Contemporary Mathematics

Weighted Laplacians and the Sigma Function of a Graph

Fan Chung and Ross M. Richardson

Abstract. We consider a general notion of the Laplacian of a graph. The weight of an edge reflects both the width and the length of an edge. Further, we allow the edge weights to vary in order to minimize the maximum eigenvalue, and using this minimum we construct the so-called $\sigma-$function of a graph. We consider a geometric interpretation of the $\sigma-$function, in particular as it applies to the detection of certain extremal configurations. Of special interest are $\sigma-$critical subgraphs. We derive several results about $\sigma-$critical graphs as well as offering conjectures about their structure. These results are related to applications in graph drawing algorithms and clique detection problems.

1. Introduction

The notion of weighted graphs, i.e. graphs for which each edge carries an associated number or cost, is fundamental to many applications of graph theory. A number of natural interpretations of edge weight exist in various contexts: in optimization, cost or capacity is natural, in electrical network theory each edge may carry resistance or capacitance, in random walks each edge carries a probabilty of from moving from one incident vertex to the other, and in geometric or analytical applications the use of edge length is often most appropriate.

The spectral theory of graphs has been well studied over the last few decades. The original body of research in spectral graph theory examined combinatorial consequences of the spectrum of the adjacency matrix, for which an excellent reference is Cvetković, Doob, and Sachs [**4**]. More recent work has focused on the spectrum associated to the *Laplacian* of a graph, which forms a discrete analog of the Laplace-Beltrami operator of spectral geometry (see [**2**] for an overview).

In this work, we shall concern ourselves with the study of the largest eigenvalue of the (normalized) Laplacian. The $\sigma-$function of a graph was introduced in [**2**] as a way of measuring how small the largest eigenvalue may become over all possible choices of edge weights. It is shown that the $\sigma-$function of a graph is bounded

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2000 *Mathematics Subject Classification.* Primary;05C75, Secondary;58J50, 81Q10, 05C80, 05C85, 90C22, 90C35.

Key words and phrases. Weighted Graph, Metric Graph, Spectral Graph Theory, Sigma Function, Lovász Theta Function, Graph Drawing, Random Graphs.

Research supported in part by NSF Grants DMS 0457215, ITR 0205061 and ITR 0426858.

between the clique and chromatic number of a graph, and in this way provides a geometric relaxation of these two fundamental combinatorial properties of a graph.

Galtman [**7**] showed that the $\sigma-$function coincides with the *Delsarte Linear Programming Bound* [**17**]. This quantity in turn is related to the celebrated $\vartheta-$function of Lovász, introduced in [**16**] as a means of estimating the *Shannon capacity* of a graph. The $\vartheta-$function (of the complement of a graph) shares the property of being bounded by the clique and chromatic number of a graph with the $\sigma-$function, and indeed the two are related by $\sigma(G) \le \vartheta(\bar{G})$. Galtman in [**7**] showed that the $\vartheta-$function may also be formulated in terms of the largest eigenvalue of a weighted Laplacian, but the characterization of allowable weights is more complicated (negative weights may occur) and might not be useful in some geometric situations. Indeed, it has been shown that there are a number of possible relaxations of the independence number of a graph besides σ and ϑ, but from the point of view of weighted Laplacians the $\sigma-$function appears to be the most natural.

The intent of this paper is to explore the relation between the $\sigma-$function of a graph and the edge weights induced by the $\sigma-$function. To this end, we introduce some necessary background in weighted graphs and the combinatorial Laplacian in section 2. We then define in section 3 the $\sigma-$function of a graph and list some basic properties useful to our study. Section 4 includes a number of alternate characterizations of the $\sigma-$function. In section 5 we introduce $\sigma-$critical graphs and prove several results regarding their structure. Finally in section 6 we discuss some conjectures and future directions for further work.

2. Preliminaries

Let $G = (V, E)$ be a simple, loopless graph with $|V| = n$. We shall assume that the vertices of G are labeled $\{1, 2, \ldots, n\}$, and further all graphs considered shall have no isolated vertices. The complete graph on n vertices, containing all possible edges, is denoted by K_n. The cycle on n vertices is C_n. A subgraph H of G on k vertices is said to be a *clique* of G if it is complete. The *clique number* of G, denoted by $\omega(G)$, is the number of vertices in a largest clique of G. For a set S, a function $f : V(G) \to S$ is said to be a proper coloring of G if $f(u) \neq f(v)$ whenever $u \sim v$. The *chromatic number* $\chi(G)$ is the size of the smallest set S for which there exists a proper coloring.

A bijection f from $V(G)$ to itself is an automorphism of G if it preservers the edge relation, i.e. $f(u) \sim f(v)$ if and only if $u \sim v$. Function composition turns the set of automorphisms into the *automorphism group* of G, denoted by $\mathrm{Aut}(G)$. A graph G is said to be *vertex-transitive* if for all $u, v \in V(G)$ there exists an automorphism which maps u to v. Similarly, a graph is edge-transitive if for all $e, f \in E(G)$ there exists an automorphism which maps e to f.

J_k is the $k \times k$ matrix consisting of all ones. A symmetric matrix $A \in M_{k\times k}(\mathbb{R})$ is said to be positive semidefinite if $x^T A x \ge 0$ for all $x \in \mathbb{R}^k$ (if the inequality is strict we say A is positive definite); we denote this by $A \succeq 0$. The largest eigenvalue of a matrix A is denoted by $\Lambda(A)$.

We say that a geometric framework for a quantum graph consists of the combinatorial graph structure $G = (V, E)$ combined with a *width* (or capacity) $c : E(G) \to \mathbb{R}_{\ge 0}$ and *length* $l : E(G) \to \mathbb{R}_{\ge 0}$. We can view each edge $e \in E(G)$ as a copy of the segment $[0, l_{ij}]$, which gives a metric graph. If we interested in the discrete case, the key object of study is the *Dirichlet sum* of a function $f : V(G) \to \mathbb{R}$:

$$\sum_{i\sim j}(f(i) - f(j))^2 w_{ij}.$$

This provides a discrete analog to the Dirichlet space metric $\int_G |u'|^2 c(x)dx$ as follows: if we interpret u' as $(f(i)-f(j))/l_{ij}$ for each point on the line, the integration yields $\sum_{i\sim j} |u'|^2 c_{ij} l_{ij} = \sum_{i\sim j}(f(i) - f(j))^2 w_{ij}$ provided we take $w_{ij} = c_{ij}/l_{ij}$. See [**6**], [**14**] for more on metric graphs.

We may associate to G a *weight matrix* $W \in M_{n\times n}$ which satisfies the following properties:

(1) $w_{ij} = w_{ji}$.
(2) $w_{ii} = 0$.
(3) $w_{ij} \geq 0$ and $w_{ij} = 0$ if i is not adjacent to j in G.

Further, we let $w_i = \sum_{j\sim i} w_{ij}$, which is referred to as the *degree* of i (the graph theoretic degree is recovered in the case where the weight matrix is given by the adjacency matrix).

We define the *weighted combinatorial Laplacian* L_W associated to W to be an operator on $\mathbb{R}^{|V|}$ for which

$$Lf(x) = \sum_{\substack{y \\ x\sim y}}(f(x) - f(y))w_{xy}.$$

Such an operator can also be given explicitly by the matrix

$$L_W(i,j) = \begin{cases} w_i & i = j, \\ -w_{ij} & i \sim j. \end{cases} \tag{1}$$

It is useful when dealing with spectral questions to work with a normalized form of the combinatorial Laplacian. Thus we next define the *weighted normalized combinatorial Laplacian* $\mathcal{L}_W$ associated to W by:

$$\mathcal{L}_W(i,j) = \begin{cases} 1 & i = j, \\ \frac{-w_{ij}}{\sqrt{w_i w_j}} & i \sim j \text{ and } w_i w_j \neq 0, \\ 0 & \text{otherwise.} \end{cases} \tag{2}$$

The operation of $\mathcal{L}_W$ then becomes

$$\mathcal{L}_W f(x) = \frac{1}{\sqrt{w_x}} \sum_{\substack{y \\ x\sim y}} \left(\frac{f(x)}{\sqrt{w_x}} - \frac{f(y)}{\sqrt{w_y}} \right).$$

The vector $(\sqrt{w_1}, \ldots, \sqrt{w_n})$ is an eigenvector for $\mathcal{L}_W$ with eigenvalue 0, and further 0 is the smallest eigenvalue. Labeling the eigenvalues associated to a given weight matrix W associated to a graph G in increasing order $0 = \lambda_0^W \leq \lambda_1^W \leq \ldots \leq \lambda_{n-1}^W$ we have the following two formulæ, which follow directly from the standard variational characterization of eigenvalues:

(3)

$$\lambda_1^W = \inf_{\substack{f \\ \sum f(x)w_x = 0}} \frac{\sum_{x\sim y}(f(x) - f(y))^2 w_{xy}}{\sum_{x\in V} f^2(x) w_x}, \quad \lambda_{n-1}^W = \sup_f \frac{\sum_{x\sim y}(f(x) - f(y))^2 w_{xy}}{\sum_{x\in V} f^2(x) w_x}.$$

Finally, we note that two weight matrices for G yield the same normalized Laplacian when they are constant positive multiples of one another. Henceforth, we consider all weight matrices related by a positive multiple to be equivalent.

A full reference to these definitions may be found in [**2**].

3. Some Facts about the $\sigma-$Function

In the study of the normalized weighted Laplacian (2), a natural question is the effect of a change in the weight matrix W associated with G to the spectrum of $\mathcal{L}_W$. If we vary the edge weights of a graph (while maintaining zero weights for non-edges), what happens to the largest eigenvalue? How large or small can this value be, and what role does the combinatorics of the underlying graph play in these extremes? We know, for example, that on a connected graph $\lambda_{n-1}^W \geq \frac{n}{n-1}$, which follows from the simple bound $\lambda_0^W + \lambda_1^W + \ldots + \lambda_{n-1}^W = n$ obtained from the trace of $\mathcal{L}_W$. With fewer edges (and thus fewer non-zero edge weights), can we obtain a larger lower bound?

For the simplest case, $G = K_2$, $\lambda_{n-1}^W(K_2) = 2$ regardless of the choice of weight matrix. However, setting $G = K_3$ the situation becomes more complicated as we can force λ_{n-1}^W to be different values in $[3/2, 2]$ with a proper choice of weight matrix. The upper bound on λ_{n-1}^W is not interesting because any graph may obtain it by having only one non-zero edge weight. The lower bound, however, depends on the underlying graph, and thus is a natural object of study.

Looking again at the example of the triangle K_3, we claim that $\lambda_{n-1}^W = 3/2$ if and only if the weights are all the same (i.e. W is the adjacency matrix). If we interpret an edge weight to be the inverse of the length of an edge (having the same capacity for the moment), then we see here that only the configuration of the triangle where all edges are the same length yields an optimal value of λ_{n-1}^W. This suggests that weight matrices corresponding to optimal values of λ_{n-1}^W carry with them geometric information about the graph.

3.1. Definition and Properties of the $\sigma-$Function. Let W be a nontrivial weight matrix for a graph G. The $\sigma-$function of G is

$$\sigma(G) = 1 + \max_W \frac{1}{\Lambda(\mathcal{L}_W) - 1}, \tag{4}$$

where the maximum is taken over all nontrivial weight matrices W associated to G.

We introduce some notation.

Definition 3.1. *A weight matrix W which achieves the maximum value in* (4) *is called an* optimal weight matrix *for G, or simply an* optimal weight matrix *if there is no confusion.*

Proposition 3.2 (Monotonicity). *For any H a subgraph of G,*

$$\sigma(H) \leq \sigma(G).$$

This follows by observing that the set of allowable weight matrices for H is a subset of those for G.

Proposition 3.3 (Connected Components). *Let G be the disjoint union of the graphs G_1 and G_2. Then*

$$\sigma(G) = \max(G_1, G_2).$$

This follows directly from the fact that $\mathcal{L}_W$ is in block diagonal form, with blocks corresponding to G_1 and G_2.

Perhaps the most important property of the $\sigma-$function is the so-called *Sandwich Theorem*, which gives combinatorial bounds on $\sigma(G)$. A self-contained proof can be found in [**2**]. The term "sandwich theorem" was coined by Knuth and explored in some depth in [**12**].

THEOREM 3.4 (Sandwich Theorem). *For a graph G,*

$$\omega(G) \leq \sigma(G) \leq \vartheta(\bar{G}) \leq \chi(G).$$

The sandwich theorem shows that $\sigma(G)$ is an estimator for $\omega(G)$ and $\chi(G)$. Moreover, $\sigma(G)$ allows us to characterize $\omega(G)$ and $\chi(G)$ on any graph where these quantities are the same (e.g. perfect graphs [**19**]).

3.2. Examples.

3.2.1. *Complete Graphs.* For a complete graph K_n, we know that $\Lambda(W) \geq n/(n-1)$ for any choice of W, so $\sigma(G) \leq n$. If A is the adjacency matrix of K_n (the matrix which is zero on the diagonal and 1 everywhere else), then we can choose $W = A$ and obtain

$$\mathcal{L}_W = I - \frac{1}{n-1}A.$$

This is of course the Laplacian associated to the adjacency matrix of K_n, which is $n/(n-1)$. Thus, the complete graph achieves $\sigma(G) = n = \omega(G) = \chi(G)$.

3.2.2. *Odd Cycles.* The odd cycles provide the simplest examples of graphs for which the clique and chromatic number are not equal. A result of Lovász states that for the odd cycle on n vertices, C_n, we have

$$\sigma(G) = \frac{1+\cos(\pi/n)}{\cos(\pi/n)}. \tag{5}$$

Observe that again, setting the weight matrix W to be the adjacency matrix A of C_n, we obtain

$$\mathcal{L}_W = I - \frac{1}{2}A.$$

Computing the largest eigenvalue of $\mathcal{L}_W$ yields this result. Thus, in both cases the weight matrix which achieves the optimal value of $\sigma(G)$ is the matrix which weights all edges evenly.

The case of even cycles is uninteresting because $\sigma = 2$ for all bipartite graphs and any nontrivial choice of weight matrix is optimal.

3.2.3. *Other Examples.* Figures 1-5 give a graphical representation of some optimal weight matrices. The weight matrices are normalized so that the largest entry of each is 1. See the key in figure 6.

4. Several Characterizations of the $\sigma-$Function

The $\sigma-$function has a number of alternate characterizations (see [**7**], [**9**], [**16**]). In particular, the $\sigma-$function is equal to a relative of the Lovász $\vartheta-$function, known as the *Delsarte linear programming bound* and often denoted $\vartheta'(\bar{G})$. We give here a few characterizations which will be useful in our study.

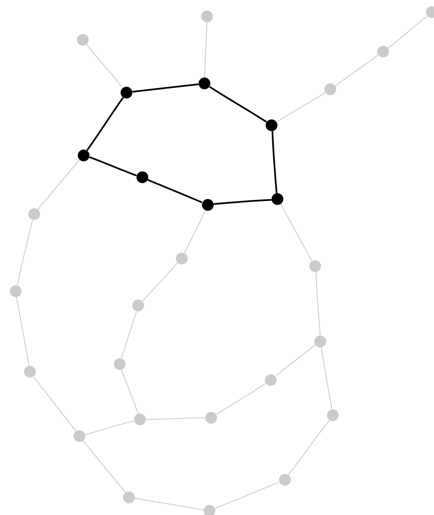

FIGURE 1. NBA Games. $\sigma = 2.1099$.

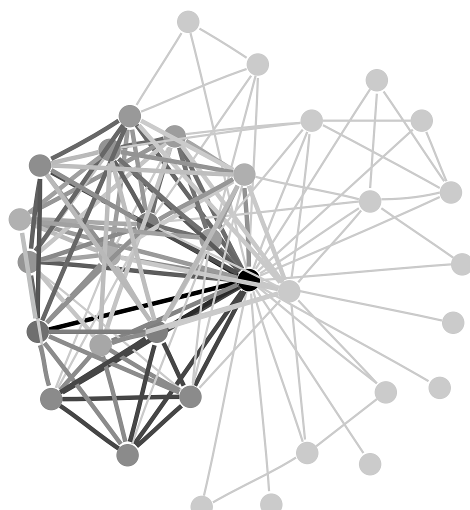

FIGURE 2. Erdős Collaboration Graph. $\sigma = 6.0270$.

4.1. σ_1**.** We denote by $\sigma_1(G)$ the optimal value obtained from the following semidefinite linear program.

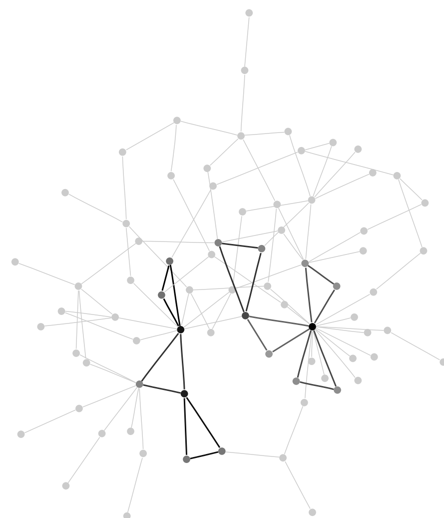

FIGURE 3. Dr. Seuss Graph. $\sigma = 3.0000$.

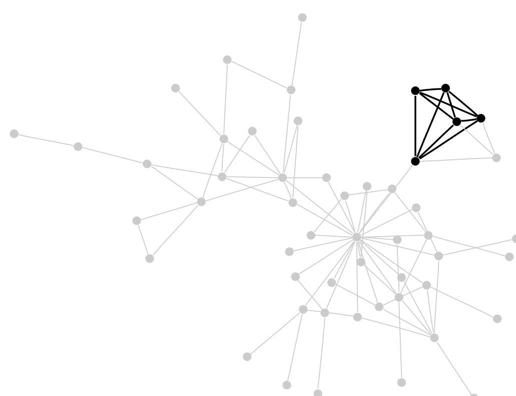

FIGURE 4. Partial Duplication Model. $\sigma = 5.0000$.

$$
\begin{aligned}
\text{maximize}\ \ & \operatorname{Tr}(J_n B) = \sum_{i,j} B_{ij} \\
\text{subject to}\ \ & B_{ij} = 0, \qquad i \not\sim j \text{ and } i \neq j \\
& \operatorname{Tr} B = 1 \\
& B \succeq 0 \\
& B_{ij} \geq 0, \qquad i, j = 1, \ldots, n.
\end{aligned}
\tag{6}
$$

This characterization proves useful when computing optimal weight matrices.

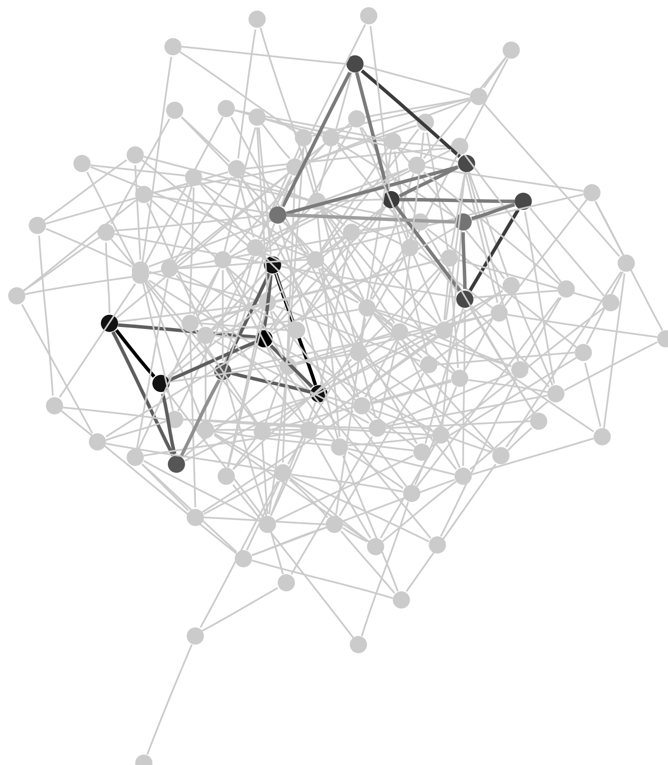

FIGURE 5. Erdős-Renyi Random Graph. $\sigma = 3.1966$.

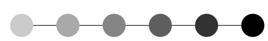

FIGURE 6. Key to graph edges and vertices. Weights increase from $0.0 - 1.0$ left to right, degrees increase from $0.0 - \max_v w_v$. Edges with weight greater than 0.0001 are shown in bold.

4.2. σ_2**.** For a graph G, let we say an $n-$tuple of vectors $v_1, \ldots, v_n$ in $\mathbb{R}^n$ is an *acute orthonormal labeling* of G if $|v_i| = 1$ for all i, $v_i \cdot v_j \geq 0$ for all i, j, and $v_i \cdot v_j = 0$ if $i \not\sim j$. Denote by $\sigma_2(G)$ the optimal value of the following:

$$\text{maximize } \sum_{i=1}^{n} (d \cdot v_i)^2, \tag{7}$$

where the maximization is taken over all acute orthonormal labellings and unit vectors d.

4.3. σ_3**.** The dual form of $\sigma_1(G)$ gives yet an alternate characterization for $\sigma(G)$, this time stated as a minimization problem. Let $A = (a_{ij})$ be an *admissible matrix* for G if $a_{ij} \geq 1$ whenever $i \sim j$ or $i = j$. The following optimal value is denoted by $\sigma_3(G)$:

$$\text{minimize } \Lambda(A), \tag{8}$$

where A is allowed to range over all admissible matrices for G.

4.4. σ_4**.** For a graph G, we say an $n-$tuple of unit vectors $v_1, \ldots, v_n$ in $\mathbb{R}^n$ is a *labeling with obtuse angles* if $v_i \cdot v_j \leq 0$ when $i \sim j$. Denote by $\sigma_4(G)$ the optimal value of the following:

$$\min_{\substack{v_1,\ldots,v_n \in \mathbb{R}^n \\ v_i \cdot d \geq 0, i=1,\ldots,n}} \max_{i=1,\ldots,n} \frac{1}{(v_i \cdot d)^2}, \tag{9}$$

where the minimum is taken over all unit vectors d and labelings with obtuse angles such that each vector v_i forms an acute angle with d.

4.5. σ_5**.** For a graph G, let $A = (a_{ij})$ be a nonnegative symmetric matrix for which $a_{ij} > 0$ only if $ij \in E(G)$. Denote by $\sigma_5(G)$ the optimal value of

$$1 + \sup_A \frac{\Lambda(A)}{\Lambda(-A)}, \tag{10}$$

where the supremum is taken over all matrices satisfying the above condition.

THEOREM 4.1 (Equivalence of Characterization).

$$\sigma_1(G) = \sigma_2(G) = \sigma_3(G) = \sigma_4(G) = \sigma_5(G) = \sigma(G).$$

For proofs, see [**7**], [**16**], and [**17**].

4.6. Conversion Formulæ. We require the following results about converting between several of the characterizations of the $\sigma-$function. Proofs can be found or adapted from [**16**] and [**7**].

We show how to generate solutions to σ_1 from σ_5 and conversely.

LEMMA 4.2. *Let A be an optimal solution to* (10)*. Let $\mathbf{v} = (v_i)_{i=1}^n$ be an nonnegative eigenvector corresponding to $\Lambda(A)$ such that $|\mathbf{v}|^2 = 1/\Lambda(-A)$. If we set $V = \mathrm{Diag}(v_1, \ldots, v_n)$ then*

$$B := V(A + \Lambda(-A)I)V$$

is an optimal solution to (6)*.*

LEMMA 4.3. *Let B be an optimal solution to* (6)*. Set*

$$v_i = \begin{cases} \sqrt{B_{ii}} & B_{ii} > 0 \\ 1 & B_{ii} = 0 \end{cases}.$$

If we set $V = \mathrm{Diag}(v_1, \ldots, v_n)$, then the matrix

$$A := V^{-1}BV^{-1} - I$$

is an optimal solution to (10)*.*

We show how optimal solutions lead to optimal weight matrices, and conversely.

LEMMA 4.4. *Let A be an optimal solution to* (10) *such that $\Lambda(A) = 1$. Set $\mathbf{v} = (v_i)_{i=1}^n$ be a positive fixed vector of A. Then an optimal weight matrix W is given by*

$$W_{ij} := v_i v_j A_{ij}.$$

LEMMA 4.5. *For a given weight matrix W, the matrix*

$$A := \mathcal{L}_W - I$$

is an optimal solution to (10)*.*

An obvious, but important, corollary of these lemmas is the following.

COROLLARY 4.6. *Given an optimal weight matrix W, there exist an optimal solution A to* (10) *and an optimal solution B to* (6) *such that*

$$w_{ij} > 0 \Leftrightarrow A_{ij} > 0 \Leftrightarrow B_{ij} > 0,$$

and similarly for A and B.

5. $\sigma-$Critical Graphs

Our goal is to explore the optimal weight matrices associated to a graph. We first show that when a graph is symmetric, the symmetric weight matrix (i.e. the adjacency matrix) is indeed optimal.

THEOREM 5.1. *Let G be an edge-transitive graph with adjacency matrix A. Then the adjacency matrix is an optimal weight matrix.*

PROOF. To show this, we appeal to the definition of $\sigma_1(G)$. We assume first that G is vertex-transitive.

Let B be an optimal solution matrix to (6), that is, $\mathrm{Tr}(B \cdot J) = \sigma(G)$. Let $\mathrm{Aut}(G)$ be represented by $n \times n$ permutation matrices P. Set

$$\tilde{B} = \frac{1}{\mathrm{Aut}(G)} \sum_{P \in \mathrm{Aut}(G)} P^{-1} B P.$$

$\tilde{B}$ is a positive linear combination of semidefinite matrices, so it is itself semidefinite. Further, $\mathrm{Tr}\,\tilde{B} = 1$, $\tilde{B}_{ij} > 0$ only if $i \sim j$ and $\mathrm{Tr}(\tilde{B}J) = \sigma(G)$, so $\tilde{B}$ optimizes (6). Because $\mathrm{Aut}(G)$ is both edge-transitive and vertex-transitive, $\tilde{B}$ is of the form $\alpha I + \beta A$. We may now appeal lemma 4.3 to note that A is thus an optimal solution to (10) which in turn implies that A is an optimal weight matrix.

When G is not vertex transitive, G is bipartite. Thus, the averaging step above produces a matrix

$$\tilde{B} = \begin{bmatrix} \alpha I & \gamma C \\ \gamma C & \beta I \end{bmatrix},$$

where $\alpha, \beta, \gamma > 0$ and C is a $0/1$ matrix corresponding to all the edges in G. This is also sufficient for the adjacency matrix to be an optimal weight matrix (by again using lemma 4.3 to conclude that A is an optimal solution to (10) and thus A is an optimal weight matrix). □

In the above proof, we showed that edge transitive bipartite graphs admit the adjacency matrix as optimal weight matrices. More generally, it is true that any nontrivial bipartite graph admits the adjacency matrix as an optimal weight matrix. To show this, we shall appeal to a more general framework.

Providing an analogy to the study of chromatic number and color-critical graphs, we introduced the notion of σ-critical graphs.

5.1. Definition of $\sigma-$Critical Graphs.

DEFINITION 5.2. *Let G be a graph with $\sigma(G) = k$. We say that G is $k - \sigma-$*critical *if $\sigma(G - e) < k$ for any edge $e \in E(G)$. A graph G is $\sigma-$critical if it is $k - \sigma-$critical for some $k = \sigma(G)$.*

REMARK 5.3. Note that the definition above allows for the inclusion or exclusion of isolated vertices. As our concern here is primarily with the edge structure of σ-critical graphs, this flexibility does not really affect our analysis. However, when we discuss the connected components of a $\sigma-$critical graph, we shall intend only the nontrivial components, i.e. those whose σ value is k.

We now consider some examples.

5.2. Examples.

5.2.1. *Cliques and Odd-Cycles.* For any edge $e \in E(K_n)$, $\sigma(K_n - e) = n - 1 < \sigma(K_n) = n$ by the sandwich theorem, so we see that cliques are color-critical. Similarly for odd cycles, removing any edge drops the σ value to 2, which is less than the σ value of an odd cycle.

We note that in both cases, the graphs involved are color critical as well as $\sigma-$critical. This leads to a conjecture.

CONJECTURE 5.4. *Every color-critical graph is $\sigma-$critical.*

The converse of this conjecture is in fact false. To see this, we look at the graph in figure 7.

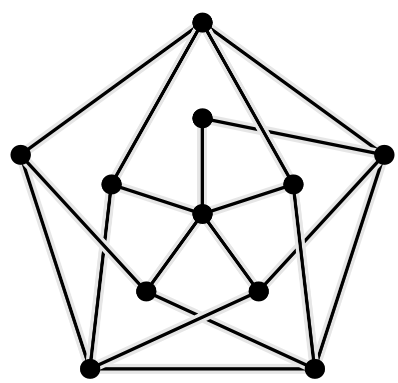

FIGURE 7. A $\sigma-$critical graph which is not color critical.

This graph is obtained by removing an edge from the Grötzsch graph, which is the five-cycle to which Mycielski's construction has been applied. Because the Grötzsch graph [**19**] is 4$-$color critical, the graph in figure 7 is 3$-$colorable. One can check that removing any single edge still leaves an embedded odd cycle, so this graph is not color critical. On the other hand, the σ value of the above graph is ≈ 2.3914 (with error less than 10^{-4}), whereas the maximum value of σ over all subgraphs obtained by removing an edge from this graph is ≈ 2.3837 (with error again less than 10^{-4}). Thus, this graph is $\sigma-$critical. These computations were performed using Matlab[1] and the SDP optimization package SeDuMi [**18**].

[1]MATLAB is a registered trademark of The MathWorks, Inc.

Thus, we see that $\sigma-$critical graphs are more difficult to characterize than color-critical graphs, and the conjecture asserts that they form a strictly larger set than the color critical graphs.

5.3. Optimal Weight Matrices. The use of $\sigma-$critical graphs allows us to characterize optimal weight matrices. We note that the non-zero entries of a weight matrix determine a subgraph. In what follows, we seek to characterize such subgraphs.

PROPOSITION 5.5. *If G is $\sigma-$critical with optimal weight matrix W, then for every edge $ij \in E(G)$, $w_{ij} > 0$.*

PROOF. If not, there would be some subgraph H of G such that $\sigma(H) = \sigma(G)$. By the monotonicity of σ, this implies that there exists some edge $e \in E(G)$ such that $\sigma(G - e) = \sigma(G)$, implying that G is not color-critical. □

For the next result, we need a definition of graph union. We say that if $H_1, \ldots, H_k$ are subgraphs of a graph G, then the *union* $\cup_{i=1}^k H_i$ is the subgraph of G with vertex set $\cup_{i=1}^k V(H_i)$ and edge set $\cup_{i=1}^k E(H_i)$.

PROPOSITION 5.6. *Let $H_1, \ldots, H_k$ be $\sigma-$critical subgraphs of a graph G. Then there exists an optimal weight matrix W for G such that $w_{ij} > 0$ only if $ij \in E(\cup_l H_l)$.*

PROOF. We shall use the characterization σ_1.

For each H_l, there is a B^l which optimizes (6) such that $B^l_{ij} > 0$ only if $ij \in E(H_l)$. As any convex combination of such matrices is also an optimal solution to (6), it follows that the matrix

$$\tilde{B} = \frac{1}{k} \sum_{i=1}^{k} B^l,$$

optimizes (6) and has the property that $\tilde{B}_{ij} > 0$ only if $ij \in E(\cup_l H_l)$. We appeal to corollary 4.6 to show that this gives an optimal weight matrix for which $w_{ij} > 0$ only if $ij \in E(\cup_l H_l)$. □

The converse of this proposition, that the $\sigma-$critical graphs characterize the full solution spaces, remains an open question. We state a (possibly) stronger conjecture, motivated by the above proof.

CONJECTURE 5.7. *Fix a graph G. Every matrix B which optimizes* (6) *may be expressed as a convex combination of matrices $B_1, \ldots, B_k$ which also optimize* (6) *and whose nonzero entries induce a $\sigma(G)$-critical subgraph.*

A positive answer to this conjecture would have important algorithmic and theoretical implications. In particular, this would imply that σ-critical graphs could be computed. From a theoretical standpoint, this would also imply that the optimal set of the semidefinite program given by (6) is polyhedral whenever B_i are finite in number (a disjoint number of cliques, for example). In general,the optimal set of an SDP is *not* polyhedral, as can be seen with the elliptope[2][**15**].

For a general $\sigma-$critical graph, it is of great interest to know when there exists a unique, or even finite number of optimal weight matrices. The only result in this

[2]The set of semidefinite matrices with diagonal entries all one.

direction is the obvious one: the complete graph on n vertices has a unique optimal weight matrix. The reader should compare this result to theorem 5.1, which asserts that for an edge-transitive graph the adjacency matrix is an optimal weight matrix but says nothing about uniqueness.

LEMMA 5.8. *There is exactly one optimal weight matrix for the complete graph on n vertices.*

PROOF. We shall use the definition of σ given by (4).

Let W be an optimal weight matrix for K_n. First observe that $w_{ij} > 0$ for all i, j, since we know that $\sigma(H) \leq n-1$ for any proper subgraph $H \subset K_n$. Without loss of generality we shall assume that the smallest entry of W has weight 1.

Let w_{uv} denote an entry which has weight 1. Recall that the second smallest eigenvalue λ_1^W is given by

$$\lambda_1^W = \inf_{\substack{f \\ \sum f(x) w_x = 0}} \frac{\sum_{x \sim y} (f(x) - f(y))^2 w_{xy}}{\sum_{x \in V} f^2(x) w_x}.$$

Choose a function f to be

$$f(x) = \begin{cases} w_u & x = v \\ -w_v & x = u. \end{cases}$$

Note that $\sum f(x) w_x = w_u w_v - w_v w_u = 0$. Thus λ_1^W is at most

$$\begin{aligned} \frac{w_u^2 w_v + w_v^2 w_u + 2 w_u w_v w_{u,v}}{w_u^2 w_v + w_v^2 w_u} &= 1 + \frac{2 w_u w_v w_{uv}}{w_u^2 w_v + w_v^2 w_u} \\ &= 1 + \frac{2}{w_u + w_v} \\ &\leq 1 + \frac{2}{2(d-1)} = \frac{n}{n-1}. \end{aligned}$$

The inequality follows from the fact that the degree of every vertex is at least $n-1$ since all entries of W are at least 1. We see that equality is reached when $w_u = w_v = n-1$, in which case $w_{ui} = w_{vi} = 1$ for all $i = 1, \ldots, n$. Now consider w_{ui} for any i. Since $w_{ui} = 1$, we may use the above argument to conclude that $w_{ij} = 1$ for any $j = 1, \ldots, n$. As i was arbitrary, we conclude that $w_{ij} = 1$ for all $i, j = 1 \ldots, n$. Thus, we conclude that the optimal weight matrix W is unique.

□

Next, we give a result adapted from Feige and Lovász [**5**] [**16**] for the important special case where $\sigma(G) = \omega(G)$. This result is useful for the problem of *clique detection* (see [**5**], [**1**]).

THEOREM 5.9. *Fix a graph G with $\sigma(G) = \omega(G)$. If the largest clique Q is unique and G has the property that $\sigma(G - v) \leq \omega(G) - 1$ for all $v \in Q$, then the unique optimal weight matrix is given by*

$$W = \begin{bmatrix} J_{\omega(G)} - I_{\omega(G)} & 0_{\omega(G) \times n - \omega(G)} \\ 0_{n - \omega(G) \times \omega(G)} & 0_{n - \omega(G) \times n - \omega(G)} \end{bmatrix},$$

where the rows are indexed to make the clique occupy the first $\omega(G)$ vertices.

Proof. We make use of the characterizations σ_1 and σ_2. Let $B = (b_{ij})$ be an optimal solution to 6. Then as B is positive semidefinite, $B = V^T V$. Denote the columns of V by $v_1, \ldots, v_n$. We then create an acute orthonormal labeling of G by setting

$$\mathbf{v}_i = v_i/|v_i| \qquad \mathbf{d} = \left(\sum_{i=1}^n v_i\right) \Big/ \left|\sum_{i=1}^n v_i\right|.$$

One may check that the vectors form an acute orthonormal representation of G. Zero columns can be chosen to be unit vectors perpendicular to $\mathbf{d}$. Further, we compute

$$\begin{aligned}
\sum_{i=1}^n (\mathbf{d}\cdot v_i)^2 &= \left(\sum_{i=1}^n |v_i|^2\right)\left(\sum_{i=1}^n (\mathbf{d}\cdot \mathbf{v}_i)^2\right) \\
&\geq \left(\sum_{i=1}^n |v_i|(\mathbf{d}\cdot\mathbf{v}_i)\right)^2 \\
&= \left(\sum_{i=1}^n \mathbf{d}\cdot v_i\right)^2 \\
&= \left(d\cdot\sum_{i=1}^n v_i\right)^2 = \left(\sum_{i=1}^n v_i\right)^2 = \sigma(G).
\end{aligned}$$

The last line follows because $\sum b_{ij} = \left(\sum_{i=1}^n v_i\right)^2 = \sigma(G)$ by definition. The inequality follows from Cauchy-Schwartz, and so equality holds exactly when

$$(\mathbf{d}\cdot v_i)^2 = \sigma(G)|v_i|^2, \tag{11}$$

since $|v_i|^2 = b_{ii}$ and $\sum b_{ii} = 1$.

Now, we claim that in any optimal acute orthonormal labeling of G, $\mathbf{d}\cdot v_i = 1$ if $i \in Q$ and 0 otherwise. If this is true, then (11) implies that $b_{ii} = 1/\omega(G)$ if $i \in Q$ and 0 otherwise. This in turn implies that the principle submatrix of B induced from Q is the matrix $(1/\omega(G))J$, and elsewhere B is zero. Appealing to corollary 4.6 we see that this implies that any optimal weight matrix W has $w_{ij} > 0$ only if $i, j \in Q$ (else we could construct an optimal solution B' to (6) which differed from B, contradicting the uniqueness of B). In this case, we appeal to proposition 5.8 to see that the principle submatrix of W induced by the clique Q is $J_{\omega(G)} - I_{\omega(G)}$, as claimed.

Finally, we prove the claim. Given some optimal acute orthonormal labeling of G by $\mathbf{w}_i$'s and unit vector $\mathbf{c}$, assume that for $i \in Q$, $(\mathbf{c}\cdot\mathbf{w}_i)^2 < 1$. Then $\sigma(G-i) \geq \sum_{j\neq i}(\mathbf{c}\cdot\mathbf{w}_j)^2 > \omega(G) - 1$. By assumption, this is impossible, as $\sigma(G-i) \leq \omega(G) - 1$. Thus our claim holds. □

Remark 5.10. The hypotheses in proposition 5.8 are applicable to the random graph model $G(n, 1/2, k)$, which is composed of the probability space of random graphs from $G(n, 1/2)$ in which a clique of size k has been planted. For $k = \Omega(\sqrt{n})$, with high probability a graph G in this model has $\sigma(G) = k$ and $\sigma(G-e) = k-1$ for any edge e. This is a model introduced by Alon et al [**1**] in the context of creating algorithms which detect large cliques.

6. Concluding Remarks

In this work we study how $\sigma-$critical subgraphs are related to optimal weight matrices associated to a graph. We have only just delved into the substance of these structures, and much remains unknown.

The biggest block to the theoretical and practical study of optimal weight matrices is the validity of conjecture 5.7 regarding the question of whether there are optimal solutions to (6) which are not convex combinations of solutions determined by $\sigma-$cricital graphs. An answer would go far in helping to understand the nature of the $\sigma-$function (or even the $\vartheta-$function). The more general study of the feasible set determined by equation 6 is posed as an important problem by Knuth in [**12**] (in the context of the Lovász $\vartheta-$function). It should be noted that the feasible region in a general SDP is very poorly understood–a sharp contrast to the theory of linear programming.

A more modest goal is the discovery of interesting families of graphs which are $\sigma-$critical. Most notable among all candidates are the color-critical graphs, as discussed earlier.

From a numerical point of view, it would be of great interest to know to what extent the $\sigma-$function can change upon edge removal. In particular, if

$$f(n) = \min_{\substack{G,H \\ H \subseteq G \\ \sigma(H) < \sigma(G) \\ |V(G)| = n}} \sigma(G) - \sigma(H)$$

then f measures how little the $\sigma-$function of a graph on n vertices can non-trivially decrease upon taking a subgraph. Is there a simple characterization for $f(n)$? Is

$$\liminf_{n\to\infty} f(n) \cdot n^k > 0$$

for some $k > 0$?

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E-mail address: `fan@math.ucsd.edu`

E-mail address: `rmrichardson@math.ucsd.edu`

Department of Mathematics, University of California, San Diego, La Jolla, CA 92093-0112, USA