.

Theorem 6.2 (Kirchhoff). *If G is a graph of order n, and $\kappa(G)$ denotes the number of spanning trees of G then*

$$\zeta'(G; 0) = -\ln(n\kappa(G)).$$

There is some evidence that one might predict chemical and physical properties of a (hypothetical) molecule, whose underlying structural graph G is known, on the basis of the ζ-function of G.

Another promising area of research might be investigating the properties of zeros or singularities of $\zeta(G;s)$. No results or experiments in this direction are known.

There are other expressions for the Riemann zeta function. A well-known formula, which shows why the properties of $\zeta(s)$ are so closely related to the distribution of primes, is the following:

$$\zeta(s) = \prod_p \left(1 - \frac{1}{p^s}\right)^{-1}, \tag{6.4}$$

where the product runs over all primes p. There is an analogous function related to the Laplacian on manifolds. It is important because of its close relationship to the geodesics on manifolds. A corresponding function on graphs was introduced by Ihara and Sunada [71] in case of regular graphs.

Let G be a k-regular graph. Let us for simplicity also assume that G is simple. A closed walk $x_0, x_1, \ldots, x_n = x_0$ is *reduced* if $x_{i-1} \neq x_{i+1}$ for $i = 1, 2, \ldots, n$. It is *prime* if it is not of the form

$$y_0, y_1, \ldots, y_t, y_0, y_1, \ldots, y_t, \ldots, y_0, y_1, \ldots, y_t$$

with the sequence $y_0, \ldots, y_t$ repeated at least twice. Call closed walks $x_0, x_1, \ldots, x_n = x_0$ and $y_0, y_1, \ldots, y_n = y_0$ *equivalent* if $y_t = x_{t+d}$ (indices modulo n) for each t and some fixed a.

The Ihara-Sunada's zeta function of the graph G is

$$Z(s) := \prod_C \left(1 - \frac{1}{(k-1)^{s \cdot l(C)}}\right)^{-1},$$

where the product runs over all equivalence classes of prime reduced closed walks C in G, and $l(C)$ denotes the length of C.

Theorem 6.3 (Sunada). *All the singularities (poles) of $Z(s)$ in the strip $0 < \operatorname{Re} s < 1$ are on the line $\operatorname{Re} s = \frac{1}{2}$ if and only if G is a Ramanujan graph.*

Let us recall that a k-regular graph G is a *Ramanujan graph* [55] if all its Laplace eigenvalues except 0 and possibly $2k$ lie in the interval $[k - 2\sqrt{k-1}, k + 2\sqrt{k-1}]$. Up to the breakthrough of Lubotzky et al. [55] and independent discovery of Margulis [56], Ramanujan graphs were known to exist only by probabilistic methods. Explicitly constructed Ramanujan graphs play an important role in the construction of several networks (e.g., the expanders and superconcentrators), in the design of explicit algorithms, and in several other problems of theoretical computer science (see, e.g., [4, 5], or the survey [60]). Therefore it is not surprising that other papers appeared with constructions of Ramanujan graphs [7, 18, 52, 66]. It should, however, be pointed out that all known constructions are number theoretic in nature.

7. Some other results

Given a walk W in graph G, the *cover time* of W is the number of steps of W required to visit every vertex of G. Considering a random walk, one can ask about the expected cover time. It turns out that the expected cover time relates to the eigenvalues of the random walk transition matrix which is, at least for regular graphs, related to the Laplacian. Upper and lower eigenvalue bounds on the expected cover time were derived by Broder and Karlin [11]. The bounds depend on $\lambda_2(G)$. Related results were obtained by some other authors [1–3, 51, 65, 69]. A similar approach gives useful results for some other problems, e.g., the rapidly mixing Markov chains [70].

Let us finally mention several papers which investigate properties (not applications) of Laplace eigenvalues of graphs, and may therefore contain useful results for applications described above or in applications to be discovered in the future. The earliest applications of Laplace eigenvalues in graph theory go back to Fiedler [31] (cf. [60] for other early works of Fiedler). His recent works in this area are [31, 33, 34]. Another source of new results about the Laplace eigenvalues of graphs emerges from Merris et al. [40–42, 57–59]. Some additional references are [73, 43].

Broder and Shamir [12] estimated the second eigenvalue of random regular graphs of fixed even valency. Their result was improved by Friedman et al. [37]. They showed that all nontrivial Laplace eigenvalues of a $2d$-regular graph of order n lie in an $O(\sqrt{d})$-interval around the mean $2d$ with high probability. More precisely, the expected value of $2d - \lambda_2(G)$ and of $\lambda_n(G) - 2d$ over all $2d$-regular graphs of order n is bounded above by

$$2\sqrt{2d-1} + 2\log d + O(1) + O\left(\frac{d^{\frac{1}{2}} \log\log n}{\log n}\right),$$

where the logarithms are base e and the constants in the oh-notation do not depend on d.

The behaviour of adjacency matrix eigenvalues of random graphs was determined by Juhász [45] and Füredi and Komlós [39]. Using their results the Laplace eigenvalues of random graphs (edge probability p) are shown in [50] to lie between $pn - f(n)$ and $pn + f(n)$ (a.s.), where

$$n = |V(G)|, \qquad f(n) = \sqrt{(3+\varepsilon)(1-p)pn \log n}$$

and $\varepsilon > 0$ arbitrary.

The eigenvalue behaviour of random graphs is important because it implies several other properties to hold for almost all graphs. More important is that many such properties are mutually equivalent and equivalent to the property that except $\lambda_1 = 0$ all other eigenvalues are close to the average degree of the graph. A graph having any of these properties possesses all others, and it is said to be *quasi-random* [21] since it shares many properties of random graphs. See Chung et al. for more details [19–22]. The idea of mimicing a random structure by

explicit objects appears also in other disciplines. Let us only mention the use of eigenvalues for such a purpose in the discrepancy theory (irregularities of partitions). See, e.g., [6].

Finally let us mention another area of mathematics where the Laplace eigenvalues of graphs came into the game. The spectral properties of the Laplacian on Riemannian manifolds are closely related to eigenvalue properties of corresponding graphs. The relation is mutual—graphs give rise to certain Riemannian manifolds with spectral properties inherited from the graph Laplacian, and conversely, the geometric dual graphs of certain 'nice' triangulations of a Riemannian manifold represent the manifold well enough in order that the graph eigenvalues give some information about the manifold. Let us mention just a recent reference [15] and an older one [13].

Note added in proof. There are several recent achievements related to the topic of this survey [74–93].

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