On extremal properties of perfect 2-colorings

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Abstract

A coloring of the vertices of a graph is called perfect if, for every vertex, the collection of colors of its neighbors depends only on its own color. The corresponding partition of the vertex set is called equitable. We note that a collection of bounds (Hoffman bound, Haemers bound, Cheeger bound, Bierbrauer–Friedman bound, etc) is only reached on perfect 2-colorings. We show that the Expander Mixing Lemma is another example of an inequality that is related to a perfect 2-coloring. For an amply regular graph G=(V,G), we prove a new upper bound for the size of a subset $S\subset V$ with the fixed average internal degree. This bound is reached on a set S if and only if $\{S,V\setminus S\}$ is an equitable partition. We improve the Hoffman bound in a special case.

Keywords: equitable partition, perfect coloring, amply regular graph, tight bound, expander mixing lemma, sensitivity of Boolean function

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1 Introduction

The concept of a perfect coloring of a graph arises independently in graph theory, algebraic combinatorics, cryptography, and coding theory. A coloring of vertices of a graph is called perfect if, for every vertex, the collection of colors of its neighbors depends only on its own color. Other terms used for this notion in the literature are "equitable partition", "partition design", "distributive coloring", "intriguing set", "extremal graphical designs", and "regular boolean function". The last three terms are used only for perfect 2-colorings. Moreover, perfect 2-colorings of a regular graph are the same as the completely regular codes with covering radius 1. A comprehensive survey of the theory of perfect colorings and related topics is available in [14].

It is very useful to formulate the definition of a perfect coloring in terms of linear algebra (see [15]). A surjective function $f: V \to \{0, \dots, k-1\}$ is a perfect k-coloring of a graph $\Gamma = (V, E)$ with quotient matrix Q of size $k \times k$ if and only if

$$M \cdot F = F \cdot Q,\tag{1}$$

where M is the $|V| \times |V|$ adjacency matrix of Γ and F is the incidence $\{0,1\}$ -matrix of size $|V| \times k$ for f. If we admit rational matrices F, then each F satisfying equation (1) is called a perfect structure (see [19]).

Some years ago, Avgustinovich [2] postulated the following principle. Each perfect coloring is a solution of some optimization problem and on the other hand, a tight (reached a theoretical bound) solution of any optimization problem in combinatorics is equivalent to a perfect coloring with some parameters that depend on the problem. The first part of this principle is not difficult. Such a problem can be formulated as Proposition 3 or as [12, Lemma 3]. Previously, we collected

many examples illustrating the second part of this principle in [18]. In this paper, we consider a number of other examples.

Indeed, perfect 2-colorings turn out to be the tight solutions of some extremal problems. If we consider the following bounds for the number of vertices, then the set of vertices attaining one of these bounds must be a perfect 2-coloring. This property holds in the cases of the Hamming and Singleton bounds in coding theory, the Hoffman bound on independent sets [11], Cheeger's bound on cut sizes [1], [9], Haemers' bounds on the subgraph degree [10], the Fon-der-Flaass [7] and Bierbrauer-Friedman bounds on orthogonal arrays (see a proof of the Bierbrauer-Friedman bound in [3], [8] and a proof of the property to be a perfect 2-coloring in [16], [17]). Binary orthogonal arrays attaining the other bound are related to perfect 3-colorings [13, Theorem 1]. In this paper we prove that the Expander Mixing Lemma is another example of an inequality whose attainment implies a perfect 2-coloring (Lemma 1).

It is possible to consider q-ary Boolean-valued function in k variables as a 2-coloring of the Hamming graph H(k,q). Then the sensitivity of the function is equal to the number of mixed-colored edges in the graph. We prove that some known bounds on the sensitivity follow from the Expander Mixing Lemma. Moreover, they are only reached on perfect 2-colorings (Corollaries 4, 5). A bound for a partition into several subsets of vertices with the fixed average internal degree was proved by Krotov [12, Sect. 3]. This bound is tight and it is only reached on perfect colorings. We note that the tight solutions of extremal problems are a rich source of combinatorial designs. The above connection can be useful for optimization theory and theory combinatorial structures.

Distance-regular graphs are one of the main topic of algebraic graph theory. There are many theorems for distance-regular graphs that are impossible for arbitrary regular graphs (see, e.g., [4]). Amply regular graphs (regular up to distance 2) occupy an intermediate position between regular and distance-regular graphs. Thus, some stronger results can be obtained for them. We prove a new upper bound for the cardinality of a subset of vertices of an amply regular graph with the fixed average internal degree (Theorem 3). The bound is tight and attained only on perfect 2-colorings. Moreover, any perfect 2-coloring of an amply regular graph attains this bound. This bound is the better than the Hoffman bound in some cases (Corollary 8).

2 Preliminaries

Next we formulate a combinatorial definition of a perfect coloring. Let G = (V, E) be a regular graph, where V is the set of vertices and E the set of edges. Throughout the article we denote by n = |V| the number of vertices of G and denote by M the adjacency matrix of G. A function $f: V \to I$ is called a perfect coloring if there are integers q_{ij} , $i, j \in I$, such that every vertex of $C_i = f^{-1}(i)$ is adjacent to q_{ij} vertices of $C_j = f^{-1}(j)$. In this case the partition $\{C_i : i \in I\}$ is called equitable. We will use the both equivalent terms "perfect coloring" and "equitable partition".

It is well known that every eigenvalue of a perfect coloring (i.e., an eigenvalue of the quotient matrix $Q = (q_{ij})$) is an eigenvalue of the adjacency matrix M. For an r-regular graph, the largest (both as a signed value and in absolute value) eigenvalue is equal to r and it coincides with the largest eigenvalue of the quotient matrix of any perfect coloring.

The following connection between perfect 2-colorings and eigenfunctions of a graph is known.

Proposition 1 ([7]) A two valued function $f: V \to \mathbb{R}$ is a perfect 2-coloring of a regular connected graph G(V, E) if and only if there exists a constant γ such that $f - \gamma \mathbf{1}_V$ is an eigenfunction of G with eigenvalue λ , where λ is an eigenvalue of the corresponding quotient matrix.

Here $\mathbf{1}_V$ is the indicator function of V. The following two propositions is well known. We prove it for the completeness.

Proposition 2 Let G = (V, E) be an r-regular connected graph with n vertices. Suppose a partition $\{A, B\}$, $B = V \setminus A$, is equitable, i. e., for some $\gamma > 0$ the function $f = \mathbf{1}_A - \gamma \mathbf{1}_V$ is an eigenfunction with an eigenvalue $\lambda \neq r$. Then the quotient matrix of the equitable partition is equal to $\left(\frac{r|A| + \lambda |B|}{n}, \frac{(r-\lambda)|B|}{n}\right)$.

Proof. Without loss of generality, the quotient matrix of an equitable partition is $Q = \begin{pmatrix} r-b & b \\ c & r-c \end{pmatrix}$ for some b and c. By double counting the number of edges that connect elements of A with elements of B, we obtain b|A| = c|B|. By Proposition 1 the second eigenvalue of Q equals $\lambda = r-b-c$. Therefore, $b = (r-\lambda)/(1+\frac{|A|}{|B|})$ and $c = (r-\lambda)/(1+\frac{|B|}{|A|})$. Since n = |A|+|B|, the proposition is proven. \Box

The simplest extremal property of perfect 2-colorings is the following.

Proposition 3 Let G = (V, E) be an r-regular graph and let $S \subset V$. For a vertex x from S, let a(x) denote the number of neighbors of x in S. We suppose $a(x) \leq a$ for some constant a. For a vertex y from $V \setminus S$, let d(y) denote the number of neighbors of y in $V \setminus S$. We suppose $d(y) \geq d$ for some constant d. Then it holds

$$\frac{|S|}{n} \le \frac{r - d}{2r - a - d}.$$

Moreover, in the case of equality, $\mathbf{1}_S$ is a perfect 2-coloring with the quotient matrix $\begin{pmatrix} a & r-a \\ r-d & d \end{pmatrix}$.

Proof. Let M be the adjacency matrix of G. It is easy to see that

$$(M\mathbf{1}_S, \mathbf{1}_S) \le a|S|, \qquad (M\mathbf{1}_S, \mathbf{1}_V - \mathbf{1}_S) = (\mathbf{1}_S, M(\mathbf{1}_V - \mathbf{1}_S)) \le (r - d)(n - |S|)$$
 (2)

and $(M\mathbf{1}_S, \mathbf{1}_V) = r|S|$. Suppose that there exists $x \in S$ such that a(x) < a or there exists $y \in V \setminus S$ such that d(y) > d. Then one of inequalities (2) should be strict.

It holds $(M\mathbf{1}_S, \mathbf{1}_V) = (M\mathbf{1}_S, \mathbf{1}_V - \mathbf{1}_S) + (M\mathbf{1}_S, \mathbf{1}_S)$. Therefore, $r|S| \leq (r-d)(n-|S|) + a|S|$, i. e., $\frac{|S|}{n} \leq \frac{r-d}{2r-d-a}$. If one of inequalities (2) is strict, then r|S| < (r-d)(n-|S|) + a|S|, i. e., $\frac{|S|}{n} < \frac{r-d}{2r-d-a}$. Thus, in the case of the equality we obtain a(x) = a for each $x \in S$ and d(y) = d for every $y \in V \setminus S$. \square

A vertex subset S in an r-regular graph is called a 1-perfect code if the partition $\{S, V \setminus S\}$ is an equitable with quotient matrix $\begin{pmatrix} 0 & r \\ 1 & r-1 \end{pmatrix}$. In the case a=0 and d=r-1, Proposition 3 corresponds to the Hamming bound and it is a routine criterion for 1-perfect codes.

Denote by λ_{\min} the minimum eigenvalue of M. The Hoffman (or Delsarte–Hoffman) upper bound [11] on the cardinality of an independent set in an r-regular graph G is equal to $\frac{-\lambda_{\min} n}{r - \lambda_{\min}}$. It is well known (see, e.g., [9]) that if an independent set S attains the Hoffman bound, then partition $\{S, V \setminus S\}$ is equitable. There exists a generalization of this fact to non independent sets. Denote by $\sigma(S)$ the average internal degree for a set $S \subset V$, i.e., $\sigma(S) = (M\mathbf{1}_S, \mathbf{1}_S)/|S|$.

Theorem 1 ([18]) Let G = (V, E) be an r-regular graph and let $S \subset V$. If $\sigma(S) \leq a$, then $|S| \leq \frac{(a - \lambda_{\min})n}{r - \lambda_{\min}}. \ Moreover, \ |S| = \frac{(a - \lambda_{\min})n}{r - \lambda_{\min}} \ if \ and \ only \ if \ \mathbf{1}_S \ is \ a \ perfect \ 2-coloring \ with \ quotient \ matrix$ $\begin{pmatrix} a & r - a \\ a - \lambda_{\min} & r + \lambda_{\min} - a \end{pmatrix}.$

$$\begin{pmatrix} a & r-a \\ a-\lambda_{\min} & r+\lambda_{\min}-a \end{pmatrix}$$

Denote by $\chi(G)$ the chromatic number of a graph G. For an r-regular graph G, the inequality $\chi(G) \geq \frac{\lambda_{\min} - r}{\lambda_{\min}}$ is a corollary of the Hoffman bound.

Corollary 1 Let G = (V, E) be an r-regular graph. If $k = \frac{\lambda_{\min} - r}{\lambda_{\min}}$, then every proper k-coloring of G is a perfect k-coloring.

Proof. By Theorem 1, the partition $\{C_i, V \setminus C_i\}$ is equitable, where C_i is the set of i-colored vertices for i = 1, ..., k. Therefore, every vertex from $V \setminus C_i$ has the same number of adjacent i-colored vertices. In particular, every vertex from C_i has the same number of adjacent i-colored vertices for each $i \neq j$. It remains to note that a vertex from C_i has no i-colored neighbors, because the coloring is proper. \square

3 Expander Mixing Lemma and its corollaries

Let A and B be arbitrary (not necessarily disjoint) nonempty subsets of V. Consider the set $\{(a,b): a \in A, b \in B, \{a,b\} \in E(G)\}$ of all arcs that connect vertices from A to vertices from B. The cardinality of this set is denoted by e(A,B). In particular, if $a,b \in A \cap B$, then the edge $\{a,b\}$ is counted twice, as the arcs (a,b) and (b,a). It is easy to see that

$$e(A,B) = (\mathbf{1}_A, M\mathbf{1}_B),\tag{3}$$

where M is the adjacency matrix of G.

The Expander Mixing Lemma is proven in [1] and it appears in a form appropriate for us, for example, in [6] (Lemma 3). Moreover, a proof of an improvement of the lemma can be found in [6]. Below, we establish that subsets attaining bound (4) correspond to a perfect 2-coloring. To prove this, we need to repeat the proof of the Expander Mixing Lemma.

Lemma 1 (Expander Mixing Lemma) Let G be an r-regular connected graph and let λ be the second largest, in absolute value, eigenvalue of G (if G is bipartite, then $\lambda = -r$). Then

$$\left| e(A,B) - \frac{r|A||B|}{n} \right| \le |\lambda| \sqrt{|A||B| \left(1 - \frac{|A|}{n}\right) \left(1 - \frac{|B|}{n}\right)}. \tag{4}$$

Moreover, this bound is reached if and only if $B = V \setminus A$ or B = A and the partition $\{A, V \setminus A\}$ is equitable with the eigenvalue λ .

Proof. Let $\lambda_k < \lambda_{k-1} < \cdots < \lambda_1 < \lambda_0 = r$ be the eigenvalues of G. By definition $\lambda = \lambda_k$ or $\lambda = \lambda_1$. Since M is a symmetric matrix, the direct sum of the eigenspaces of all of M's eigenvalues is the entire vector space. Consider the indicator functions $\mathbf{1}_A$ and $\mathbf{1}_B$ as linear combinations of eigenfunctions of G, i.e., $\mathbf{1}_A = \sum_i \alpha_i \phi_i$ and $\mathbf{1}_B = \sum_i \beta_i \phi_i'$, where ϕ_i and ϕ_i' correspond to the eigenvalue λ_i . Note that ϕ_i and ϕ'_i may be different. Without loss of generality, we require that $\|\phi_i\|_2 = 1$ for all i. We assume $\lambda_0 = r$, so the corresponding eigenfunction is $\phi_0 = 1/\sqrt{n}$. Therefore $\alpha_0 = (\mathbf{1}_A, \phi_0) = |A|/\sqrt{n}$ and $\beta_0 = (\mathbf{1}_B, \phi_0) = |B|/\sqrt{n}$. Then

$$(\mathbf{1}_A - \alpha_0 \phi_0, M(\mathbf{1}_B - \beta_0 \phi_0)) = \sum_{i \neq 0} \lambda_i \alpha_i \beta_i (\phi_i, \phi_i').$$
 (5)

By the Cauchy-Schwarz inequality, we obtain

$$\left| \sum_{i \neq 0} \lambda_i \alpha_i \beta_i(\phi_i, \phi_i') \right| \leq |\lambda| \sum_{i \neq 0} |\alpha_i \beta_i| \leq |\lambda| \left(\sum_{i \neq 0} \alpha_i^2 \right)^{1/2} \left(\sum_{i \neq 0} \beta_i^2 \right)^{1/2}. \tag{6}$$

By (3), it holds

$$(\mathbf{1}_{A} - \alpha_{0}\phi_{0}, M(\mathbf{1}_{B} - \beta_{0}\phi_{0})) =$$

$$= (\mathbf{1}_{A}, M\mathbf{1}_{B}) - \beta_{0}(\mathbf{1}_{A} - \alpha_{0}\phi_{0}, M\phi_{0}) - \alpha_{0}(M\phi_{0}, \mathbf{1}_{B} - \beta_{0}\phi_{0}) - (\alpha_{0}\phi_{0}, M(\beta_{0}\phi_{0}))$$

$$= e(A, B) - \frac{r|A||B|}{n}. \quad (7)$$

From $(\mathbf{1}_A, \mathbf{1}_A) = \sum_i \alpha_i^2$, we derive

$$\sum_{i \neq 0} \alpha_i^2 = (\mathbf{1}_A, \mathbf{1}_A) - \alpha_0^2 = |A| - |A|^2 / n.$$
 (8)

A similar equation takes place for B. Summarizing (5)–(7), we get

$$\left| e(A,B) - \frac{r|A||B|}{n} \right| = \left| (\mathbf{1}_A - \alpha_0 \phi_0, M(\mathbf{1}_B - \beta_0 \phi_0)) \right| \le |\lambda| \sqrt{(|A| - |A|^2/n)(|B| - |B|^2/n)}.$$

In order to obtain the equality in the Cauchy-Schwarz inequality, it is necessary vector $\mathbf{1}_A - \alpha_0 \phi_0$ to be collinear to the vector $\mathbf{1}_B - \beta_0 \phi_0$. So, we obtain that $\phi_i = \phi_i'$ and $\alpha_i = \beta_i$ or $\alpha_i = -\beta_i$ for all $i \neq 0$. Moreover, in order to obtain equality in the first inequality of (6), it is necessary the function $\mathbf{1}_B - \beta_0 \phi_0$ to be an eigenfunction with the eigenvalue $\pm \lambda$. By Proposition 1, we see that $\mathbf{1}_B$ is a perfect 2-coloring. If the vector $\mathbf{1}_A - \alpha_0 \phi_0$ has the same direction as $\mathbf{1}_B - \beta_0 \phi_0$, then B = A. If $\mathbf{1}_A - \alpha_0 \phi_0$ has the direction opposite to $\mathbf{1}_B - \beta_0 \phi_0$, then $A = V \setminus B$.

Let $\{A,V\setminus A\}$ be an equitable partition with the eigenvalue λ . Consider the case $B=V\setminus A$. We have $1-\frac{|A|}{n}=\frac{|B|}{n}$ and $|A|-\frac{|A|^2}{n}=\frac{|A||B|}{n}=|B|-\frac{|B|^2}{n}$. From the quotient matrix of the equitable partition (see Proposition 2), we derive $e(A,B)=\frac{(r-\lambda)|A||B|}{n}$. The equality in (4) is now straightforward. The second case A=B is similar. \square

As stated in [6] inequality (4) is one of the form of Cheeger's bound. Let $A \subset V$ and $B = V \setminus A$. The set of all edges that connect A and B is called a cut-set. The cardinality e(A, B) of the cut-set is called the cut size.

Corollary 2 ([9]) Let G be an r-regular connected graph and let $\lambda_k < \lambda_{k-1} < \cdots < \lambda_1 < \lambda_0 = r$ be the eigenvalues of G. Then for any nonempty $A \subset V$ and $B = V \setminus A$, it holds

$$\frac{(r-\lambda_1)|A||B|}{n} \le e(A,B) \le \frac{(r-\lambda_k)|A||B|}{n}.$$

Moreover, one of this two bounds is reached if and only if $\{A, B\}$ is an equitable partition with the eigenvalue λ_1 or λ_k respectively.

Proof. We will use the notation from the proof of Lemma 1. Since $\mathbf{1}_B = \mathbf{1}_V - \mathbf{1}_A = \mathbf{1}_V - \sum_i \alpha_i \phi_i$, (5) is equivalent to the equation

$$(\mathbf{1}_A - \alpha_0 \phi_0, M(\mathbf{1}_B - \beta_0 \phi_0)) = -\sum_{i \neq 0} \lambda_i \alpha_i^2.$$

By the hypothesis of the corollary, it holds

$$-\lambda_1 \sum_{i \neq 0} \alpha_i^2 \le -\sum_{i \neq 0} \lambda_i \alpha_i^2 \le -\lambda_k \sum_{i \neq 0} \alpha_i^2.$$

Utilizing (7) and (8), we obtain the required inequality. The left (or right) side of the inequality holds with equality if and only if $\mathbf{1}_A - \alpha_0 \phi_0$ is an eigenfunction of G with eigenvalue λ_1 (or λ_k respectively). In these cases, the partition $\{A, B\}$ is equitable by Proposition 1. \square

By Corollary 2, we obtain that the maximum cut size $(r - \lambda_k)n/4$ corresponds to an equitable partition with the minimum eigenvalue.

As mentioned above an indicator functions of each subset $C \subset V$ is the linear combination $\mathbf{1}_C = \sum_i \phi_i$, where ϕ_i is an eigenfunction of G with eigenvalue λ_i and $\lambda_k < \lambda_{k-1} < \cdots < \lambda_1 < \lambda_0 = r$. In an arbitrary regular graph G = (V, E), a nonempty set C of vertices is called an algebraic T-design if $\phi_i = 0$ as $i \in T$ in the this decomposition (see [5]).

Corollary 3 Let G be an r-regular connected graph and let $\lambda_k < \lambda_{k-1} < \cdots < \lambda_1 < \lambda_0 = r$ be the eigenvalues of G.

(a) Let $T = \{j+1, \ldots, k\}$. Then for any nonempty T-design $C \subset V$, it holds

$$e(C, V \setminus C) \le \frac{(r - \lambda_j)|C|(n - |C|)}{n}.$$

(b) Let $T = \{1, ..., j-1\}$. Then for any nonempty T-design $C \subset V$, it holds

$$e(C, V \setminus C) \ge \frac{(r - \lambda_j)|C|(n - |C|)}{n}.$$

Moreover, any of this two bounds is reached if and only if $\{C, V \setminus C\}$ is an equitable partition with the eigenvalue λ_i .

A proof of Corollary 3 is similar to the proof of Corollary 2.

Let G be the Hamming graph H(k,q). It is well known that in this case $\lambda_i = k(q-1) - iq$. We can consider $f = \mathbf{1}_C$ as a q-ary Boolean-valued function in k variables. If C is an algebraic T-design and $T = \{1, \ldots, j\}$, then f is a correlation-immune function of order j (see, e.g., [17], Proposition 2). If C is an algebraic T-design and $T = \{j+1, \ldots, k\}$, then f has degree j (see, e.g., [20]). In the theory of Boolean functions the value $e(C, V \setminus C)/n$ is called the average sensitivity of f and is denoted by I(f). The value |C|/n is denoted by $\rho(f)$.

By Corollary 3 we immediately obtain the following statements.

Corollary 4 ([17], Theorem 1) Let f be a q-ary Boolean-valued function in k variables, and let cor(f) be the maximal order of its correlation immunity. Then it holds

$$I(f) \ge q(\text{cor}(f) + 1)\rho(f)(1 - \rho(f)).$$
 (9)

Moreover, this bound is reached if and only if f is a perfect 2-coloring.

Note that (9) coincides with the Bierbrauer bound [3] if C is an independent set. Indeed, in this case $I(f) = \rho(f)k(q-1)$, so $1 - \rho(f) \le \frac{k(q-1)}{q(\operatorname{cor}(f)+1)}$.

Corollary 5 Let f be a q-ary Boolean-valued function in k variables with degree d. Then it holds

$$I(f) \le qd\rho(f)(1-\rho(f)).$$

Moreover, this bound is reached if and only if f is a perfect 2-coloring.

Corollary 5 is similar to the result by Valyuzhenich ([20], Corollary 1) in the case $\rho(f) = \frac{1}{2}$. By the definition, e(C, C) is the doubled number of pairs of adjacent vertices in $C \subset V$. The following inequalities are well known. We establish only the connection with equitable partitions.

Corollary 6 ([10]) Let G be an r-regular connected graph, let $C \subset V$, and let $\lambda_k < \lambda_{k-1} < \cdots < \lambda_1 < \lambda_0 = r$ be the eigenvalues of G. Then it holds

$$\lambda_k|C| + \frac{(r-\lambda_k)|C|^2}{n} \le e(C,C) \le \lambda_1|C| + \frac{(r-\lambda_1)|C|^2}{n}.$$

Moreover, one of this two bounds is reached if and only if $\{C, V \setminus C\}$ is an equitable partition with the eigenvalue λ_1 or λ_k respectively.

Proof. We will use the notation from the proof of Lemma 1. Put B=A=C. In this case, (5) is equivalent to the equation

$$(\mathbf{1}_C - \alpha_0 \phi_0, M(\mathbf{1}_C - \alpha_0 \phi_0)) = \sum_{i \neq 0} \lambda_i \alpha_i^2.$$

By the hypothesis of the corollary, it holds

$$\lambda_k \sum_{i \neq 0} \alpha_i^2 \le \sum_{i \neq 0} \lambda_i \alpha_i^2 \le \lambda_1 \sum_{i \neq 0} \alpha_i^2.$$

Utilizing (7) and (8), we obtain the required inequality. The left (or right) side of the inequality holds with equality if and only if $\mathbf{1}_C - c\phi_0$ is an eigenfunction of G with eigenvalue λ_k (or λ_1 respectively). In these cases, the partition $\{C, V \setminus C\}$ is equitable by Proposition 1. \square

4 Perfect 2-colorings of amply regular graphs

A graph G is called amply regular if the distance-2 adjacency matrix $M_2(G)$ is a polynomial

$$M_2(G) = p(M) = p_2 M^2 + p_1 M + p_0 I$$
(10)

on the adjacency matrix M. It is easy to see that any amply regular graph is an r_p -regular, where $r_p = -p_0/p_2$. Denote by $\sigma_2(S)$ the average number of vertices at distance 2 in the set $S \subset V$, i.e., $\sigma_2(S) = (M_2(G)\mathbf{1}_S, \mathbf{1}_S)/|S|$. Recall that $\sigma(S) = (M\mathbf{1}_S, \mathbf{1}_S)/|S|$.

The following theorem is true for any number of elements in an equitable partition. We formulate the case of two elements in the partition, which is sufficient for our objectives.

Theorem 2 ([12]) Let G be an amply regular graph with polynomial p and let $S \subset V$. If $\sigma(S) = a$ and $\sigma(V \setminus S) = d$, then $\sigma_2(S) \leq (p(Q))_{11}$ and $\sigma_2(V \setminus S) \leq (p(Q))_{22}$, where $Q = \begin{pmatrix} a & r_p - a \\ r_p - d & d \end{pmatrix}$. Moreover, the inequalities both hold with equality if and only if $\mathbf{1}_S$ is a perfect 2-coloring with quotient matrix Q.

By Theorem 2, we can easy obtain the following criterium for perfect 2-colorings with the minimum eigenvalue in amply graphs.

Corollary 7 Let G be an amply r-regular graph with polynomial p and let $S \subset V$ be an independent set. Then $\sigma_2(S) \leq -p_2r(\lambda_{\min}+1)$, where λ_{\min} is the minimum eigenvalue of G. Moreover, $\sigma_2(S) = -p_2r(\lambda_{\min}+1)$ if and only if $\mathbf{1}_S$ is a perfect 2-coloring with the eigenvalue λ_{\min} .

Proof. It is clear that $\sigma(S) = 0$ and $\sigma(V \setminus S) = r(1 - \frac{|S|}{n - |S|})$ for each independent set S. It is easy to find that $(p(Q))_{11} = p_2(r(r-d)-r)$. By Theorem 2, it holds $\sigma_2(S) \leq p_2(\frac{r^2|S|}{n-|S|}-r)$. By the Hoffman bound, we get $\frac{r^2|S|}{n-|S|} \leq -\lambda_{\min}r$. Thus $\sigma_2(S) \leq -p_2r(\lambda_{\min}+1)$. If $\sigma_2(S) = -p_2r(\lambda_{\min}+1)$ then $\mathbf{1}_S$ is a perfect 2-coloring by Theorem 1. For any perfect 2-coloring with the eigenvalue λ_{\min} , the equality $\sigma_2(S) = -p_2r(\lambda_{\min}+1)$ is straightforward. \square

Suppose that the adjacency matrix M satisfies (10). Then by the definition of a perfect 2-coloring, it is possible to count the number of vertices from C_j at distance 2 from any vertex from C_i . If the quotient matrix of the perfect 2-coloring is equal to $\begin{pmatrix} a & b \\ c & d \end{pmatrix}$, then there hold $(M\mathbf{1}_{C_1},\mathbf{1}_{C_1})=a|C_1|, \ (M_2\mathbf{1}_{C_1},\mathbf{1}_{C_1})=(p_2(a^2+bc)+p_1a+p_0)|C_1|, \ \text{and} \ |C_1|=\frac{cn}{b+c}.$ Let $\beta=\sigma_2(C_1)=p_2(a^2+bc)+p_1a+p_0$. It is clear that $\frac{c}{b+c}=\frac{bc}{b^2+bc}=\frac{\beta-p(a)}{p_2b^2+\beta-p(a)}$. Thus we obtain that $|C|=\frac{(\beta-p(a))n}{p_2(r_p-a)^2+\beta-p(a)}$ for any perfect 2-coloring $\mathbf{1}_C$ of G.

Next we prove that a fixed $\sigma(C)$ and a bounded $\sigma_2(C)$ provide an upper bound for the cardinality of C. Moreover, if this upper bound is reached on C then the partition $\{C, V \setminus C\}$ is equitable.

Theorem 3 Let G be an amply r-regular graph with polynomial p and let $C \subset V$. If $\sigma(C) = a$ and $\beta = \sigma_2(C)$ then $|C| \leq \frac{(\beta - p(a))n}{p_2(r-a)^2 + \beta - p(a)}$. Moreover, if $|C| = \frac{(\beta - p(a))n}{p_2(r-a)^2 + \beta - p(a)}$ then $\mathbf{1}_C$ is a perfect 2-coloring of G.

Proof. Without loss of generality, we suppose that G is connected. In the other case, we can prove the theorem separately for each component of connectivity. Consider $\mathbf{1}_C$ as a linear combination of eigenfunctions of G. It holds $\mathbf{1}_C = \sum_i \alpha_i \phi_i$, where ϕ_i is an eigenfunction of M with eigenvalue λ_i . Without loss of generality, we assume $\|\phi_i\|_2 = 1$ for all i. The eigenfunction with eigenvalue r is equal to $\phi_0 = \mathbf{1}_V/\sqrt{n}$. From $(\mathbf{1}_C, \mathbf{1}_C) = \sum_i \alpha_i^2$ we derive

(I)
$$\sum_{i \neq 0} \alpha_i^2 = (\mathbf{1}_C, \mathbf{1}_C) - \alpha_0^2 = |C| - \varrho |C|,$$

where $\varrho = |C|/n$. From $(M\mathbf{1}_C, \mathbf{1}_C) = a|C|$ and $(M\mathbf{1}_C, \mathbf{1}_C) = \sum_i \alpha_i^2 \lambda_i$, it follows

(II)
$$r\varrho|C| + \sum_{i \neq 0} \alpha_i^2 \lambda_i = a|C|.$$

From (10) and the hypothesis of the theorem we obtain

$$(M^2\mathbf{1}_C, \mathbf{1}_C) = \frac{1}{p_2}((M_2 - p_1M - p_0I)\mathbf{1}_C, \mathbf{1}_C) = \frac{|C|}{p_2}(\beta - p_1a - p_0).$$

Hence,

(III)
$$r^2 \varrho |C| + \sum_{i \neq 0} \alpha_i^2 \lambda_i^2 = \frac{|C|}{p_2} (\beta - p_1 a - p_0).$$

Let us combine the left and right parts of equations (I)–(III) according to the following formula (III) $-2\theta(II) + \theta^2(I)$. Then for any $\theta \in \mathbb{R}$ we obtain the inequalities

$$r^{2} \varrho |C| - 2r \varrho \theta |C| + \sum_{i \neq 0} \alpha_{i}^{2} (\lambda_{i} - \theta)^{2} = \frac{|C|}{p_{2}} (\beta - p_{1}a - p_{0}) - 2a\theta |C| + |C|(1 - \varrho)\theta^{2},$$

$$r^{2}\varrho - 2r\varrho\theta \leq \frac{1}{p_{2}}(\beta - p_{1}a - p_{0}) - 2a\theta + (1 - \varrho)\theta^{2},$$

$$\varrho \leq \frac{\frac{1}{p_{2}}(\beta - p(a)) + (a - \theta)^{2}}{(r - \theta)^{2}}.$$
(11)

Let $\theta = a - \frac{\beta - p(a)}{p_2(r-a)}$. Then we conclude that

$$\varrho \le \frac{(a-\theta)(r-a) + (a-\theta)^2}{(r-a+a-\theta)^2} = \frac{a-\theta}{r-\theta} = \frac{\beta - p(a)}{p_2(r-a)^2 + \beta - p(a)}.$$

It is clear that (11) holds with equality if and only if $f = \phi + \alpha_0 \varphi_0$, where ϕ is an eigenfunction with eigenvalue θ . By Proposition 1 we obtain that $\mathbf{1}_C$ is a perfect 2-coloring in this case. \square

For a=0 and $\beta=0$, the new bound coincides with the Hamming bound $|C| \leq \frac{n}{r+1}$. If C is an independent set, then a=0, $p(0)=p_0=-rp_2$ and $\varrho \leq 1/(1+\frac{p_2r^2}{\beta+p_2r})$. This bound and the Hoffman bound are reached simultaneously on perfect 2-colorings with the minimum eigenvalue. In this case, it holds $\sigma_2(C)=-p_2r(\lambda_{\min}+1)$. By Corollary 7, we have $\sigma_2(C)\leq -p_2r(\lambda_{\min}+1)$ for any independent set C. Consequently, meaningfully consider only the case of $\beta<-p_2r(\lambda_{\min}+1)$.

Corollary 8 Let C be an independent set in an amply regular graph G with polynomial p. If $\beta = \sigma_2(C) < -p_2 r(\lambda_{\min} + 1)$, then the bound $\frac{|C|}{n} \le 1/(1 + \frac{p_2 r^2}{\beta + p_2 r})$ is the better than the Hoffman bound.

Proof.
$$1/(1+\frac{p_2r^2}{\beta+p_2r}) < 1/(1+\frac{p_2r^2}{-p_2r\lambda_{\min}}) = \frac{-\lambda_{\min}}{r-\lambda_{\min}}$$
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