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Semidefinite Approximations for Bicliques and Bi-Independent Pairs

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Abstract. We investigate some graph parameters dealing with bi-independent pairs (A, B) in a bipartite graph $G = (V_1 \cup V_2, E)$, that is, pairs (A, B) where $A \subseteq V_1$, $B \subseteq V_2$, and $A \cup B$ are independent. These parameters also allow us to study bicliques in general graphs. When maximizing the cardinality $|A \cup B|$, one finds the stability number $\alpha(G)$, well-known to be polynomial-time computable. When maximizing the product $|A| \cdot |B|$, one finds the parameter $g(G)$, shown to be NP-hard by Peeters in 2003, and when maximizing the ratio $|A| \cdot |B| / |A \cup B|$, one finds $h(G)$, introduced by Vallentin in 2020 for bounding product-free sets in finite groups. We show that $h(G)$ is an NP-hard parameter and, as a crucial ingredient, that it is NP-complete to decide whether a bipartite graph G has a balanced maximum independent set. These hardness results motivate introducing semidefinite programming (SDP) bounds for $g(G)$, $h(G)$, and $\alpha_{\mathrm{bal}}(G)$ (the maximum cardinality of a balanced independent set). We show that these bounds can be seen as natural variations of the Lovász ϑ-number, a well-known semidefinite bound on $\alpha(G)$. In addition, we formulate closed-form eigenvalue bounds, and we show relationships among them as well as with earlier spectral parameters by Hoffman and Haemers in 2001 and Vallentin in 2020.

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Keywords: independent set • biclique • bi-independent pair • Lovász theta number • semidefinite programming • polynomial optimization • eigenvalue bound • stability number of a graph • Hoffman's ratio bound

1. Introduction

Given a bipartite graph $G = (V_1 \cup V_2, E)$, a *bipartite bi-independent pair* in G is a pair (A, B) of subsets $A \subseteq V_1$ and $B \subseteq V_2$ such that no pair of nodes $\{i, j\} \in A \times B$ is an edge of G. The adjective "bipartite" is used to indicate that we restrict to the pairs (A, B) that respect the bipartite structure of G, that is, with $A \subseteq V_1$ and $B \subseteq V_2$; we will, however, sometimes omit it for the sake of brevity. The maximum sum $|A| + |B|$ taken over all bipartite bi-independent pairs (A, B) is the well-studied parameter $\alpha(G)$, known as the *stability number* of G. We consider the following two other parameters, asking for the maximum product $|A| \cdot |B|$ and the maximum ratio $(|A| \cdot |B|)/(|A| + |B|)$,

$$g(G) := \max\{|A| \cdot |B| : (A, B) \text{ is a bipartite bi-independent pair in } G\}, \tag{1}$$

$$h(G) := \max\left\{\frac{|A| \cdot |B|}{|A| + |B|} : (A, B) \text{ is a bipartite bi-independent pair in } G\right\}. \tag{2}$$

If G is a complete bipartite graph, then any bipartite bi-independent pair has $A = \emptyset$ or $B = \emptyset$ (and thus, $g(G) = h(G) = 0$); such a pair is called *trivial*. Otherwise, in the definition of $g(G)$ and $h(G)$, one may restrict the optimization to *nontrivial* pairs (A, B), that is, with $A, B \neq \emptyset$. A pair (A, B) is called *balanced* if $|A| = |B|$. Then, a related parameter of interest is $\alpha_{\mathrm{bal}}(G)$, the maximum number of vertices in a balanced bi-independent pair, given by

$$\alpha_{\mathrm{bal}}(G) := \max\{|A| + |B| : (A, B) \text{ is a balanced bipartite biindependent pair in } G\}.$$

One can also define the parameters $g_{\mathrm{bal}}(G)$ and $h_{\mathrm{bal}}(G)$ as the analogs of $g(G)$ and $h(G)$, where one restricts the optimization to balanced pairs in (1) and (2), respectively. Here are some easy relations that hold among these parameters.

Lemma 1. *Let G be a bipartite graph. Then, we have*

$$\frac{1}{4}\alpha_{\mathrm{bal}}(G)=\frac{1}{2}\sqrt{g_{\mathrm{bal}}(G)}=h_{\mathrm{bal}}(G)\ \le\ h(G)\ \le\ \frac{1}{2}\sqrt{g(G)}\ \le\ \frac{1}{4}\alpha(G), \tag{3}$$

$$h(G)=\frac{1}{4}\alpha(G)\Longleftrightarrow\frac{1}{2}\sqrt{g(G)}=\frac{1}{4}\alpha(G)\Longleftrightarrow\alpha(G)=\alpha_{\mathrm{bal}}(G), \tag{4}$$

Proof. The equalities $\frac{1}{4}\alpha_{\mathrm{bal}}(G)=\frac{1}{2}\sqrt{g_{\mathrm{bal}}(G)}=h_{\mathrm{bal}}(G)$ follow from the definitions. We now show the inequalities in (3). First, if (A,B) is optimal for $\alpha_{\mathrm{bal}}(G)$, then $|A|=|B|$, and thus, we have $h(G)\ge\frac{|A|\cdot|B|}{|A|+|B|}=|A|/2=\alpha_{\mathrm{bal}}(G)/4$. Second, if (A,B) is optimal for $h(G)$, then

$$\frac{1}{2}\sqrt{g(G)}\ge\frac{1}{2}\sqrt{|A|\cdot|B|}\ge\frac{|A|\cdot|B|}{|A|+|B|}=h(G),$$

where the last inequality holds as $(\sqrt{|A|}-\sqrt{|B|})^2\ge 0$. Third, if (A,B) is optimal for $g(G)$, then

$$\frac{1}{4}\alpha(G)\ge\frac{1}{4}(|A|+|B|)\ge\frac{1}{2}\sqrt{|A|\cdot|B|}=\frac{1}{2}\sqrt{g(G)},$$

where, again, the last inequality holds as $(\sqrt{|A|}-\sqrt{|B|})^2\ge 0$. This concludes the proof of (3). Moreover, equality $\alpha(G)/4=\sqrt{g(G)}/2$ implies $|A|=|B|$, and thus, (A,B) is a balanced optimal solution for $\alpha(G)$ so that $\alpha(G)=\alpha_{\mathrm{bal}}(G)$. In addition, if $h(G)=\alpha(G)/4$, then $\alpha(G)/4=\sqrt{g(G)}/2$ by (3), which, as we just observed, implies $\alpha(G)=\alpha_{\mathrm{bal}}(G)$. The other implications follow directly from (3). □

In the rest of this section, we first explain how these parameters also permit us to model problems about bicliques (in arbitrary graphs), and we mention some applications. Then, we present a roadmap through our main results that deal with complexity questions and with designing semidefinite bounds and closed-form eigenvalue-based bounds, topics to which we come back to in detail in Sections 2, 3, 4, and 6.

1.1. Bi-Independent Pairs and Bicliques in Arbitrary Graphs

Bipartite bi-independent pairs in *bipartite* graphs also permit to model *general* bi-independent pairs and bicliques in *arbitrary* graphs. Consider an arbitrary graph $G=(V,E)$ (not necessarily bipartite). A *bi-independent* pair in G is a pair (A,B) of disjoint subsets of V such that no pair of nodes $\{i,j\}\in A\times B$ is an edge of G (but edges are allowed within A or B). One then defines analogously the parameters $g_{\mathrm{bi}}(G)$ and $h_{\mathrm{bi}}(G)$, respectively, as the maximum product $|A|\cdot|B|$ and the maximum ratio $(|A|\cdot|B|)/(|A|+|B|)$, taken over all bi-independent pairs in G. The analog of relation (3) holds:

$$h_{\mathrm{bi}}(G)\le\frac{1}{2}\sqrt{g_{\mathrm{bi}}(G)}\le\frac{1}{4}|V|.$$

Note that $h_{\mathrm{bi}}(G)\ge\frac{1}{4}\alpha(G)$ if $\alpha(G)$ is even and $h_{\mathrm{bi}}(G)\ge\frac{1}{4}\left(\alpha(G)-\frac{1}{\alpha(G)}\right)$ if $\alpha(G)$ is odd (which can be seen by partitioning a maximum stable set into two almost equally sized parts). The parameters $h_{\mathrm{bi}}(G)$ and $g_{\mathrm{bi}}(G)$ can, in fact, be reformulated in terms of the parameters $g(\cdot)$ and $h(\cdot)$ for an associated bipartite graph $B_0(G)$, the *extended bipartite double* of G, defined as follows. First, we define the *bipartite double* $B(G)$, whose node set is $V\cup V'$, where $V'=\{i':i\in V\}$ is a disjoint copy of V and whose edges are the pairs $\{i,j'\}$ and $\{j,i'\}$ for $\{i,j\}\in E$. Then, the *extended bipartite double* $B_0(G)$ is obtained by adding all pairs $\{i,i'\}$ $(i\in V)$ as edges to $B(G)$. Now, observe that a pair (A,B) is bi-independent in G precisely when the pair $(A\subseteq V, B':=\{i':i\in B\}\subseteq V')$ is bipartite bi-independent in $B_0(G)$. Therefore, we have

$$g_{\mathrm{bi}}(G)=g(B_0(G))\quad\text{and}\quad h_{\mathrm{bi}}(G)=h(B_0(G))\quad\text{for any graph } G. \tag{5}$$

One can also model bicliques in an arbitrary graph $G=(V,E)$. A *biclique* in G is a pair (A,B) of disjoint subsets of V such that $A\times B\subseteq E$ or, equivalently, (A,B) is a bi-independent pair in the complementary graph $\overline{G}=(V,\overline{E})$ of G. In analogy, let $g_{\mathrm{bc}}(G)$ and $h_{\mathrm{bc}}(G)$ denote the maximum product $|A|\cdot|B|$ and ratio $(|A|\cdot|B|)/(|A|+|B|)$, taken over all bicliques (A,B) in G so that

$$g_{\mathrm{bc}}(G)=g_{\mathrm{bi}}(\overline{G})=g(B_0(\overline{G}))\quad\text{and}\quad h_{\mathrm{bc}}(G)=h_{\mathrm{bi}}(\overline{G})=h(B_0(\overline{G}))\quad\text{for any graph } G. \tag{6}$$

In the case when $G=(V_1\cup V_2,E)$ is a bipartite graph, nontrivial bicliques in G correspond to nontrivial bipartite bi-independent pairs in the bipartite graph $\overline{G}^b:=(V_1\cup V_2,(V_1\times V_2)\setminus E)$, known as the *bipartite complement* of G. Therefore, we also have

$$g_{\mathrm{bc}}(G)=g(\overline{G}^b)\quad\text{and}\quad h_{\mathrm{bc}}(G)=h(\overline{G}^b)\quad\text{for any graph } G. \tag{7}$$

Therefore, Relations (6) and (7) offer different formulations for the parameters $g_{\text{bc}}(\cdot)$ and $h_{\text{bc}}(\cdot)$; we will investigate in Section 4.3 how the associated semidefinite bounds relate.

1.2. Complexity Results

As is well-known, there are polynomial-time algorithms for computing the stability number $\alpha(G)$ of a bipartite graph G. On the other hand, Peeters [38] shows that, given an integer k, deciding whether a bipartite graph G has a biclique (A, B) with $|A| \cdot |B| \geq k$ is an NP-complete problem. Hence, computing the parameter $g(G)$ is an NP-hard problem (by switching between bicliques and bi-independent pairs).

We will show that also $h(G)$ is hard to compute. For this, we show that the problem (denoted α-BAL-BIP in Section 2) of deciding whether a bipartite graph G has a *balanced* maximum independent set, that is, whether $\alpha(G) = \alpha_{\text{bal}}(G)$ is NP-complete (see Theorem 1). Combining with Lemma 1, it follows that deciding whether $h(G) \geq \alpha(G)/4$ is an NP-complete problem.

It is known that, given an integer k, deciding whether a bipartite graph G contains a bipartite bi-independent pair (A, B) with $|A| = |B| = k$ is an NP-complete problem (Garey and Johnson [16] and Jonhson [24]) (switching between bi-independent pairs and bicliques). Hence, our hardness result for problem α-BAL-BIP shows hardness of this problem already for the case $k = \alpha(G)/2$.

Our proof technique will, in fact, permit us to show NP-hardness for a broader set of problems, namely, for deciding whether any of the following equalities holds:

$$g(G) = g_{\text{bal}}(G),\ \ h(G) = h_{\text{bal}}(G),\ \ h(G) = \frac{1}{2}\sqrt{g(G)},\ \text{ or }\ \frac{1}{2}\sqrt{g(G)} = \frac{1}{4}\alpha(G)$$

(thus, whether the inequalities in (3) hold at equality). See Theorem 3 and Corollary 3.

1.3. Some Applications for the Parameters $g(\cdot)$ and $h(\cdot)$

As explained earlier, the parameter $g(\cdot)$ also allows us to model maximum edge cardinality bicliques in bipartite (or general) graphs. This problem has many real-life applications, such as reducing assembly times in product manufacturing lines and in the area of formal concept analysis, as explained in Dawande et al. [8] (see also Dawande et al. [7] and Swaminathan and Tayur [43]). The related parameter asking for the maximum number of vertices in a balanced biclique has also many applications, for example, in very large-scale integration (VLSI) design (e.g., Al-Yamani et al. [2], Ravi and Lloyd [40], Tahoori [44]), in the analysis of biological data (as in the instance of bicluster, e.g., Yang et al. [47]), and of interactions of proteins (e.g., Mukhopadhyay et al. [35]).

The parameter $g(\cdot)$ appears naturally in the study of cross-intersecting set (or subspace) families. For integers $n \geq k \geq \ell \geq 1$, let $\mathcal{P}_k$ denote the collection of k-subsets of $[n]$ and similarly for $\mathcal{P}_\ell$. Two set families, $\mathcal{A} \subseteq \mathcal{P}_k$ and $\mathcal{B} \subseteq \mathcal{P}_\ell$, are called *cross-intersecting* if $A \cap B \neq \emptyset$ for all $A \in \mathcal{A}$ and $B \in \mathcal{B}$. Then, the maximum product $|\mathcal{A}| \cdot |\mathcal{B}|$ for such a cross-intersecting pair is the parameter $g(G^n_{k,\ell})$, where $G^n_{k,\ell}$ is the bipartite graph with bipartition $\mathcal{P}_k \cup \mathcal{P}_\ell$ and an edge $(A, B) \in \mathcal{P}_k \times \mathcal{P}_\ell$ if $A \cap B = \emptyset$. Pyber [39] gives bounds on this parameter $g(G^n_{k,\ell})$ as an extension of the classical Erdös-Ko-Rado result (Erdös et al. [11]). Suda and Tanaka [41] consider the analogous question for subspace families. Given a finite field $\mathbb{F}_q$ ($q \geq 2$), let Ω_k denote the set of all k-dimensional subspaces of $(\mathbb{F}_q)^n$ and define analogously Ω_ℓ. Consider the bipartite graph $G^{n,q}_{k,\ell}$ with bipartition $\Omega_k \cup \Omega_\ell$, where there is an edge $(A, B) \in \Omega_k \times \Omega_\ell$ if $A \cap B = \{0\}$. Then, bi-independent pairs in $G^{n,q}_{k,\ell}$ correspond to cross-intersecting families of subspaces. Suda and Tanaka [41] give bounds on the parameter $g(G^{n,q}_{k,\ell})$ based on semidefinite programming (see also Remark 2). We also refer to Suda et al. [42], who consider an extension to cross-intersecting families with measures.

The parameter $g(\cdot)$ is also relevant for bounding the nonnegative rank of a matrix. Given a matrix $M \in \mathbb{R}_+^{|V_1| \times |V_2|}$, its *nonnegative rank* $\text{rank}_+(M)$ is the smallest integer $r \in \mathbb{N}$ such that $M = \sum_{\ell=1}^r a_\ell b_\ell^{\mathsf{T}}$ for some nonnegative vectors $a_\ell \in \mathbb{R}_+^{|V_1|}$ and $b_\ell \in \mathbb{R}_+^{|V_2|}$; computing $\text{rank}_+(\cdot)$ is an NP-hard problem (Vavasis [46]). A classical combinatorial lower bound for $\text{rank}_+(M)$ is the *rectangle covering bound* $\text{rc}(M)$, defined as the smallest number of rectangles $A \times B \subseteq V_1 \times V_2$ whose union is equal to the support $S_M := \{(i,j) \in V_1 \times V_2 : M_{ij} \neq 0\}$ of M (see, e.g., Fiorini et al. [13]). The rectangle covering bound was used, for example, in Fiorini et al. [14], to show an exponential lower bound on the extension complexity of combinatorial polytopes such as the traveling salesman and correlation polytopes. Also, the parameter $\text{rc}(M)$ is not easy to compute. To approximate it, one can consider the bipartite graph B_M, with vertex set $V_1 \cup V_2$ and edge set $E_M := (V_1 \times V_2) \setminus S_M$. Then, one can show that $\text{rc}(M) \cdot g(B_M) \geq |S_M|$. Hence, an upper bound on $g(B_M)$ gives directly a lower bound on $\text{rc}(M)$ and thus a lower bound on the nonnegative rank $\text{rank}_+(M)$.

The parameter $h(\cdot)$ was introduced by Vallentin [45], who observed its relevance to maximum product-free subsets in groups in the work of Gowers [18]. Let Γ be a finite group. A set $A \subseteq \Gamma$ is called *product-free* if $ab \notin A$ for all $a, b \in A$ and one is interested in finding the largest cardinality of a product-free set in Γ (see Gowers [18] and Kedlaya [27] for a background on this problem). We now briefly indicate how to bound this parameter using the parameter $h(\cdot)$; for the interested reader, we will present this connection in more detail in Appendix A.

Assume $A \subseteq \Gamma$ is product-free. Let $G_{\Gamma,A} = (V_1 \cup V_2, E)$ be the associated bipartite Cayley graph, where V_1 and V_2 are disjoint copies of Γ and there is an edge between $v_1 \in V_1$ and $v_2 \in V_2$ if their product $v_1 v_2$ belongs to A. The crucial observation now is that because A is product-free, the pair (A_1, A_2) is (balanced) bipartite bi-independent in $G_{\Gamma,A}$, where $A_1 \subseteq V_1, A_2 \subseteq V_2$ are the corresponding disjoint copies of A. This implies $|A|/2 \le h(G_{\Gamma,A})$. Hence, upper bounds on $h(G_{\Gamma,A})$ give upper bounds on product-free sets in Γ. Vallentin [45] introduced the eigenvalue-based upper bound $h(G) \le \frac{|V|}{2r}\lambda_2(A_G)$ for any r-regular bipartite graph G. Applying it to the $|A|$-regular bipartite graph $G_{\Gamma,A}$, he could recover a result by Gowers [18], which states that a product-free subset A in Γ has cardinality $|A| \le |\Gamma|/k^{1/3}$, where k is the minimum dimension of a nontrivial representation of Γ. We will show the sharper eigenvalue-based bound

$$h(G) \le \widehat{h}(G) = \frac{|V|}{4}\frac{\lambda_2(A_G)}{r + \lambda(A_G)}$$

(see Proposition 3) and use it to show a slight sharpening of Gowers's bound, replacing $\frac{|\Gamma|}{k^{1/3}}$ by $\frac{|\Gamma|}{1+k^{1/3}}$ (see Theorem A.1).

In fact, for this application, one is only interested in *balanced* bi-independent pairs in the graph $G_{\Gamma,A}$, and we have $2|A| \le \alpha_{\text{bal}}(G_A)$ if A is product-free in Γ. This motivates investigating whether sharper semidefinite and eigenvalue-based bounds can be found for the balanced parameters. We come back briefly to this question later in the introduction, and it will be investigated in detail in Section 6.

1.4. Semidefinite Approximations

The parameters $g(G)$ and $h(G)$ can be formulated as polynomial optimization problems that lead to hierarchies of semidefinite programming upper bounds $g_r(G)$ and $h_r(G)$ (for $r \ge 1$) able to find the original parameters at order $r = \alpha(G)$. We investigate, in particular, the SDP bounds obtained at the first-order $r = 1$. As we will see, they take the form

$$g_1(G) = \max_{X \in \mathcal{S}^{|V|}} \left\{ \langle C, X \rangle : \begin{pmatrix} 1 & \text{diag}(X)^{\mathsf{T}} \\ \text{diag}(X) & X \end{pmatrix} \succeq 0,\ X_{ij} = 0 \text{ if } \{i,j\} \in E \right\}, \tag{8}$$

$$h_1(G) = \max_{X \in \mathcal{S}^{|V|}} \{\langle C, X \rangle : X \succeq 0,\ \text{Tr}(X) = 1,\ X_{ij} = 0 \text{ if } \{i,j\} \in E\}. \tag{9}$$

Here, $C = \frac{1}{2}\begin{pmatrix} 0 & J \\ J & 0 \end{pmatrix} \in \mathbb{R}^{|V_1|+|V_2|}$, where J denotes the all-ones matrix of appropriate size. The parameters $g_1(G)$ and $h_1(G)$ can be seen as variations of the parameter $\vartheta(G)$, introduced by Lovász [33] as upper bound on $\alpha(G)$ for any G (and equal to $\alpha(G)$ when G is bipartite). Indeed, if we replace the objective $\langle C, X \rangle$ by $\text{Tr}(X)$ in Program (8) and by $\langle J, X \rangle$ in Program (9), then we obtain $\vartheta(G)$ in both cases (see (23) and (24)). We will show the following relations between the parameters $h(G), g(G), h_1(G), g_1(G)$, and $\alpha(G)$.

Proposition 1. *For any bipartite graph G, we have*

$$h(G) \le \frac{1}{2}\sqrt{g(G)} \le h_1(G) \le \frac{1}{2}\sqrt{g_1(G)} \le \frac{1}{4}\alpha(G).$$

It is interesting to note that $h_1(G)$ may improve the bound $\frac{1}{2}\sqrt{g_1(G)}$ for $\frac{1}{2}\sqrt{g(G)}$. Indeed, the inequality $h_1(G) \le \frac{1}{2}\sqrt{g_1(G)}$ can be strict, for example, when G is $K_{n,n}$ minus a perfect matching with $n \ge 5$, as we see in Section 5. The key ingredient to show this is getting eigenvalue-based reformulations for the parameters when G enjoys symmetry properties, as we discuss next.

1.5. Eigenvalue Bounds

When G is a bipartite r-regular graph, we can give closed-form bounds in terms of the second-largest eigenvalue of the adjacency matrix A_G of G. These bounds are obtained by restricting, in the definitions (8) and (9) of $g_1(G)$ and $h_1(G)$, the optimization to matrices with some symmetry.

Proposition 2. *Assume G is a bipartite r-regular graph, set $n := |V_1| = |V_2|$, and let λ_2 be the second-largest eigenvalue of the adjacency matrix A_G of G. Then, we have*

$$g_1(G) \le \widehat{g}(G) := \begin{cases} \dfrac{n^2\lambda_2^2}{(\lambda_2+r)^2} & \text{if } r \le 3\lambda_2, \\ \dfrac{n^2\lambda_2}{8(r-\lambda_2)} & \text{otherwise,} \end{cases} \quad \text{and} \quad h_1(G) \le \widehat{h}(G) := \frac{n\lambda_2}{2(\lambda_2+r)}.$$

Moreover, we have equality $g_1(G) = \widehat{g}(G)$ if G is vertex-and edge-transitive and equality $h_1(G) = \widehat{h}(G)$ if G is edge-transitive.

Observe that the bound $h(G) \le \widehat{h}(G)$ sharpens the bound $h(G) \le \frac{n}{r}\lambda_2$ by Vallentin [45]. Moreover, one can check that $\widehat{h}(G) \le \frac{1}{2}\sqrt{\widehat{g}(G)}$, which mirrors the inequalities $h(G) \le \frac{1}{2}\sqrt{g(G)}$ and $h_1(G) \le \frac{1}{2}\sqrt{g_1(G)}$ (in Proposition 1). We will see, in Section 5, several classes of graphs for which strict inequality $\widehat{h}(G) < \frac{1}{2}\sqrt{\widehat{g}(G)}$ holds, and in Section 4, we will compare the parameter $\widehat{h}(\cdot)$ with other eigenvalue bounds by Hoffman and by Haemers [21, 22].

1.6. Bounds for the Balanced Parameters

As we have seen earlier, the parameter $\alpha_{\text{bal}}(G)$, asking for the maximum cardinality of a balanced independent set in G, arises naturally when considering the parameters $h(\cdot)$ and $g(\cdot)$. An additional motivation comes from its relevance to product-free sets in groups and other applications as in Al-Yamani et al. [2], Mukhopadhyay et al. [35], Ravi and Lloyd [40], Tahoori [44], and Yang et al. [47]. The question thus arises of finding semidefinite and eigenvalue-based bounds for $\alpha_{\text{bal}}(G)$ (and the related parameters $h_{\text{bal}}(G)$ and $g_{\text{bal}}(G)$) that improve on the bounds $h_1(G)$ and $\widehat{h}(G)$ designed for the general (not necessarily balanced) parameters. We investigate this question in detail in Section 6. We define semidefinite bounds $\text{las}_{\text{bal},1}(G)$ and $\vartheta_{\text{bal}}(G)$ for $\alpha_{\text{bal}}(G)$, $g_{\text{bal},1}(G)$ for $g_{\text{bal}}(G)$, and $h_{\text{bal},1}(G)$ for $h_{\text{bal}}(G)$, and we show they satisfy

$$\frac{1}{4}\text{las}_{\text{bal},1}(G) \le \frac{1}{2}\sqrt{g_{\text{bal},1}(G)} \le h_{\text{bal},1}(G) = \frac{1}{4}\vartheta_{\text{bal}}(G)$$

(see Proposition 9). Interestingly, the "balanced versions" of the theta number may lead to different parameters; that is, $\text{las}_{\text{bal},1}(G) < \vartheta_{\text{bal}}(G)$ may hold (see Example 2). On the other hand, we show that the closed-form values obtained by restricting the optimization to symmetric solutions in each of these semidefinite bounds, in fact, recover (up to the correct transformation) the eigenvalue-bound $\widehat{h}(G)$ (see Proposition 12).

1.7. Organization of the Paper

The paper is organized as follows. Section 2 is devoted to the study of the complexity status of the parameters $h(\cdot)$, $g(\cdot)$ and their balanced analogs $\alpha_{\text{bal}}(\cdot)$, $g_{\text{bal}}(\cdot)$, and $h_{\text{bal}}(\cdot)$. In Section 3, we investigate semidefinite bounds for $g(\cdot)$ and $h(\cdot)$, and in Section 4, we study the corresponding eigenvalue-based bounds. In Section 5, we illustrate the behavior of the various parameters on several classes of regular bipartite graphs. We turn our attention to bounds for the balanced parameters in Section 6 and conclude with several remarks and open questions in the final Section 7. In Appendix A, we briefly present the application of the parameters $h(\cdot), \widehat{h}(\cdot), \alpha_{\text{bal}}(\cdot)$ to bounding product-free sets in finite groups, and we group several technical proofs in Appendices B, C, and D.

1.8. Some Notation and Preliminaries

Throughout, $\mathcal{S}^n$ denotes the set of real symmetric $n \times n$ matrices. Let $I_n, J_n \in \mathcal{S}^n$ denote, respectively, the identity matrix and the all-ones matrix (also denoted as I, J when the dimension is clear from the context). Given integers $a, b \ge 1$, we also let $J_{a,b}$ denote the $a \times b$ all-ones matrix, given that a graph $G = (V = [n], E)$, $\mathcal{S}_G$ denotes the set of matrices $M \in \mathcal{S}^n$ that are *supported* by G, that is, such that $M_{ij} = 0$ for all $i, j \in V$ such that $\{i, j\} \notin E$. For a matrix $X \in \mathcal{S}^n$, $\text{diag}(X) = (X_{ii})_{i=1}^n \in \mathbb{R}^n$ denotes the vector of its diagonal entries, and for a vector $x \in \mathbb{R}^n$, $\text{Diag}(x) \in \mathcal{S}^n$ is the diagonal matrix with the x_i's as its diagonal entries. We use the symbol $e \in \mathbb{R}^n$ to denote the all-ones vector (whose dimension should be clear from the context).

For a real symmetric matrix $A \in \mathcal{S}^{|V|}$, we denote its eigenvalues as $\lambda_1(A) \ge \cdots \ge \lambda_{|V|}(A)$. We will often consider the case when A has a bipartite structure of the form

$$A = \begin{pmatrix} 0 & M \\ M^{\mathsf{T}} & 0 \end{pmatrix} \in \mathcal{S}^{|V|}, \tag{10}$$

where V is partitioned as $V = V_1 \cup V_2$ with $|V_1| = |V_2| =: n$ and $M \in \mathbb{R}^{|V_1| \times |V_2|}$. Then, the eigenvalues of A are $\pm\sqrt{\lambda_1(MM^{\mathsf{T}})}, \ldots, \pm\sqrt{\lambda_n(MM^{\mathsf{T}})}$, thus arising from the singular values of M.

For a subset $U \subseteq V$, we let $\chi^U \in \mathbb{R}^{|V|}$ denote its characteristic vector, whose i-th entry is one if $i \in U$ and zero if $i \in V \setminus U$. For a matrix $M \in \mathcal{S}^{|V|}$, $M[U] = (M_{ij})_{i,j \in U}$ denotes the principal submatrix of M indexed by U.

2. Complexity Results

In this section, we prove several complexity results. Recall that a *clique* in G is a set of pairwise adjacent vertices, and $\omega(G)$ denotes the maximum cardinality of a clique in G so that $\omega(G) = \alpha(\overline{G})$. We consider the following problems.

Problem 1 ($\boldsymbol{\alpha}$-BAL-BIP). Given a bipartite graph G, decide whether $\alpha(G) = \alpha_{\text{bal}}(G)$, that is, whether G has a balanced maximum independent set.

Problem 2 (HALF-SIZE-CLIQUE-EDGE). Given a graph $G = (V, E)$ with $|V|$ even and $|E| = \frac{1}{4}|V|(|V| - 2)$, decide whether $\omega(G) \geq \frac{|V|}{2}$.

Problem 3 (HALF-SIZE-CLIQUE). Given a graph $G = (V, E)$ with $|V|$ even, decide whether $\omega(G) \geq \frac{|V|}{2}$.

Problem 4 (CLIQUE). Given a graph G and an integer $k \in \mathbb{N}$, decide whether $\omega(G) \geq k$.

It is well-known that CLIQUE is an NP-complete problem (Karp [26]) as well as problem HALF-SIZE-CLIQUE; we refer, for example, to Alon et al. [1] for an easy reduction of CLIQUE to HALF-SIZE-CLIQUE. In what follows, we will show the following reductions:

$$\text{HALF-SIZE-CLIQUE} \leq_P \text{HALF-SIZE-CLIQUE-EDGE} \leq_P \alpha\text{-BAL-BIP}. \tag{11}$$

Here, we say that $L_1 \leq_P L_2$ if we have a polynomial-time algorithm permitting us to encode an instance of L_1 as an instance of L_2. We will show the first reduction in Theorem 2 and the second one in Theorem 3. Then, using the reductions in (11), we obtain the following complexity results.

Theorem 1. *Problem 1 (α-BAL-BIP) is an NP-complete problem.*

Corollary 1. *Computing the parameter $h(G)$ for G bipartite is NP-hard.*

Proof. Recall that computing $\alpha(G)$ in bipartite graphs can be done in polynomial time. Hence, if there is a polynomial time algorithm for computing $h(G)$, then one can decide in polynomial time whether $h(G) = \frac{\alpha(G)}{4}$, which is equivalent to Problem 1 in view of Lemma 1. □

The proof technique used to show the reduction from problem HALF-SIZE-CLIQUE-EDGE to problem α-BAL-BIP will, in fact, allow us to show a broader set of results. Namely, it permits us to show hardness of testing whether any of the following equalities hold: $g(G) = g_{\text{bal}}(G)$, $h(G) = h_{\text{bal}}(G)$, or $h(G) = \frac{1}{2}\sqrt{g(G)}$. In other words, it is NP-hard to check whether any of the inequalities in Relation (3) hold at equality. See Corollary 3 for these and other hardness results.

In the rest of the section, we will prove the two reductions from Relation (11) and related hardness results for the other (balanced) parameters. For this, we use, as a first ingredient, the following graph constructions.

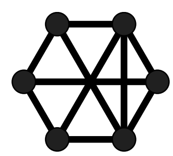
Definition 1. Let $G = (V(G), E(G))$ and $H = (V(H), E(H))$ be two graphs with disjoint vertex sets, and let $k \geq 1$ be an integer.

(i) The disjoint union of G and H, denoted by $G \oplus H$, is the graph with vertex set $V(G) \cup V(H)$ and edge set $E(G) \cup E(H)$.

(ii) The joining of G and H, denoted by $G \bowtie H$, is the graph with vertex set $V(G) \cup V(H)$ and edge set $E(G) \cup E(H) \cup (V(G) \times V(H))$.

(iii) The k-th expansion of G, denoted by $G^{(k)}$, is the graph constructed as follows: its vertex set is $\cup_{v \in V(G)} X_v$, where X_v are disjoint sets, each of size k, and we have a clique on each X_v and a complete bipartite graph between X_u and X_v whenever $\{u, v\} \in E(G)$.

Figure 1. Graph F, $\omega(F) = 3$, 6 nodes, 10 edges.



Clearly, we have the following relations:

$$|V(G \oplus H)| = |V(G)| + |V(H)|, |E(G \oplus H)| = |E(G)| + |E(H)|, \tag{12}$$

$$\omega(G \oplus H) = \max\{\omega(G), \omega(H)\}, \tag{13}$$

$$|V(G \bowtie H)| = |V(G)| + |V(H)|, |E(G \bowtie H)| = |E(G)| + |E(H)| + |V(G)| \cdot |V(H)|, \tag{14}$$

$$\omega(G \bowtie H) = \omega(G) + \omega(H), \tag{15}$$

$$|V(G^{(k)})| = k|V(G)|,\ |E(G^{(k)})| = \binom{k}{2}|V(G)| + k^2|E(G)|,\ \omega(G^{(k)}) = k\omega(G). \tag{16}$$

Theorem 2. *HALF-SIZE-CLIQUE $\leq_P$ HALF-SIZE-CLIQUE-EDGE.*

Proof. Let G be an instance of HALF-SIZE-CLIQUE; set $|V(G)| = 2n, |E(G)| = m$. Let t be the smallest integer such that $\binom{t}{2} \geq 9n^2 + n + m$. Consider the graph F from Figure 1 and define the graph $H := ((G \bowtie F^{(n)}) \bowtie K_t) \oplus H_0$, where H_0 is a graph with t nodes and $\binom{t}{2} - (9n^2 + n + m)$ edges. Therefore, the role of H_0 is to add enough edges in order to ensure that $|E(H)| = |V(H)|(|V(H)| - 2)/4$. Observe that H can be constructed in polynomial time. Using (12)–(16), we obtain

$$|V(H)| = 8n + 2t,$$
$$|E(H)| = \left(m + 6\binom{n}{2} + 10n^2 + 12n^2\right) + \binom{t}{2} + 8nt + \left(\binom{t}{2} - 9n^2 - n - m\right)$$
$$= (4n + t)(4n + t - 1) = \frac{1}{4}(8n + 2t)(8n + 2t - 2),$$
$$\omega(H) = \omega(G) + 3n + t.$$

Hence, H is an instance of HALF-SIZE-CLIQUE-EDGE and $\omega(H) \geq |V(H)|/2$ if and only if $\omega(G) \geq |V(G)|/2$. Therefore, if there is a polynomial time algorithm for solving HALF-SIZE-CLIQUE-EDGE, then we can solve HALF-SIZE-CLIQUE in polynomial time. □

As a next step, we show the reduction of HALF-SIZE-CLIQUE-EDGE to α-BAL-BIP. Our proof is inspired from an argument in Chen and Kanj [4], where the authors consider minimum vertex covers in a bipartite graph restricted to have at least k_1 vertices in one side of the bipartition and at least k_2 vertices in the other side. In Chen and Kanj [4, theorem 3.1], it is shown that deciding the existence of such vertex covers is NP-complete by giving a reduction from CLIQUE. We adapt this reduction by suitably selecting the values of k_1 and k_2, considering independent sets (complements of vertex covers) instead of vertex covers, and modifying the graph construction used in Chen and Kanj [4].

The following graph construction will play a central role for the reduction of HALF-SIZE-CLIQUE-EDGE to α-BAL-BIP (and other related problems).

Definition 2. Given a graph $G = (V, E)$ with $n := |V|$ and $m := |E|$, consider the bipartite graph $H_G = (V_1 \cup V_2, E_H)$ constructed as follows.

(i) For each vertex $v \in V$, we construct two vertices, $v_1 \in V_1$ and $v_2 \in V_2$, and add the edge $\{v_1, v_2\}$ to E_H.

(ii) For each edge $e \in E$, we construct two vertex sets, $L_e \subseteq V_1$ and $R_e \subseteq V_2$ with $|L_e| = |R_e| = n + 1$, and add all edges in $L_e \times R_e$ to E_H.

(iii) If $v \in V$ is incident to $e \in E$, then we let v_1 be adjacent in H_G to all vertices of R_e.

Hence, setting $L_V := \{v_1 : v \in V\}$, $R_V := \{v_2 : v \in V\}$, $L_E := \cup_{e \in E} L_e$, and $R_E := \cup_{e \in E} R_e$, we have $V_1 = L_V \cup L_E$ and $V_2 = R_V \cup R_E$; there is a perfect matching between L_V and R_V, there is a complete bipartite graph between L_e and R_e for each $e \in E$, and there is a complete bipartite graph between $v_1 \in V_1$ and R_e for each edge $e \in E$ containing $v \in V$.

The next lemma shows that the maximal independent sets in the bipartite graph H_G have a very special structure, which will be useful for the Proof of Theorem 3.

Lemma 2. *Let $G = (V, E)$ be a graph, $n := |V|$, $m := |E|$, and let H_G be the associated bipartite graph as in Definition 2. Assume $I \subseteq V(H_G) = V_1 \cup V_2$ is a maximal independent set of H_G. Then, I takes the following form:*

$$I \cap V_1 = \{v_1 : v \in A\} \cup \bigcup_{e \in E_1} L_e, \quad I \cap V_2 = \{v_2 : v \in B\} \cup \bigcup_{e \in E_2} R_e, \tag{17}$$

where $A \subseteq V$, $B = V \setminus A$, E_1 is the set of edges $e \in E$ that are incident to some node $v \in A$, and $E_2 = E \setminus E_1$ (thus, the set of edges $e \in E$ contained in B). Moreover, I is a maximum independent set of H_G and $\alpha(H_G) = n + m(n+1)$. Conversely, any set I as in (17) is a (maximum) independent set of H_G.

Proof. Assume $I \subseteq V_1 \cup V_2$ is a maximal independent set of H_G. Set $A := \{v \in V : v_1 \in I\}$, $B := \{v \in V : v_2 \in I\}$, and $E_2 := E \setminus E_1$, where E_1 is the set of edges $e \in E$ that are incident to some node $v \in A$; we show that (17) holds. First, we have $A \cap B = \emptyset$ (for, if $v \in A \cap B$, then the edge $\{v_1, v_2\}$ of H_G would be contained in I, contradicting that I is independent). Moreover, $A \cup B = V$ (for, if $v \in V \setminus (A \cup B)$, then the set $I \cup \{v_2\}$ would be independent in H_G, contradicting the maximality of I). Therefore, we have $I \cap L_V = \{v_1 : v \in A\}$ and $I \cap R_V = \{v_2 : v \in B\}$. We now claim that $I \cap L_E = \cup_{e \in E_1} L_e$ and $I \cap R_E = \cup_{e \in E_1} R_e$. First, note that if $I \cap R_e \neq \emptyset$, then e is not incident to any node of A and thus $e \in E_2$. Moreover, by maximality of I, we have $R_e \subseteq I$ for any $e \in E_2$. Therefore, we indeed have $I \cap R_E = \cup_{e \in E_2} R_e$, and, in turn, this implies $I \cap L_E = \cup_{e \in E_1} L_e$. Therefore, we have $|I| = n + m(n+1)$, which implies that $\alpha(H_G) = n + m(n+1)$ and that I is maximum independent. This concludes the proof (because the last (reverse) claim is straightforward to check). □

Corollary 2. *Let $G = (V, E)$ be a graph, and let H_G be the bipartite graph as in Definition 2. The following assertions are equivalent.*
(i) $\alpha_{\text{bal}}(H_G) = \alpha(H_G)$.
(ii) $g_{\text{bal}}(H_G) = g(H_G)$.
(iii) $h_{\text{bal}}(H_G) = h(H_G)$.

Proof. The implications (i) ⇒ (ii) and (i) ⇒ (iii) follow from Relation (3). Conversely, assume (ii) holds, and let (A, B) be a balanced optimal solution for $g(H_G)$. Then, $A \cup B$ is maximal independent in H_G, and thus, by Lemma 2, it is maximum so that $\alpha(H_G) = |A \cup B| = \alpha_{\text{bal}}(H_G)$ as (A, B) is balanced. The same argument shows the implication (iii) ⇒ (i). □

Now, we show the main result of the section, which, combined with Theorem 2, implies Theorem 1.

Theorem 3. *Let $G = (V, E)$ be a graph satisfying $|E| = \frac{1}{4}|V|(|V| - 2)$, and let H_G be the associated bipartite graph as in Definition 2. The following assertions are equivalent.*
(i) *G has a clique of size $|V|/2$, that is, $\omega(G) \geq |V|/2$.*
(ii) $\alpha(H_G) = \alpha_{\text{bal}}(H_G)$.
Therefore, HALF-SIZE-CLIQUE-EDGE $\leq_P$ α-BAL-BIP.

Proof. We first show (i) ⇒ (ii). Assume C is a clique of G with $|C| = |V|/2$. Let E_2 be the set of edges of G that are contained in C so that $E_1 := E \setminus E_2$ is the set of edges of G that are incident to some node in $V \setminus C$. By the assumption on G, we have $\binom{|V|/2}{2} = \frac{|E|}{2}$, and thus, $|E_2| = \binom{|V|/2}{2} = \frac{|E|}{2} = |E_1|$. Consider the subset $I \subseteq V_1 \cup V_2$ of $V(H_G)$, which is defined by

$$I \cap V_1 = \{v_1 : v \notin C\} \cup \bigcup_{e \in E_1} L_e, \quad I \cap V_2 = \{v_2 : v \in C\} \cup \bigcup_{e \in E_2} R_e.$$

By Lemma 2, I is a maximum independent set in H_G, and $\alpha(H_G) = n + m(n+1)$. Moreover, we have $|I \cap V_1| = |I \cap V_2|$, which shows that $\alpha_{\text{bal}}(H_G) = \alpha(H_G)$.

Now, we show (ii) ⇒ (i). By the assumption (ii), H_G has a balanced maximum independent set I. By Lemma 2, I takes the form as in (17). As I is balanced, we have $|I \cap V_1| = |I \cap V_2|$, and thus,

$$||A| - |B|| = (n+1)||E_2| - |E_1||.$$

If $|E_1| \neq |E_2|$, then the left-hand side is at most n, whereas the right-hand side is at least $n+1$. Therefore, we have $|E_1| = |E_2| = |E|/2$ and $|A| = |B| = |V|/2$. Moreover, $|E_2| \leq \binom{|B|}{2} = \binom{|V|/2}{2}$ because E_2 consists of the edges that are contained in B. This gives $|E| = 2|E_2| \leq 2\binom{|V|/2}{2} = |V|(|V| - 2)/4$. We now use the assumption $|E| = |V|(|V| - 2)/4$ on the number of edges of G, which implies that equality holds throughout and, thus, that B is a clique in G of size $|B| = |V|/2$, showing (i). □

Corollary 3. *Given a bipartite graph G, it is NP-hard to decide whether any of the following equalities holds.*
(i) $g(G) = g_{\text{bal}}(G)$.
(ii) $h(G) = h_{\text{bal}}(G)$.
(iii) $h(G) = \frac{1}{4}\alpha(G)$.
(iv) $\frac{1}{2}\sqrt{g(G)} = \frac{1}{4}\alpha(G)$.
(v) $h(G) = \frac{1}{2}\sqrt{g(G)}$.

Proof. We show that it is NP-hard to check any of the equalities (i)–(v) for the class of bipartite graphs that are of the form H_G (as in Definition 2) for some graph G with $|E| = \frac{1}{4}|V|(|V|-2)$. The key fact is that for bipartite graphs of the form H_G, any of the assertions (i)–(v) are equivalent to $\alpha(H_G) = \alpha_{\text{bal}}(H_G)$; this was shown in Corollary 2 for (i)–(ii) and in Relation (4) for (iii)–(iv), and one can easily verify that (v) implies (i). Then, the corollary follows using Theorems 2 and 3 together with hardness of HALF-SIZE-CLIQUE. □

Remark 1. The hardness results in Corollary 3 hold, in fact, for a broader class of bipartite graph parameters. For this, consider a bivariate function $f : \mathbb{R}_+^2 \to \mathbb{R}$ that satisfies the condition

$$f(a,b) \le \frac{a+b}{4}, \text{ and } f(a,b) = \frac{a+b}{4} \Longleftrightarrow a = b, \quad \text{for all } a,b \in \mathbb{N} \tag{18}$$

and define the corresponding graph parameter

$$f(G) := \max\{f(|A|,|B|) : (A,B) \text{ is bipartite biindependent in } G\} \quad \text{for } G \text{ bipartite.}$$

Using Relation (18), one can check the inequalities $\frac{\alpha_{\text{bal}}(G)}{4} \le f(G) \le \frac{\alpha(G)}{4}$ and the equivalence

$$f(G) = \frac{\alpha(G)}{4} \Longleftrightarrow \alpha(G) = \alpha_{\text{bal}}(G).$$

Using Theorem 3, it follows that computing $f(\cdot)$ is NP-hard (already for the bipartite graphs of the form H_G for some graph G with $|V|(|V|-2)/4$ edges).

Examples of functions satisfying (18) include $f(a,b) = \frac{ab}{a+b}$ (giving the parameter $h(G)$) and $f(a,b) = \frac{1}{2}\sqrt{ab}$ (giving $\frac{1}{2}\sqrt{g(G)}$), or any $f(\cdot)$ nested between $h(\cdot)$ and $\frac{1}{2}\sqrt{g(\cdot)}$. As another example, consider $f(a,b) := \left(\frac{1}{2}\sqrt{ab}\right)^p \left(\frac{a+b}{4}\right)^{1-p}$ with $0 \le p \le 1$, which gives a graph parameter $f(\cdot)$ nested between $\frac{1}{2}\sqrt{g(\cdot)}$ and $\frac{\alpha(\cdot)}{4}$.

3. Semidefinite Approximations for the Parameters *g*(*G*) and *h*(*G*)

In this section, we introduce semidefinite approximations for the parameters $g(\cdot)$ and $h(\cdot)$ from (1) and (2), which are both NP-hard to compute, as we saw in the previous sections. Let $G = (V = V_1 \cup V_2, E)$ be a bipartite graph, and let C be the matrix from Relation (26). The starting point is to formulate the parameters $g(G)$ and $h(G)$ as maximizing, respectively, the quadratic polynomial $x^{\mathsf{T}}Cx$ and the rational function $\frac{x^{\mathsf{T}}Cx}{x^{\mathsf{T}}x}$ over the vectors $x \in \{0,1\}^{|V|}$ such that $x_ix_j = 0$ for all $\{i,j\} \in E$. Then, to get a tractable approximation, a common approach is to linearize the quadratic terms by introducing a matrix X modeling xx^{T} in the case of $g(G)$ and modeling $\frac{xx^{\mathsf{T}}}{x^{\mathsf{T}}x}$ in the case of $h(G)$. In this way, one obtains the semidefinite bounds $g_1(G)$ and $h_1(G)$ introduced earlier in (8) and (9). More generally, one can define hierarchies of semidefinite parameters $(h_r(G))_{r\in\mathbb{N}}$ and $(g_r(G))_{r\in\mathbb{N}}$ that upper bound $h(G)$ and $g(G)$, respectively, using polynomial optimization techniques. Then, the parameters $h_1(G)$ and $g_1(G)$ correspond to the bounds at the first level $r=1$ in these hierarchies. We will next briefly recall how the polynomial optimization approach applies for bounding the parameters $g(G)$ and $h(G)$, and after that, we investigate the bounds $g_1(G)$ and $h_1(G)$ in more detail.

3.1. Polynomial Optimization Formulations and Bounds

We begin with a short recap on notation about polynomials and their use for approximating stable sets in graphs. Throughout, $\mathbb{R}[x] = \mathbb{R}[x_1,\dots,x_n]$ denotes the ring of n-variate polynomials. For an integer $r \in \mathbb{N}$, $\mathbb{R}[x]_r$ denotes the subset of n-variate polynomials with degree at most r. Then, $\Sigma_r \subseteq \mathbb{R}[x]_{2r}$ denotes the set of sums of squares of polynomials of the form $\sum_{i=1}^k u_i^2$ with $u_i \in \mathbb{R}[x]_r$ and $k \in \mathbb{N}$. Recall that one can test whether a polynomial $f \in \mathbb{R}[x]_{2r}$ belongs to Σ_r via semidefinite optimization. Indeed, $f \in \Sigma_r$ if and only if there exists a positive semidefinite matrix Q that satisfies the polynomial identity $f(x) = [x]_r^{\mathsf{T}}Q[x]_r$, where $[x]_r$ denotes the vector of square-free (a.k.a. multilinear) monomials of degree at most r. In particular, $[x]_1$ denotes the (column) vector $(1,x_1,\dots,x_n)^{\mathsf{T}}$.

Let $G = (V = [n], E)$ be a graph. Define the ideal $I_G \subseteq \mathbb{R}[x]$ generated by the polynomials $x_i^2 - x_i$ ($i \in V$) and x_ix_j ($\{i,j\} \in E$), which consists of the polynomials $q = \sum_{i\in V} u_i(x_i^2 - x_i) + \sum_{\{i,j\}\in E} u_{ij}x_ix_j$ with $u_i, u_{ij} \in \mathbb{R}[x]$. For an integer $r \in \mathbb{N}$, let $I_{G,2r} \subseteq \mathbb{R}[x]_{2r}$ denote its degree $2r$ truncation consisting of the polynomials q, where we require that u_i and u_{ij} have degree at most $2r-2$. The motivation for considering the ideal I_G comes from the fact that the stable sets in

G correspond to the vectors in its variety $V(I_G)$, that is, to the vectors $x \in \mathbb{R}^n$ satisfying $x_i^2 - x_i = 0$ for $i \in V$ and $x_i x_j = 0$ for $\{i,j\} \in E$. This enables reformulating the stability number of G as

$$\alpha(G) = \max\left\{\sum_{i\in V} x_i : x \in V(I_G)\right\} = \min\left\{\lambda : \lambda - \sum_{i\in V} x_i \geq 0 \text{ for all } x \in V(I_G)\right\} \tag{19}$$

$$= \min\left\{\lambda : \lambda - \sum_{i\in V} x_i \in \Sigma_{\alpha(G)} + I_{G,2\alpha(G)}\right\}. \tag{20}$$

Here, the last equality follows from the following well-known key fact: for a polynomial $p \in \mathbb{R}[x]$,

$$p(x) \geq 0 \text{ for all } x \in V(I_G) \Longleftrightarrow p \in \Sigma_{\alpha(G)} + I_G. \tag{21}$$

(see Lasserre [30] and Laurent [31]). This motivates defining the parameters

$$\text{las}_r(G) := \min\left\{\lambda : \lambda - \sum_{i\in V} x_i \in \Sigma_r + I_{G,2r}\right\} \quad \text{for any } \ r \in \mathbb{N}, \tag{22}$$

also known as the Lasserre bounds, for $\alpha(G)$. The parameter $\text{las}_r(G)$ can be expressed via a semidefinite program, and we have $\alpha(G) \leq \text{las}_{r+1}(G) \leq \text{las}_r(G)$, with equality $\alpha(G) = \text{las}_r(G)$ if $r \geq \alpha(G)$ [31]. At order $r = 1$, we obtain the bound $\text{las}_1(G)$, which, after applying SDP duality, can be checked to take the form

$$\text{las}_1(G) = \max\left\{\langle I, X\rangle : X \in \mathcal{S}^n, \begin{pmatrix} 1 & \text{diag}(X)^\mathsf{T} \\ \text{diag}(X) & X \end{pmatrix} \succeq 0, X_{ij} = 0 \text{ for } \{i,j\} \in E\right\}. \tag{23}$$

Another upper bound on $\alpha(G)$ is the theta number by Lovász [33], defined by

$$\vartheta(G) = \max\{\langle J, X\rangle : X \in \mathcal{S}^n, X \succeq 0, \langle I, X\rangle = 1, X_{ij} = 0 \text{ for } \{i,j\} \in E\}. \tag{24}$$

As is well-known, these two bounds coincide:

$$\text{las}_1(G) = \vartheta(G) \tag{25}$$

(see, e.g., Grötschel et al. [19]; see also Remark 4). Moreover, $\vartheta(G) = \alpha(G)$ if G is bipartite (more generally, if G is perfect, see Grötschel et al. [19]). We now indicate how the polynomial optimization approach sketched earlier also applies to the parameters $g(\cdot)$ and $h(\cdot)$.

Assume now that $G = (V = V_1 \cup V_2, E)$ is a bipartite graph. Define the matrix

$$C := \frac{1}{2}\begin{pmatrix} 0 & J_{|V_1|,|V_2|} \\ J_{|V_2|,|V_1|} & 0 \end{pmatrix} \in \mathcal{S}^{|V|} \tag{26}$$

so that $x^\mathsf{T} C x = (\sum_{i\in V_1} x_i)(\sum_{j\in V_2} x_j)$. As observed, one can encode a bi-independent pair (A, B) with $A \subseteq V_1$ and $B \subseteq V_2$ by its characteristic vector $x = \chi^{A\cup B}$, which belongs to the variety $V(I_G)$. Then, we can express the parameters $g(G)$ and $h(G)$ as

$$g(G) = \max\{x^\mathsf{T} C x : x_i^2 = x_i \,(i \in V), \, x_i x_j = 0 \,(\{i,j\} \in E)\}, \tag{27}$$

$$h(G) = \max\left\{\frac{x^\mathsf{T} C x}{x^\mathsf{T} x} : x_i^2 = x_i \,(i \in V), \, x_i x_j = 0 \,(\{i,j\} \in E)\right\}. \tag{28}$$

The Lasserre bounds of order r for $g(G)$ and $h(G)$ read, respectively,

$$g_r(G) := \min\{\lambda : \lambda - x^\mathsf{T} C x \in \Sigma_r + I_{G,2r}\}, \tag{29}$$

$$h_r(G) := \min\{\lambda : x^\mathsf{T}(\lambda I - C)x \in \Sigma_r + I_{G,2r}\}, \tag{30}$$

and the next result follows as a direct application of Relation (21).

Lemma 3. *Let G be a bipartite graph. For any integer $r \geq 1$, we have $g(G) \leq g_r(G)$ and $h(G) \leq h_r(G)$, with equality if $r \geq \alpha(G)$.*

As sums of squares of polynomials can be modeled using positive semidefinite matrices, the parameters $\text{las}_r(G)$, $g_r(G)$, $h_r(G)$ can be formulated using a semidefinite program. In later sections, we will give the explicit semidefinite programs for the parameters $g_1(G)$ and $h_1(G)$, their symmetric versions, and their balanced analogs. An important property that we will use is that strong duality holds for all these semidefinite programs, which follows from a result in Josz and Henrion [25] (thanks to the presence of the equations $x_i^2 - x_i = 0$ for $i \in V$ in the original polynomial optimization problems).

3.2. Semidefinite Formulations for the Lasserre Bounds $h_1(G)$ and $g_1(G)$

In this section, we give explicit semidefinite formulations for the Lasserre Bounds (29) and (30) of order $r = 1$ for $g(G)$ and $h(G)$. In particular, we indicate how to obtain the formulations given earlier in (8) and (9). Recall that $\mathcal{S}_G$ consists of the matrices in $\mathcal{S}^{|V|}$ that are supported by G. We begin with a claim expressing polynomials in the truncated ideal $I_{G,2}$ that we will repeatedly use.

Lemma 4. *Given a graph $G = (V, E)$ and a matrix $M \in \mathcal{S}^{1+|V|}$ (indexed by $\{0\} \cup V$), we have $[x]_1^{\mathsf{T}} M [x]_1 \in I_{G,2}$ if and only if M takes the form*

$$M = \begin{pmatrix} 0 & -u^{\mathsf{T}}/2 \\ -u/2 & \text{Diag}(u) + Z \end{pmatrix} \text{ for some } u \in \mathbb{R}^{|V|},\ Z \in \mathcal{S}_G. \tag{31}$$

Proof. By definition, $[x]_1^{\mathsf{T}} M [x]_1 \in I_{G,2}$ if $[x]_1^{\mathsf{T}} M [x]_1 = \sum_{i \in V} u_i(x_i^2 - x_i) + \sum_{\{i,j\} \in E} u_{ij} x_i x_j$ for some $u_i, u_{ij} \in \mathbb{R}$. The result follows by equating coefficients at both sides of this polynomial identity. □

We now give semidefinite formulations for the parameters $h_1(G)$ and $g_1(G)$.

Lemma 5. *Let $G = (V = V_1 \cup V_2, E)$ be a bipartite graph. Then, the Lasserre bound of order $r = 1$ for $h(G)$ can be reformulated as*

$$h_1(G) = \min_{\lambda \in \mathbb{R}, Z \in \mathcal{S}^{|V|}} \{\lambda : \lambda I + Z - C \succeq 0,\ Z \in \mathcal{S}_G\}, \tag{32}$$

$$= \max_{X \in \mathcal{S}^{|V|}} \{\langle C, X \rangle : X \succeq 0,\ \text{Tr}(X) = 1,\ X_{ij} = 0 \text{ for } \{i,j\} \in E\}. \tag{33}$$

Proof. By definition, $h_1(G)$ is the smallest scalar λ for which $x^{\mathsf{T}}(\lambda I - C)x \in \Sigma_2 + I_{G,2}$, that is, the smallest λ for which $[x]_1^{\mathsf{T}} Q [x]_1 - x^{\mathsf{T}}(\lambda I - C)x \in I_{G,2}$ for some matrix $Q \succeq 0$ (indexed by $\{0\} \cup V$). Using Lemma 4,we obtain that $Q_{00} = 0$, and thus, $Q_{0i} = 0$ for all $i \in V$ (as $Q \succeq 0$). From this follows that the principal submatrix indexed by V takes the form $Q[V] = Z + \lambda I - C$ for some $Z \in \mathcal{S}_G$, and we arrive at Formulation (32) for $h_1(G)$. By taking the semidefinite dual, we obtain Formulation (33). As already noted, strong duality holds as an application of Josz and Henrion [25]. □

Remark 2. After submission of our paper, H. Tanaka attended us on Suda and Tanaka [41] and Suda et al. [42], where the following bound on $\sqrt{g(G)}$ is studied. Let $I_{V_1} = \text{Diag}(\chi^{V_1})$ and $I_{V_2} = \text{Diag}(\chi^{V_2})$, and define the parameter

$$T(G) := \max_{X \in \mathcal{S}^{|V|}} \{\langle C, X \rangle : X \succeq 0, \langle X, I_{V_1} \rangle = \langle X, I_{V_2} \rangle = 1,\ X_{ij} = 0 \text{ for } \{i,j\} \in E,\ X \geq 0\}. \tag{34}$$

Note that if we let $T'(G)$ denote the same parameter without the entrywise nonnegativity constraint on X, then we have equality $T'(G) = 2h_1(G)$. It is clear that $T'(G) \leq 2h_1(G)$ because an optimal solution X for $T'(G)$ gives a feasible matrix $X/2$ for Program (33) defining $h_1(G)$. Conversely, if X is optimal for $h_1(G)$, then $2X$ is feasible for $T'(G)$. Indeed, one can show that such X satisfies $\langle X, I_{V_1} \rangle = \langle X, I_{V_2} \rangle = 1/2$ (using Relations (40) and (41) in the following proof). Therefore, we have the inequalities $\sqrt{g(G)} \leq T(G) \leq 2h_1(G)$.

Lemma 6. *Let G be a bipartite graph. Then, we have*

$$g_1(G) = \min_{\lambda \in \mathbb{R}, u \in \mathbb{R}^{|V|}, Z \in \mathcal{S}^{|V|}} \left\{\lambda : \begin{pmatrix} \lambda & u^{\mathsf{T}}/2 \\ u/2 & \text{Diag}(u) - C + Z \end{pmatrix} \succeq 0,\ Z \in \mathcal{S}_G\right\}, \tag{35}$$

$$= \max_{X\in\mathcal{S}^{|V|}} \left\{ \langle C, X\rangle : \begin{pmatrix} 1 & \operatorname{diag}(X)^{\mathsf{T}} \\ \operatorname{diag}(X) & X \end{pmatrix} \succeq 0,\ X_{ij} = 0 \text{ for } \{i,j\}\in E \right\}. \tag{36}$$

Proof. By definition, $g_1(G)$ is the smallest scalar λ for which $\lambda - x^{\mathsf{T}}Cx \in \Sigma_2 + I_{G,2}$. In other words, this is the smallest λ for which there exists $Q \succeq 0$ such that $[x]_1^{\mathsf{T}}\left(Q - \begin{pmatrix} \lambda & 0 \\ 0 & -C\end{pmatrix}\right)[x]_1 \in I_{G,2}$. Using Lemma 4, we obtain the formulation of $g_1(G)$ as in (35). Then, Formulation (36) follows by taking the dual of the semidefinite program (35) and strong duality holds by a result in Josz and Henrion [25]. □

Remark 3. In order to highlight some similarities and differences between the parameters $\text{las}_1(G)$, $g_1(G)$ and $h_1(G)$, we indicate how to derive Formulation (23) of $\text{las}_1(G)$. Let us start with the definition of $\text{las}_1(G)$ as the smallest λ for which $\lambda - \sum_{i\in V} x_i \in \Sigma_2 + I_{G,2}$. As $\sum_{i\in V} x_i - x^{\mathsf{T}}Ix \in I_{G,2}$, we can alternatively search for the smallest λ for which $[x]_1^{\mathsf{T}}\left(Q - \begin{pmatrix} \lambda & 0 \\ 0 & -I\end{pmatrix}\right)[x]_1 \in I_{G,2}$. Using Lemma 4, we obtain

$$\text{las}_1(G) = \min_{\lambda\in\mathbb{R},\, u\in\mathbb{R}^{|V|},\, Z\in\mathcal{S}^{|V|}} \left\{ \lambda : \begin{pmatrix} \lambda & u^{\mathsf{T}}/2 \\ u/2 & \operatorname{Diag}(u) - I + Z \end{pmatrix} \succeq 0,\ Z \in \mathcal{S}_G \right\}. \tag{37}$$

Taking the dual semidefinite program of (37), we arrive at Formulation (23).

Note the similarity between Programs (35) and (37), which are the same up to exchanging the matrices C and I. Note also that it is possible to simplify Program (37) and bring it in the form

$$\text{las}_1(G) = \min_{\lambda\in\mathbb{R},\, Z\in\mathcal{S}^{|V|}} \left\{ \lambda : \begin{pmatrix} \lambda & e^{\mathsf{T}} \\ e & I + Z \end{pmatrix} \succeq 0,\ Z \in \mathcal{S}_G \right\}, \tag{38}$$

which is another well-known formulation of $\vartheta(G)$. To see this, call Q the matrix in Program (37). As $Q_{ii} = u_i - 1 \geq 0$, we have $u_i \geq 1$ for all $i \in V$. By scaling the i-th column/row of Q by $2/u_i$ and adding $1 - \frac{4}{u_i^2}(u_i - 1) = \frac{(u_i-2)^2}{u_i^2} \geq 0$ to entry Q_{ii}, we obtain a new matrix $Q' \succeq 0$ satisfying $Q'_{0i} = Q'_{ii} = 1$ for all $i \in V$ and thus is feasible for (38). This shows the equivalence of (37) and (38).

Note, however, that this rescaling trick could not be applied to program (35); indeed, if Q denotes the matrix appearing in (35), then one must have $Q_{ij} = -1/2$ for all positions $(i,j) \in V_1 \times V_2$ corresponding to nonedges of G.

Finally, we mention a natural strengthening of $h_1(G)$, obtained by adding one row/column to the matrix variable (as in the definition (36) of $g_1(G)$):

$$h_1'(G) := \max\left\{ \langle C, X\rangle : \begin{pmatrix} 1 & x^{\mathsf{T}} \\ x & X \end{pmatrix} \succeq 0,\ \operatorname{Tr}(X) = 1,\ x = \operatorname{diag}(X),\ X_{ij} = 0 \text{ for } \{i,j\}\in E \right\}. \tag{39}$$

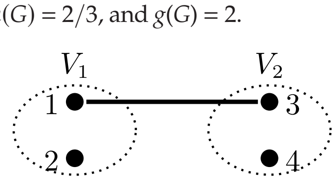
We have

$$h(G) \leq h_1'(G) \leq h_1(G).$$

The inequality $h_1'(G) \leq h_1(G)$ is clear because any feasible solution of (39) gives a feasible solution of (33). To see that $h(G) \leq h_1'(G)$, let (A, B) be an optimal solution for $h(G)$, and set $y := \chi^{A\cup B}$. Then, $x := y/e^{\mathsf{T}}y$ and $X := yy^{\mathsf{T}}/e^{\mathsf{T}}y$ provide a feasible solution for $h_1'(G)$, with value $\langle C, X\rangle = |A|\cdot|B|/|A\cup B| = h(G)$ (using the fact that $X - xx^{\mathsf{T}} = yy^{\mathsf{T}}(e^{\mathsf{T}}y - 1)/(e^{\mathsf{T}}y)^2 \succeq 0$). In the next section, we will show that $h_1(G)$ upper bounds also $\frac{1}{2}\sqrt{g(G)}$; the next example shows this is not true for $h_1'(G)$.

Example 1. Let $G = (V_1 \cup V_2, E)$ be the bipartite graph with $V_1 = \{1,2\}$, $V_2 = \{3,4\}$ and a single edge $\{1, 3\}$; see Figure 2. We have $h_1'(G) < \left(\frac{\sqrt{2}}{2} = \right)\frac{1}{2}\sqrt{g(G)} = h_1(G)$. Indeed, $h_1(G) \geq \frac{1}{2}\sqrt{g(G)}$ holds by Proposition 1, and $h_1(G) \leq \frac{\sqrt{2}}{2}$ follows from the fact that $\frac{\sqrt{2}}{2}I + A_G - C \succeq 0$, which exhibits a feasible solution to (32). Moreover, the strict

Figure 2. Graph G with $\alpha(G) = 3$, $\alpha_{\text{bal}}(G) = 2$, $h(G) = 2/3$, and $g(G) = 2$.



inequality $h_1'(G) < \frac{\sqrt{2}}{2}$ follows from the fact that the dual program (50) (defined later) of (39) has feasible solution $\lambda = 0.0002$, $\eta = 0.7068$, $u = (-0.01, 0.004, -0.01, 0.004)^\top$, $Z = 0.99A_G$, with objective value $0.707 < \frac{\sqrt{2}}{2}$.

3.3. Comparison of the Lasserre Bounds $h_1(G)$ and $g_1(G)$

In this section, we show the following inequalities

$$h(G) \leq \frac{1}{2}\sqrt{g(G)} \leq h_1(G) \leq \frac{1}{2}\sqrt{g_1(G)} \leq \frac{1}{4}\alpha(G) \quad \text{for any bipartite graph } G$$

that were claimed in Proposition 1. One may have strict inequalities $h_1(G) < \frac{1}{2}\sqrt{g_1(G)} < \frac{1}{4}\alpha(G)$, for example, when G is the complete bipartite graph $K_{n,n}$ minus a perfect matching and $n \geq 5$ (see Section 5.2). To show these inequalities, we will use, in particular, the fact that the theta number $\vartheta(G)$ admits the two equivalent formulations that were given earlier in (23) and (24) (recall (25); see also Remark 4) and the fact that $\vartheta(G) = \alpha(G)$ when G is a bipartite graph. Recall that we already know $h(G) \leq \frac{1}{2}\sqrt{g(G)}$ from Lemma 1. Hence, in order to show Proposition 1, it suffices to show the inequalities

$$\frac{1}{2}\sqrt{g(G)} \leq h_1(G),\ h_1(G) \leq \frac{1}{2}\sqrt{g_1(G)},\ h_1(G) \leq \frac{1}{4}\alpha(G), \text{ and } g_1(G) \leq \alpha(G)h_1(G).$$

Proof of $\frac{1}{2}\sqrt{g(G)} \leq h_1(G)$. Let (A, B) be an optimal solution for $g(G)$ with $|A| =: a$, $|B| =: b$, and let (λ, Z) be a feasible solution for Formulation (32) of $h_1(G)$; we show that $\lambda \geq \frac{1}{2}\sqrt{ab}$. By assumption, the matrix $M := \lambda I + Z - C$ is positive semidefinite, and thus, also its principal submatrix $M[A \cup B]$ is positive semidefinite. Observe that $M[A \cup B]$ has the block-form

$$M[A \cup B] = \begin{pmatrix} \lambda I_a & -\frac{1}{2}J_{a,b} \\ -\frac{1}{2}J_{b,a} & \lambda I_b \end{pmatrix},$$

because $Z_{ij} = 0$ for $i \in A, j \in B$ as $A \cup B$ is independent. By taking a Schur complement, we obtain that $M[A \cup B] \succeq 0$ if and only if $\lambda I_a - \frac{b}{4\lambda}J_{a,a} \succeq 0$. This implies $\lambda \geq \frac{1}{2}\sqrt{ab} = \frac{1}{2}\sqrt{g(G)}$ and thus $h_1(G) \geq \frac{1}{2}\sqrt{g(G)}$. □

Proof of $h_1(G) \leq \frac{1}{2}\sqrt{g_1(G)}$. Let X be an optimal solution for Formulation (33) of $h_1(G)$. Then, $X \succeq 0$, and thus, $X = (y_i^\top y_j)_{i,j \in V}$ for some vectors $y_i \in \mathbb{R}^{|V|}$ $(i \in V)$. We may assume without loss of generality that $y_i \neq 0$ for $i \in V$ (because if $y_i = 0$, then we just replace X by its principal submatrix indexed by $V \setminus \{i\}$). Define the vectors $y' := \sum_{i \in V_1} y_i$ and $y'' := \sum_{i \in V_2} y_i$ so that $h_1(G) = \langle C, X \rangle = (y')^\top y''$. To shorten notation, we set $h := h_1(G) = (y')^\top y''$. We may assume $h > 0$, or else there is nothing to prove. For $\epsilon = \pm 1$, define the vector $d_\epsilon := \frac{y' + \epsilon y''}{\|y' + \epsilon y''\|}$. Here, the convention is that we consider the vector d_ϵ only if $y' + \epsilon y'' \neq 0$. Note that at least one of d_1 and d_{-1} is well defined (because, otherwise, one would have $y' = y'' = 0$, implying $h_1(G) = 0$, a contradiction). Then, let X_ϵ denote the Gram matrix of the vectors $\frac{d_\epsilon^\top y_i}{\|y_i\|^2} y_i$ for $i \in V$; we claim that X_ϵ is feasible for Formulation (36) of $g_1(G)$. To see it, consider the matrix Y_ϵ, defined as the Gram matrix of the vectors d_ϵ and $\frac{d_\epsilon^\top y_i}{\|y_i\|^2} y_i$ for $i \in V$, so that X_ϵ is its principal submatrix indexed by V, and note that $Y_\epsilon \succeq 0$, $(Y_\epsilon)_{00} = 1$, $(Y_\epsilon)_{0i} = (Y_\epsilon)_{ii}$ for $i \in V$, and $(Y_\epsilon)_{ij} = 0$ if $\{i, j\} \in E$. Hence, if one can show that $\langle C, X_\epsilon \rangle \geq 4\langle C, X \rangle^2$ for some $\epsilon \in \{\pm 1\}$, then this implies $g_1(G) \geq \langle C, X_\epsilon \rangle \geq 4\langle C, X \rangle^2 = 4h_1(G)^2$, and the proof is complete. The rest of the proof is devoted to showing that $\langle C, X_\epsilon \rangle \geq 4\langle C, X \rangle^2$ for some $\epsilon \in \{\pm 1\}$ and is a bit technical.

In a first step, we show that the vectors y_i $(i \in V)$ satisfy the following relations:

$$y_i^\top y'' = 2h\,\|y_i\|^2 \quad (i \in V_1), \tag{40}$$

$$y_j^\top y' = 2h\,\|y_j\|^2 \quad (j \in V_2). \tag{41}$$

For this, consider an optimal solution $S := hI + Z - C$ of Program (32) defining $h_1(G)$, where $Z \in \mathcal{S}_G$. As X and S are primal and dual optimal solutions, we must have $XS = 0$; that is, $0 = hX + XZ - XC$. We now compute the diagonal entries. Note that $(XZ)_{ii} = 0$ for all $i \in V$ (because, for each $k \in V$, we have $X_{ik} = 0$ or $Z_{ki} = 0$). Hence, for $i \in V_1$, we have $h\|y_i\|^2 = hX_{ii} = (XC)_{ii} = \frac{1}{2}\sum_{j \in V_2} X_{ij} = \frac{1}{2}y_i^\top y''$, and for $j \in V_2$, we have $h\|y_j\|^2 = hX_{jj} = (XC)_{jj} = \frac{1}{2}\sum_{i \in V_1} X_{ij} = \frac{1}{2}y_j^\top y'$. Therefore, (40) and (41) hold.

We now proceed to compute

$$\langle C, X_\epsilon\rangle = \sum_{(i,j)\in V_1\times V_2} \frac{d_\epsilon^{\mathsf T} y_i \cdot d_\epsilon^{\mathsf T} y_j}{\|y_i\|^2\|y_j\|^2}\cdot y_i^{\mathsf T} y_j. \tag{42}$$

First, we compute (part of) the inner term for $i \in V_1$ and $j \in V_2$:

$$\frac{d_\epsilon^{\mathsf T} y_i \cdot d_\epsilon^{\mathsf T} y_j}{\|y_i\|^2\|y_j\|^2} = \frac{1}{\|y' + \epsilon y''\|^2}\frac{(y'+\epsilon y'')^{\mathsf T} y_i \cdot (y'+\epsilon y'')^{\mathsf T} y_j}{\|y_i\|^2\|y_j\|^2} \tag{43}$$

$$= \frac{1}{\|y' + \epsilon y''\|^2}\left(2h\frac{(y')^{\mathsf T} y_i}{\|y_i\|^2} + 2h\frac{(y'')^{\mathsf T} y_j}{\|y_j\|^2} + \epsilon\frac{(y')^{\mathsf T} y_i\cdot (y'')^{\mathsf T} y_j}{\|y_i\|^2\|y_j\|^2} + 4h^2\epsilon\right), \tag{44}$$

where we have used relations (40) and (41) and that $\epsilon^2 = 1$ to carry out the simplifications. Next, observe that

$$\sum_{(i,j)\in V_1\times V_2}\frac{(y')^{\mathsf T} y_i}{\|y_i\|^2} y_i^{\mathsf T} y_j = \sum_{i\in V_1}\frac{(y')^{\mathsf T} y_i}{\|y_i\|^2}\left(\sum_{j\in V_2} y_i^{\mathsf T} y_j\right) = \sum_{i\in V_1}\frac{(y')^{\mathsf T} y_i}{\|y_i\|^2} y_i^{\mathsf T} y'' = 2h\sum_{i\in V_1}(y')^{\mathsf T} y_i = 2h\|y'\|^2, \tag{45}$$

where we have again used Relation (40). In the same way, we have

$$\sum_{(i,j)\in V_1\times V_2}\frac{(y'')^{\mathsf T} y_j}{\|y_j\|^2} y_i^{\mathsf T} y_j = 2h\|y''\|^2. \tag{46}$$

Combining (42), (44), (45), and (46), we obtain

$$\langle C, X_\epsilon\rangle = \frac{1}{\|y'+\epsilon y''\|^2}\left(4h^2(\|y'\|^2 + \|y''\|^2 + \epsilon (y')^{\mathsf T} y'') + \epsilon\sum_{(i,j)\in V_1\times V_2}\frac{(y')^{\mathsf T} y_i\cdot (y'')^{\mathsf T} y_j\cdot y_i^{\mathsf T} y_j}{\|y_i\|^2\|y_j\|^2}\right)$$

$$= \frac{1}{\|y'+\epsilon y''\|^2}\left(4h^2\|y'+\epsilon y''\|^2 - 4h^2\epsilon (y')^{\mathsf T} y'' + \epsilon\sum_{(i,j)\in V_1\times V_2}\frac{(y')^{\mathsf T} y_i\cdot (y'')^{\mathsf T} y_j\cdot y_i^{\mathsf T} y_j}{\|y_i\|^2\|y_j\|^2}\right)$$

$$= 4h^2 + \frac{\epsilon}{\|y'+\epsilon y''\|^2}\underbrace{\left(\sum_{(i,j)\in V_1\times V_2}\frac{(y')^{\mathsf T} y_i\cdot (y'')^{\mathsf T} y_j\cdot y_i^{\mathsf T} y_j}{\|y_i\|^2\|y_j\|^2} - 4h^3\right)}_{=:\varphi} = 4h^2 + \frac{\epsilon\cdot\varphi}{\|y'+\epsilon y''\|^2}.$$

We can now conclude the proof. Assume first $y' \pm y'' \neq 0$ so that both d_1 and d_{-1} are well defined. If $\varphi \geq 0$, then $\langle C, X_1\rangle \geq 4h^2$. Otherwise, if $\varphi < 0$, then $\langle C, X_{-1}\rangle \geq 4h^2$. Therefore, we have shown the desired result: $\langle C, X_\epsilon\rangle \geq 4h^2$ for some $\epsilon \in \{\pm 1\}$. Consider, now, the case when $y' = \epsilon y''$ for some $\epsilon\in\{\pm 1\}$. Then, using Relations (40) and (41), we obtain that $\varphi = 0$. Hence, if $y' = y''$ (resp., $y' = -y''$), then we have $\langle C, X_1\rangle \geq 4h^2$ (resp., $\langle C, X_{-1}\rangle \geq 4h^2$), which concludes the proof. □

Remark 4. Note that the proof for the inequality $h_1(G) \leq \frac{1}{2}\sqrt{g_1(G)}$ resembles—but is technically more involved than—the classical proof for the inequality $\text{las}_1(G) \geq \vartheta(G)$, where $\text{las}_1(G)$ is given by (23) and $\vartheta(G)$ by (24), and G is an arbitrary graph. (The reverse inequality $\vartheta(G) \geq \text{las}_1(G)$ is straightforward.) We sketch the proof for $\text{las}_1(G) \geq \vartheta(G)$ in order to highlight the resemblance with the proof for $\frac{1}{2}\sqrt{g_1(G)} \geq h_1(G)$. Therefore, assume X is optimal for (24) (defined as the Gram matrix of vectors y_i for $i\in V$) and construct the matrix X_1 (as the Gram matrix of the vectors $\frac{d_1^{\mathsf T} y_i}{\|y_i\|^2} y_i$ for $i \in V$, where $d_1 := (\sum_{i\in V} y_i)/\|\sum_{i\in V} y_i\|$). Then, $\vartheta(G) = \langle J, X\rangle = \|\sum_{i\in V} y_i\|^2$, $1 = \langle I, X\rangle = \sum_{i\in V}\|y_i\|^2$, and $y_i^{\mathsf T} y_j = 0$ if $\{i,j\}\in E$. This implies X_1 is feasible for (23), and thus, $\text{las}_1(G) \geq \langle X_1, I\rangle$. It suffices now to check that $\langle X_1, I\rangle = \sum_{i\in V}\frac{(d_1^{\mathsf T} y_i)^2}{\|y_i\|^2} \geq \|\sum_{i\in V} y_i\|^2 = \vartheta(G)$. But this follows easily using the Cauchy-Schwartz inequality, namely,

$$\left\|\sum_{i\in V} y_i\right\|^2 = \left(d_1^{\mathsf T}\sum_{i\in V} y_i\right)^2 = \left(\sum_{i\in V}\frac{d_1^{\mathsf T} y_i}{\|y_i\|}\|y_i\|\right)^2 \leq \left(\sum_{i\in V}\frac{(d_1^{\mathsf T} y_i)^2}{\|y_i\|^2}\right)\left(\sum_{i\in V}\|y_i\|^2\right) = \sum_{i\in V}\frac{(d_1^{\mathsf T} y_i)^2}{\|y_i\|^2}.$$

Proof of $h_1(G) \le \frac{1}{4}\alpha(G)$. Let X be optimal for the formulation (33) of $h_1(G)$. Then, X is feasible for (24), and thus, $\vartheta(G) \ge \langle J, X\rangle$. Because $J - 4C \ge 0$, this implies $\langle J, X\rangle \ge 4\langle C, X\rangle = 4h_1(G)$. Combining both inequalities, we get $4h_1(G) \le \vartheta(G) = \alpha(G)$. □

Proof of $g_1(G) \le \alpha(G)h_1(G)$. Let X be an optimal solution for the formulation (36) of $g_1(G)$. Then, $\frac{X}{\mathrm{Tr}(X)}$ is feasible for $h_1(G)$, and thus, $g_1(G) = \langle C, X\rangle \le h_1(G)\cdot \mathrm{Tr}(X)$. On the other hand, X is feasible for (23), which gives $\vartheta(G) \ge \mathrm{Tr}(X)$. Combining these two facts, we obtain that $g_1(G) \le h_1(G)\cdot\vartheta(G) = h_1(G)\cdot\alpha(G)$. □

Remark 5. Therefore, we have the following chain of inequalities for any bipartite graph G,

$$\frac{1}{4}\alpha_{\mathrm{bal}}(G) \le h(G) \le \frac{1}{2}\sqrt{g(G)} \le h_1(G) \le \frac{1}{4}\alpha(G)$$

(Proposition 1 and Lemma 1). Hence, equality $\alpha(G) = \alpha_{\mathrm{bal}}(G)$ implies $h_1(G) = h(G)$. Observe that the reverse implication holds when restricting to the bipartite graphs of the form H_G (constructed from some graph G as in Definition 2). Indeed, $h_1(H_G) = h(H_G)$ implies $\frac{1}{2}\sqrt{g(H_G)} = h(H_G)$, which, in turn, implies $g(H_G) = g_{\mathrm{bal}}(H_G)$ (Corollary 3 and its proof), and thus, $\alpha(H_G) = \alpha_{\mathrm{bal}}(H_G)$ (Corollary 2). This shows that deciding whether the parameter $h(\cdot)$ coincides with its semidefinite relaxation $h_1(\cdot)$ is an NP-hard problem (already when restricting to the bipartite graphs of the form H_G; recall Theorem 3). This can be seen as an analog of the hardness of deciding whether the basic semidefinite relaxation of the maximum cut problem is exact, as shown in Delorme and Poljak [9].

4. Eigenvalue Bounds for the Parameters $g(G)$ and $h(G)$

Let $G = (V, E)$ be a bipartite graph with adjacency matrix A_G. We have introduced in Lemmas 5 and 6 the parameters $g_1(G)$ and $h_1(G)$ that, respectively, upper bound the parameters $g(G)$ and $h(G)$. For convenience, we repeat their formulations

$$g_1(G) = \min_{\lambda\in\mathbb{R}, Z\in\mathcal{S}^{|V|}, u\in\mathbb{R}^{|V|}} \left\{\lambda : \lambda(\mathrm{Diag}(u) - C + Z) - \frac{1}{4}uu^{\mathsf{T}} \ge 0,\ \lambda \ge 0,\ Z \in \mathcal{S}_G\right\},$$

$$h_1(G) = \min_{\lambda\in\mathbb{R}, Z\in\mathcal{S}^{|V|}} \{\lambda : \lambda I + Z - C \ge 0, Z \in \mathcal{S}_G\}$$

(where the formulation for $g_1(G)$ follows from (35) after taking the Schur complement with respect to the upper left corner λ). In order to obtain closed-form parameters, one may restrict the optimization in each of the programs to matrices $Z = tA_G$ (for some $t \in \mathbb{R}$) and, for the parameter $g_1(G)$, to vectors $u = \mu e$ (for some $\mu \in \mathbb{R}$). Let $\widehat{g}(G)$ and $\widehat{h}(G)$ denote the parameters obtained in this way so that $g_1(G) \le \widehat{g}(G)$ and $h_1(G) \le \widehat{h}(G)$. When the graph G is regular, the all-ones vector is an eigenvector of the matrices involved in the programs defining $\widehat{g}(G)$ and $\widehat{h}(G)$, and as we will show, this allows us to show the closed-form expressions claimed in Proposition 2 for $\widehat{g}(G)$ and $\widehat{h}(G)$ in terms of the second-largest eigenvalue λ_2 of A_G and $n := |V_1| = |V_2|$.

We will use the following basic result about the eigenvalues of A_G. We refer, for example, to the book by Brouwer and Haemers [3] for a general background about eigenvalues of graphs.

Lemma 7. *Assume $G = (V_1 \cup V_2, E)$ is a bipartite r-regular graph with $|V_1| = |V_2| =: n \ge 2$. Then, its adjacency matrix is of the form*

$$A_G = \begin{pmatrix} 0 & M_G \\ M_G^{\mathsf{T}} & 0 \end{pmatrix}, \quad \text{where } M_G \in \mathbb{R}^{|V_1|\times|V_2|}, \tag{47}$$

the eigenvalues of A_G are $\pm\sqrt{\lambda_i(M_G M_G^{\mathsf{T}})}$ for $i \in [n]$, $\lambda_1(A_G) = r$, $\lambda_{2n}(A_G) = -r$, and $\lambda_2(A_G) \ge 0$, with equality $\lambda_2(A_G) = 0$ if and only if G is complete bipartite. In the case when $G = B(H)$ is the bipartite double of an r-regular graph H, we have $M_G = A_H$, the eigenvalues of $A_{B(H)}$ are $\pm\lambda_i(A_H)$ for $i \in [n]$, and thus, $\lambda_2(A_{B(H)}) = \max\{\lambda_2(A_H), -\lambda_n(A_H)\}$. When $G = B_0(H)$ is the extended bipartite double of H, we have $M_G = A_H + I$ and $\lambda_2(A_{B_0(H)}) = \max\{\lambda_2(A_H) + 1, -\lambda_n(A_H) - 1\}$.

4.1. An Eigenvalue-Based Upper Bound $\widehat{h}(G)$ for $h(G)$

We give a closed-form eigenvalue-based upper bound for the parameter $h(G)$ in the case when the bipartite graph G is r-regular. Let $n := |V_1| = |V_2|$, and let λ_2 denote the second-largest eigenvalue of A_G (i.e., the second-largest singular value of M_G by Lemma 7). Vallentin [45] shows that $h(G) \le \frac{n}{r}\lambda_2$; our next result gives a sharpening of this bound.

Proposition 3. *Assume G is a bipartite r-regular graph, set $|V_1| = |V_2| =: n$, and let λ_2 be the second-largest eigenvalue of its adjacency matrix A_G. Then, we have*

$$h_1(G) \le \widehat{h}(G) = \frac{n}{2}\frac{\lambda_2}{r+\lambda_2} \le \frac{n}{r}\lambda_2. \tag{48}$$

Moreover, equality $h_1(G) = \frac{n}{2}\frac{\lambda_2}{r+\lambda_2}$ holds when G is edge-transitive.

Proof. We may assume G is not complete bipartite (or else $\lambda_2 = 0$ and $h(G) = h_1(G) = \widehat{h}(G) = 0$). The inequality $\frac{n}{2}\frac{\lambda_2}{r+\lambda_2} \le \frac{n}{2}\lambda_2$ is clear; we now show $h_1(G) \le \frac{n}{2}\frac{\lambda_2}{r+\lambda_2}$. For this, we use the formulation of $h_1(G)$ from (32), where we restrict the optimization to matrices Z of the form $Z = tA_G$ for some scalar $t \in \mathbb{R}$; we will show that the resulting optimal value is equal to $\frac{n}{2}\frac{\lambda_2}{r+\lambda_2}$. Note that when G is edge-transitive, this restriction can be made without loss of generality. Thus, we aim to compute the optimum value of the program

$$\widehat{h}(G) := \min_{\lambda, t\in\mathbb{R}} \{\lambda : \lambda I + tA_G - C \succeq 0\}, \tag{49}$$

which upper bounds $h_1(G)$ and is equal to it when G is edge-transitive. By taking a Schur complement, the matrix

$$\lambda I + tA_G - C = \begin{pmatrix} \lambda I & tM_G - \frac{1}{2}J \\ tM_G^{\mathsf{T}} - \frac{1}{2}J & \lambda I \end{pmatrix}$$

is positive semidefinite if and only if $\lambda > 0$ and the matrix

$$\begin{aligned}\lambda^2 I - \left(tM_G - \frac{1}{2}J\right)\left(tM_G^{\mathsf{T}} - \frac{1}{2}J\right) &= \lambda^2 I - \left(t^2 M_G M_G^{\mathsf{T}} - \frac{t}{2}M_G J - \frac{t}{2}JM_G^{\mathsf{T}} + \frac{1}{4}J^2\right) \\ &= \lambda^2 I - t^2 M_G M_G^{\mathsf{T}} + \frac{rt}{2}J + \frac{rt}{2}J - \frac{n}{4}J \\ &= \lambda^2 I - t^2 M_G M_G^{\mathsf{T}} + \left(rt - \frac{n}{4}\right)J =: Q\end{aligned}$$

is positive semidefinite. Because G is not complete bipartite, we have $\lambda > 0$. We now analyze when Q is positive semidefinite. The all-ones vector e is an eigenvector of $M_G M_G^{\mathsf{T}}$ and J and, thus, also of Q. Any eigenvector $w \perp e$ of $M_G M_G^{\mathsf{T}}$ for $\lambda_i(M_G M_G^{\mathsf{T}})$ $(2 \le i \le n)$ is an eigenvector of Q. Then, the eigenvalues of Q at these eigenvectors are as follows:

$$\text{at } e: \quad \lambda^2 - t^2 r^2 + n\left(tr - \frac{n}{4}\right),$$

$$\text{at } w \perp e: \quad \lambda^2 - t^2 \lambda_i(M_G M_G^{\mathsf{T}}) \quad \text{for } i = 2, \ldots, n.$$

Hence, $Q \succeq 0$ if and only if $\lambda^2 - t^2 r^2 + n(tr - \frac{n}{4}) \ge 0$ and $\lambda^2 - t^2\lambda_i(M_G M_G^{\mathsf{T}}) \ge 0$ for any $i \ge 2$, which is equivalent to $\lambda^2 - t^2\lambda_2^2 \ge 0$ (recall Lemma 7). Therefore, we must select t such that

$$\max\left\{t^2\lambda_2^2, t^2 r^2 - ntr + \frac{n^2}{4}\right\} \text{ is smallest possible.}$$

This maximum value is minimized at a root of the quadratic function $\phi(t) := \left(t^2 r^2 - trn + \frac{n^2}{4}\right) - t^2\lambda_2^2 = t^2(r^2 - \lambda_2^2) - trn + \frac{n^2}{4}$. Its discriminant is $r^2 n^2 - n^2(r^2 - \lambda_2^2) = n^2\lambda_2^2$, and $\phi(t)$ has two roots,

$$\frac{rn + \epsilon n\lambda_2}{2(r^2 - \lambda_2^2)} = \frac{n}{2(r - \epsilon\lambda_2)}$$

for

$$\epsilon = \pm 1.$$

Therefore, $\max\{t^2\lambda_2^2, t^2 r^2 - ntr + \frac{n^2}{4}\}$ is minimized at the smallest root $t := \frac{n}{2(r+\lambda_2)}$. Therefore, we have $\widehat{h}(G) = t\lambda_2 = \frac{n\lambda_2}{2(r+\lambda_2)}$, which proves (48). □

The parameter $h_1'(G)$ introduced in (39) provides an upper bound for $h(G)$ that is at least as good as $h_1(G)$. A natural question is whether one can derive from it another closed-form bound for $h(G)$ that may improve on $\widehat{h}(G)$ when G is regular. To define such a bound, one follows the same strategy as for $\widehat{h}(G)$. First, one writes the dual formulation of (39), which reads

$$\min_{\lambda,\eta\in\mathbb{R},u\in\mathbb{R}^n,Z\in\mathcal{S}^n}\left\{\lambda+\eta:\begin{pmatrix}\lambda & -u^{\mathsf{T}}/2\\ -u^{\mathsf{T}}/2 & \mathrm{Diag}(u)+\eta I+Z-C\end{pmatrix}\succeq 0,\ Z\in\mathcal{S}_G\right\}. \tag{50}$$

Then, one restricts the optimization to $u=\mu e$ and $Z=tA_G$ for scalars $\mu,t\in\mathbb{R}$, and after that, one takes again the dual, which gives the parameter

$$\widehat{h}'(G):=\max\left\{\langle C,X\rangle:\begin{pmatrix}1 & x^{\mathsf{T}}\\ x & X\end{pmatrix}\succeq 0,\ \mathrm{Tr}(X)=1,\ e^{\mathsf{T}}x=1,\ \langle A_G,X\rangle=0\right\}. \tag{51}$$

To ease the comparison with $\widehat{h}(G)$, let us also write the dual program of (49), which reads

$$\widehat{h}(G)=\max\{\langle C,X\rangle:X\succeq 0,\ \mathrm{Tr}(X)=1,\langle A_G,X\rangle=0\}. \tag{52}$$

(Strong duality holds because (49) is strictly feasible.) Both parameters $\widehat{h}(G)$ and $\widehat{h}'(G)$, in fact, coincide. To show this, we need the following auxiliary result, whose proof is postponed to Appendix B.

Lemma 8. *Assume $X\in\mathcal{S}^n$ satisfies $X\succeq 0$ and $\mathrm{Tr}(X)=1$. Then, there exists a vector $x\in\mathbb{R}^n$ such that $\begin{pmatrix}1 & x^{\mathsf{T}}\\ x & X\end{pmatrix}\succeq 0$ and $e^{\mathsf{T}}x=1$ if and only if $\langle J,X\rangle\geq 1$.*

Proposition 4. *For any bipartite regular graph G, we have $\widehat{h}(G)=\widehat{h}'(G)$.*

Proof. Comparing (51) with (52), it is clear that $\widehat{h}'(G)\leq\widehat{h}(G)$. If $G=K_{n,n}$, then both bounds are equal to zero. Assume $G\neq K_{n,n}$, and let X be an optimal solution for (52). As $J-4C\succeq 0$, we have $\langle J,X\rangle\geq 4\langle C,X\rangle=4\cdot\widehat{h}(G)\geq 4\cdot h(G)\geq 2$ (where $h(G)\geq 1/2$ follows by considering a bi-independent pair $(\{a\},\{b\})$ with $a\in V_1$ and $b\in V_2$). Hence, we can apply Lemma 8 and find a vector x such that (x,X) is feasible for (51), which shows that $\widehat{h}'(G)\geq\langle C,X\rangle=\widehat{h}(G)$. □

4.2. An Eigenvalue-Based Upper Bound $\widehat{g}(G)$ for $g(G)$

In the same way, one can give an eigenvalue-based upper bound $\widehat{g}(G)$ for the parameter $g(G)$ when G is bipartite r-regular. It is obtained by solving analytically the following optimization problem:

$$\widehat{g}(G):=\min_{\lambda,\mu,t\in\mathbb{R}}\left\{\lambda:\lambda(\mu I-C+tA_G)-\frac{\mu^2}{4}J\succeq 0,\ \lambda\geq 0\right\}.$$

The details are analogous to those for the parameter $\widehat{h}(G)$ considered in the previous section, but technically more involved. Therefore, we postpone the proof of the next result to Appendix C.

Proposition 5. *Assume G is a bipartite r-regular graph, set $n:=|V_1|=|V_2|$, and let λ_2 be the second-largest eigenvalue of the adjacency matrix A_G of G. Then, we have*

$$g_1(G)\leq\widehat{g}(G)=\begin{cases}\dfrac{n^2\lambda_2^2}{(\lambda_2+r)^2} & \text{if } r\leq 3\lambda_2,\\[2mm] \dfrac{n^2\lambda_2}{8(r-\lambda_2)} & \text{otherwise.}\end{cases}$$

Moreover, equality $g_1(G)=\widehat{g}(G)$ holds if G is vertex and edge-transitive.

Remark 6. Here are examples of regular bipartite graphs satisfying $r\leq 3\lambda_2$ or the reverse inequality $3\lambda_2\leq r$: if G is a perfect matching on $2n$ vertices, then $\lambda_2=r=1$, and thus, $r<3\lambda_2$ (see Section 5.1); on the other hand, if G is the complete bipartite graph $K_{n,n}$ minus a perfect matching, then $r=n-1$ and $\lambda_2=1$, and thus, $r\geq 3\lambda_2$ if $n\geq 4$ (see Section 5.2).

Recall the inequalities $h(G)\leq\frac{1}{2}\sqrt{g(G)}$ (from Lemma 1) and $h_1(G)\leq\frac{1}{2}\sqrt{g_1(G)}$ (from Proposition 1). One can check that also the eigenvalue bounds satisfy the analogous relation $\widehat{h}(G)\leq\frac{1}{2}\sqrt{\widehat{g}(G)}$, with equality if and only if $r\leq 3\lambda_2$. Hence, in the regime $3\lambda_2<r$, the parameter $\widehat{h}(G)$ provides a strictly better bound than $\frac{1}{2}\sqrt{\widehat{g}(G)}$ for both $h(G)$ and $\frac{1}{2}\sqrt{g(G)}$.

Therefore, we have

$$h_1(G) \le \min\{\widehat{h}(G), \frac{1}{2}\sqrt{g_1(G)}\} \le \max\{\widehat{h}(G), \frac{1}{2}\sqrt{g_1(G)}\} \le \frac{1}{2}\sqrt{\widehat{g}(G)}.$$

We now observe that the two parameters $\widehat{h}(G)$ and $\frac{1}{2}\sqrt{g_1(G)}$ are incomparable. Indeed, as observed, strict inequality $\widehat{h}(G) < \frac{1}{2}\sqrt{g_1(G)}$ may hold (e.g., for $K_{n,n}$ minus a perfect matching). On the other hand, there are regular bipartite graphs satisfying $\frac{1}{2}\sqrt{g_1(G)} < \widehat{h}(G)$ (such G is not edge-transitive). As an example, let G be the disjoint union of C_4 and C_6, thus two-regular with $\lambda_2 = 2$. Then, we verified that

$$\frac{1}{2}\sqrt{g_1(G)} = \frac{1}{2}\sqrt{6} < \frac{5}{4} = \widehat{h}(G).$$

4.3. Links to Some Other Eigenvalue Bounds

In this section, we investigate links between the new bounds introduced in previous sections and some known eigenvalue bounds in the literature. First, we point out a natural link between $\widehat{h}(\cdot)$ and Hoffman's ratio bound (53) for the stability number of a graph. After that, we present links to some spectral parameters $\varphi(G)$, $\varphi'(G)$ and $\varphi_H(G)$ by Haemers [21, 22], which he used to bound the parameter $g_{\mathrm{bc}}(G)$, the maximum number of edges in a biclique of an arbitrary graph G; see (55), (58), and (61) for the exact definitions. As $g_{\mathrm{bc}}(G) = g_{\mathrm{bi}}(\overline{G}) = g(B_0(\overline{G}))$, also the parameter $h_1(B_0(\overline{G}))$ provides an upper bound for $g_{\mathrm{bc}}(G)$. We will review the parameters of Haemers and investigate their relationships with the parameters $h_1(\cdot)$ and $\widehat{h}(\cdot)$.

4.3.1. Linking the Parameter $\widehat{h}(B(G))$ to Hoffman's Bound for $\alpha(G)$. Let $G = (V = [n], E)$ be an arbitrary graph, and let $\lambda_n(A_G)$ be the smallest eigenvalue of its adjacency matrix. If G is r-regular, then the following bound holds for its stability number:

$$\alpha(G) \le n\frac{-\lambda_n(A_G)}{r - \lambda_n(A_G)}. \tag{53}$$

This bound was proved by Hoffman (unpublished) and is known as Hoffman's ratio bound (see Haemers [23] for a short proof and a historical account). There is a tight link between Hoffman's ratio bound for G and the parameter $\widehat{h}(\cdot)$ for its bipartite double $B(G)$. Indeed, if $A \subseteq V$ is an independent set in G, then the pair (A, A) is a balanced bi-independent pair in $B(G)$. Therefore, $|A| \le \alpha(G)$ and $2|A| \le \alpha_{\mathrm{bal}}(B(G)) \le 4 \cdot \widehat{h}(B(G))$, giving

$$\alpha(G) \le \frac{1}{2}\alpha_{\mathrm{bal}}(B(G)) \le 2 \cdot \widehat{h}(B(G)) = n\frac{\lambda_2(A_{B(G)})}{r + \lambda_2(A_{B(G)})}. \tag{54}$$

By Lemma 7, we have $\lambda_2(A_{B(G)}) = \max\{\lambda_2(A_G), -\lambda_n(A_G)\}$, and thus,

$$n\frac{-\lambda_n(A_G)}{r - \lambda_n(A_G)} \le 2 \cdot \widehat{h}(B(G)) = n\frac{\lambda_2(A_{B(G)})}{r + \lambda_2(A_{B(G)})}.$$

Lovász [33] showed that also $\vartheta(G)$ is upper bounded by Hoffman's ratio bound. The parameters $\vartheta(G)$ and $h_1(B(G))$ satisfy the analogous relationship: $\vartheta(G) \le 2 \cdot h_1(B(G))$. Indeed, if X is an optimal solution to Program (24), then the matrix $X' := \frac{1}{2}\begin{pmatrix} X & X \\ X & X \end{pmatrix}$ is feasible for (33) with objective value $\langle C, X'\rangle = \frac{1}{2}\langle J, X\rangle = \frac{1}{2}\vartheta(G)$, giving the desired inequality.

4.3.2. Linking the Parameter $h_1(B_0(G))$ to Haemers's Spectral Bound $\varphi(G)$. As we saw earlier, for any bipartite graph G, the parameter $h_1(G)$ provides an upper bound for the parameter $g(G)$ via $\frac{1}{2}\sqrt{g(G)} \le h_1(G)$. This also directly gives a bound for the parameter $g_{\mathrm{bi}}(G) = g(B_0(G))$ when G is an arbitrary graph, namely, $\frac{1}{2}\sqrt{g_{\mathrm{bi}}(G)} \le h_1(B_0(G))$.

For an arbitrary graph $G = (V, E)$, Haemers [22] introduces the spectral parameter

$$\varphi(G) := \min_{M \in \mathcal{S}^{|V|}} \{\lambda_{abs}(M) : M_{ij} = 1 \text{ for all } \{i,j\} \in E\}, \tag{55}$$

where $\lambda_{abs}(M)$ denotes the maximum absolute value of an eigenvalue of M, and he shows that $\varphi(G)$ provides an upper bound for the parameter $g_{\mathrm{bc}}(G) = g_{\mathrm{bi}}(\overline{G})$ via the inequality

$$\sqrt{g_{\mathrm{bc}}(G)} \le \varphi(G). \tag{56}$$

Therefore, we have two bounds for $g_{\mathrm{bc}}(G)$, namely, $\frac{1}{2}\sqrt{g_{\mathrm{bc}}(G)} \le \frac{1}{2}\varphi(G)$ and $\frac{1}{2}\sqrt{g_{\mathrm{bc}}(G)} \le h_1(B_0(\overline{G}))$. We now show that these two upper bounds, in fact, coincide.

Lemma 9. *For any graph G, we have* $h_1(B_0(G)) = \frac{1}{2}\varphi(\overline{G})$.

Proof. Let $G = (V, E)$ and $\overline{G} = (V, \overline{E})$. First, observe the parameter $\varphi(\overline{G})$ can be reformulated as

$$\varphi(\overline{G}) = \min\left\{\lambda_{\max}(Y) : Y = \begin{pmatrix} 0 & M \\ M & 0 \end{pmatrix}, M \in \mathcal{S}^{|V|}, M_{ij} = 1 \text{ for all } \{i,j\} \in \overline{E}\right\}; \tag{57}$$

this follows from the fact that the eigenvalues of any Y in (57) are $\pm\lambda_i(M)$ for $i \in [|V|]$. Let $V \cup V'$ be the vertex set of the extended bipartite double $B_0(G)$, where V' is a disjoint copy of V, and let C be the matrix from (26), which is now indexed by $V \cup V'$. We use Formulation (32) of $h_1(B_0(G))$, defined as the smallest scalar λ for which $\lambda I - C + Z \succeq 0$ for some $Z \in \mathcal{S}_{B_0(G)}$ or, equivalently, as the minimum value of $\lambda_{\max}(C - Z)$ for $Z \in \mathcal{S}_{B_0(G)}$. As the condition $Z \in \mathcal{S}_{B_0(G)}$ corresponds to $Y := 2(C - Z)$ being feasible for (57), we can conclude that $2h_1(B_0(G)) = \varphi(\overline{G})$. □

4.3.3. Linking $h_1(B_0(G))$ to Haemers's Spectral Bounds $\varphi'(G)$ and $\varphi_H(G)$.

In the previous section, we mentioned the spectral bound $\varphi(G)$ from (55) of Haemers [22] for the parameter $g_{\text{bc}}(G)$ and observed its link to the parameter $h_1(\cdot)$; recall (56) and Lemma 9. In some earlier work [21], Haemers introduced the following spectral parameter for an arbitrary graph $G = (V = [n], E)$,

$$\varphi'(G) := \min_{M \in \mathcal{S}^{|V|}}\left\{n\frac{\lambda(M)}{1 + \lambda(M)} : Me = e, M_{ij} = 0 \text{ for } \{i,j\} \in E\right\}, \tag{58}$$

where $\lambda(M)$ denotes the second-largest absolute value of an eigenvalue of M. Haemers [22] showed that $\varphi(G) \le \varphi'(G)$ for all G and that there are graphs G for which the inequality is strict.

Let L_G denote the Laplacian matrix of G that is defined as $L_G = D_G - A_G$, where $D_G \in \mathcal{S}^n$ is the diagonal matrix whose i-th entry is the degree of vertex $i \in V$ in G. In what follows, we let $0 = \mu_1 \le \mu_2 \le \cdots \le \mu_n$ denote the eigenvalues of the Laplacian matrix L_G. In Haemers [21, theorem 2.4], he shows the inequality

$$\varphi'(\overline{G}) \le \varphi_H(G) := \frac{n}{2}\left(1 - \frac{\mu_2}{\mu_n}\right) \tag{59}$$

for any graph G (on n nodes), and he shows that equality holds in (59) if G is vertex- and edge-transitive. Therefore, we have the following inequalities:

$$(h_1(B_0(G)) =)\,\frac{1}{2}\varphi(\overline{G}) \le \frac{1}{2}\varphi'(\overline{G}) \le \frac{1}{2}\varphi_H(G) = \frac{n}{4}\left(1 - \frac{\mu_2}{\mu_n}\right), \tag{60}$$

where the right-most inequality is an equality if G is vertex- and edge-transitive. We next sharpen this latter result and show that $h_1(B_0(G)) = \frac{n}{4}\left(1 - \frac{\mu_2}{\mu_n}\right)$ if G is vertex- and edge-transitive.

Proposition 6. *Let $G = (V, E)$ be a graph, set $n := |V|$, and let $0 = \mu_1 \le \mu_2 \le \cdots \le \mu_n$ denote the eigenvalues of the Laplacian matrix of G. Then, we have*

$$h_1(B_0(G)) = \frac{1}{2}\varphi(\overline{G}) \le \frac{1}{2}\varphi_H(G) = \frac{n}{4}\left(1 - \frac{\mu_2}{\mu_n}\right),$$

with equality if G is vertex- and edge-transitive.

Proof. Consider the parameter $\tilde{h}(G)$ obtained from the definition of $h_1(B_0(G))$ in (32), where we restrict the optimization to matrices Z of the form $Z = \begin{pmatrix} 0 & tL_G + \mu I \\ tL_G + \mu I & 0 \end{pmatrix}$ for scalars $t, \mu \in \mathbb{R}$. Hence, $h_1(B_0(G)) \le \tilde{h}(G)$. First, we show that if G is vertex- and edge-transitive (hence regular), then this restriction can be made without loss of generality, and thus, $h_1(B_0(G)) = \tilde{h}(G)$.

For this, for any permutation σ of V, consider the associated permutation $\tilde{\sigma}$ of $V \cup V'$ (the vertex set of $B_0(G)$, where V' is a disjoint copy of V) defined by $\tilde{\sigma}(i) = \sigma(i)$ and $\tilde{\sigma}(i') := \sigma(i)'$ for $i \in V$; clearly, $\tilde{\sigma}$ is an automorphism of $B_0(G)$ if σ is an automorphism of G. Consider, in addition, the automorphism π of $B_0(G)$ obtained by flipping V and V': $\pi(i) = i'$ and $\pi(i') = i$ for $i \in V$. Then, under the action of the group of automorphisms of $B_0(G)$ generated by π and $\tilde{\sigma}$ (for σ automorphism of G), the edge set of $B_0(G)$ is partitioned into two orbits, the orbit $\Omega_V := \{\{i, i'\} : i \in V\}$ and the orbit $\Omega_E := \{\{i, j'\}, \{i', j\} : \{i, j\} \in E\}$. Now, if (λ, Z) is feasible for $h_1(B_0(G))$, then the same holds for its symmetrization obtained by averaging over the group of automorphisms of $B_0(G)$ just described. This gives a new feasible solution, (λ, Z), where the entries of Z take two possible nonzero values, depending on whether the entry corresponds to an edge in Ω_V or in Ω_E, and thus, Z has indeed the desired form claimed earlier.

We now aim to compute the optimum value of the program

$$\tilde{h}(G) = \min_{\lambda, t, \mu \in \mathbb{R}} \left\{ \lambda : \begin{pmatrix} \lambda I & tL_G + \mu I - \frac{1}{2}J \\ tL_G + \mu I - \frac{1}{2}J & \lambda I \end{pmatrix} \succeq 0 \right\}$$

and show it is equal to $\frac{n}{4}\left(1 - \frac{\mu_2}{\mu_n}\right)$. By taking a Schur complement (and assuming $\lambda > 0$), the matrix in the semidefinite program is positive semidefinite if and only if the matrix

$$\lambda^2 I - \left(tL_G + \mu I - \frac{1}{2}J\right)\left(tL_G + \mu I - \frac{1}{2}J\right) = (\lambda^2 - \mu^2)I - t^2 L_G^2 - 2t\mu L_G + \left(\mu - \frac{n}{4}\right)J =: Q$$

is positive semidefinite. Let e denote the all-ones vector, which is an eigenvector of L_G for its smallest eigenvalue $\mu_1 = 0$, and let $w_i \perp e$ be an eigenvector of L_G for its eigenvalue μ_i with $i \geq 2$. Then, the eigenvalues of Q at these eigenvectors are as follows:

$$\text{at } e: \quad \lambda^2 - \mu^2 + n\left(\mu - \frac{n}{4}\right) = \lambda^2 - \left(\mu - \frac{n}{2}\right)^2,$$

$$\text{at } w_i \perp e: \quad \lambda^2 - (t\mu_i + \mu)^2, \quad \text{for } i = 2, \ldots, n.$$

Hence, $Q \succeq 0$ if and only if all these eigenvalues are nonnegative, and thus, we must select t, μ such that

$$\max\left\{ \left(\mu - \frac{n}{2}\right)^2, (t\mu_2 + \mu)^2, (t\mu_n + \mu)^2 \right\} \text{ is smallest possible.}$$

Therefore, we must find the smallest value of λ for which there exist t, μ satisfying the system

$$\lambda \geq |t\mu_2 + \mu|, \quad \lambda \geq |t\mu_n + \mu|, \quad \lambda \geq |\mu - \frac{n}{2}|.$$

First, note that taking $\mu := \frac{n}{4} + \frac{n\mu_2}{4\mu_n}$, $t := \frac{-n}{2\mu_n}$ and $\lambda := \frac{n}{4}\left(1 - \frac{\mu_2}{\mu_n}\right)$ is feasible for the system shown (because $t\mu_2 + \mu = \lambda$, $t\mu_n + \mu = \mu - \frac{n}{2} = -\lambda$), which shows $\tilde{h}(G) \leq \frac{n}{4}\left(1 - \frac{\mu_2}{\mu_n}\right)$. We now show the reverse inequality. Assume λ, t, μ satisfy this system. The conditions $\lambda \geq -t\mu_n - \mu$ and $\lambda \geq t\mu_2 + \mu$ together give $\lambda \geq \frac{1}{2}(\mu_2 - \mu_n)t$, and the conditions $\lambda \geq t\mu_2 + \mu$ and $\lambda \geq -\mu + \frac{n}{2}$ give $\lambda \geq \frac{\mu_2}{2}t + \frac{n}{4}$. Therefore, $\tilde{h}(G)$ is at least the smallest value of λ for which there exists t such that $\lambda \geq \max\{\frac{1}{2}(\mu_2 - \mu_n)t, \frac{\mu_2}{2}t + \frac{n}{4}\}$. Now, observe that this maximum is minimized at the intersection point where $t = -\frac{n}{2\mu_n}$ (because $\mu_2 - \mu_n \leq 0$ and $\mu_2 \geq 0$). This gives the desired relation

$$\tilde{h}(G) \geq \frac{1}{2}(\mu_2 - \mu_n)\left(\frac{n}{-2\mu_n}\right) = \frac{n}{4}\left(1 - \frac{\mu_2}{\mu_n}\right),$$

which concludes the proof. □

An interesting feature of the closed-form bound $\frac{1}{2}\varphi_H(G) = \frac{n}{4}\left(1 - \frac{\mu_2}{\mu_n}\right)$ in Proposition 6 is that it is valid without any regularity assumption on the graph G.

Assume now G is r-regular, still arbitrary (not necessarily bipartite) on n nodes. Then, its adjacency matrix A_G satisfies $A_G = rI - L_G$, and thus, its eigenvalues are $\lambda_i = r - \mu_i$ for $i \in [n]$, with $\lambda_1 = r \geq \lambda_2 \geq \cdots \geq \lambda_n$. Therefore, for any r-regular graph G, we have

$$h_1(B_0(G)) \leq \frac{1}{2}\varphi_H(G) = \frac{n}{4}\left(1 - \frac{\mu_2}{\mu_n}\right) = \frac{n}{4}\frac{\lambda_2 - \lambda_n}{r - \lambda_n}. \tag{61}$$

As shown in Proposition 6, equality $h_1(B_0(G)) = \frac{1}{2}\varphi_H(G)$ holds if G is vertex- and edge-transitive. As the extended bipartite double graph $B_0(G)$ is $(r+1)$-regular, one can also upper bound $h_1(B_0(G))$ by the parameter $\widehat{h}(B_0(G))$ (as defined in Proposition 2). By Lemma 7, the second-largest eigenvalue of the adjacency matrix of $B_0(G)$ equals $\max\{\lambda_2 + 1, -\lambda_n - 1\}$, and thus,

$$h_1(B_0(G)) \leq \widehat{h}(B_0(G)) = \frac{n}{2}\frac{\max\{\lambda_2 + 1, -\lambda_n - 1\}}{\max\{\lambda_2 + 1, -\lambda_n - 1\} + r + 1}. \tag{62}$$

Next, we compare the upper bounds in (61) and (62).

Proposition 7. *Let G be an r-regular graph. Then, we have $\frac{1}{2}\varphi_H(G) \le \widehat{h}(B_0(G))$, with equality if and only if $\lambda_2 = r$ or $\lambda_2 + \lambda_n + 2 = 0$.*

Proof. Set $\mu := \max\{\lambda_2 + 1, -\lambda_n - 1\}$, and note that $\frac{1}{2}\varphi_H(G) \le \widehat{h}(B_0(G))$ is equivalent to $\psi := \mu(\lambda_2 + \lambda_n - 2r) + (r+1)(\lambda_2 - \lambda_n) \le 0$. If $\lambda_2 + \lambda_n + 2 \ge 0$, then $\mu = \lambda_2 + 1$, and we have $\psi = (\lambda_2 - r)(\lambda_2 + \lambda_n + 2) \le 0$. Otherwise, $\lambda_2 + \lambda_n + 2 \le 0$, $\mu = -\lambda_n - 1$, and we have $\psi = (r - \lambda_2)(\lambda_2 + \lambda_n + 2) \le 0$. □

Therefore, Haemers's bound $\varphi_H(G)$ improves on the bound $\widehat{h}(B_0(G))$ for any regular graph G. On the other hand, also the reverse situation may occur, where the parameter $\widehat{h}$ improves on Haemers's bound φ_H. For this, consider a bipartite graph $G = (V_1 \cup V_2, E)$. As observed in (7), we have $g_{\rm bc}(G) = g(\overline{G}^b)$, where $\overline{G}^b = (V_1 \cup V_2, (V_1 \times V_2) \setminus E)$ is the bipartite complement of G. Hence, we have the inequalities

$$\begin{aligned}\frac{1}{2}\sqrt{g_{\rm bc}(G)} &= \frac{1}{2}\sqrt{g(\overline{G}^b)} \le h_1(\overline{G}^b) \le \widehat{h}(\overline{G}^b),\\ \frac{1}{2}\sqrt{g_{\rm bc}(G)} &= \frac{1}{2}\sqrt{g(B_0(\overline{G}))} \le h_1(B_0(\overline{G})) \le \frac{1}{2}\varphi_H(\overline{G}),\end{aligned} \tag{63}$$

where we assume that G is regular when considering the parameters $\widehat{h}(\overline{G}^b)$ and $\varphi_H(\overline{G})$. Next, we show that $h_1(B_0(\overline{G})) = h_1(\overline{G}^b)$ and that $\widehat{h}(\overline{G}^b) \le \frac{1}{2}\varphi_H(\overline{G})$.

Proposition 8. *Let G be a bipartite graph. Then, we have $h_1(B_0(\overline{G})) = h_1(\overline{G}^b)$. Moreover, if G is r-regular, $n := |V_1| = |V_2|$, and λ_2 denotes the second-largest eigenvalue of A_G, then we have*

$$\widehat{h}(\overline{G}^b) = \frac{n}{2}\frac{\lambda_2}{\lambda_2 + n - r} \le \frac{1}{2}\varphi_H(\overline{G}) = \frac{n}{2}\frac{\lambda_2 + r}{2n - r + \lambda_2}, \tag{64}$$

with strict inequality precisely when $\lambda_2 < r < n$, that is, when G is connected and $G \ne K_{n,n}$.

Proof. First, we prove $h_1(B_0(\overline{G})) = h_1(\overline{G}^b)$. For this, we use Formulation (33) for the parameter $h_1(\cdot)$. Recall the definition (26) of the matrix $C \in \mathcal{S}^{|V|}$ for the bipartition $V = V_1 \cup V_2$, and let $\tilde{C} \in \mathcal{S}^{|V|+|V'|}$ denote the analogous matrix corresponding now to the bipartition $V \cup V'$, where $V = V_1 \cup V_2$ and $V' = V_1{}' \cup V_2{}'$ is a disjoint copy of V. The matrices $\tilde{C}$ and $A_{B_0(\overline{G})}$ have the form $\tilde{C} = \frac{1}{2}\begin{pmatrix} 0 & J & J & 0\\ J & 0 & 0 & J\\ J & 0 & 0 & J\\ 0 & J & J & 0\end{pmatrix}$ and $A_{B_0(\overline{G})} = \begin{pmatrix} 0 & A(\overline{G}^b) & I & 0\\ A(\overline{G}^b) & 0 & 0 & I\\ I & 0 & 0 & A(\overline{G}^b)\\ 0 & I & A(\overline{G}^b) & 0\end{pmatrix}$ with respect to the partition $V_1 \cup V_2' \cup V_1' \cup V_2$ (taken in that order), setting $A(\overline{G}^b) := A_{\overline{G}^b}$ for easier notation. If $X \in \mathcal{S}^{|V|}$ is optimal for $h_1(\overline{G}^b)$, then $Y := \frac{1}{2}\begin{pmatrix} X & 0\\ 0 & X\end{pmatrix}$ is feasible for $h_1(B_0(\overline{G}))$ with $\langle \tilde{C}, Y\rangle = \langle C, X\rangle$, which shows $h_1(B_0(G)) \ge h_1(\overline{G}^b)$. Conversely, assume $Y \in \mathcal{S}^{|V|+|V'|}$ is optimal for $h_1(B_0(\overline{G}))$. Let X (resp., X') denote the principal submatrix of Y indexed by $V_1 \cup V_2'$ (resp., $V_1' \cup V_2$). Then, $X/\mathrm{Tr}(X)$ and $X'/\mathrm{Tr}(X')$ are both feasible for $h_1(\overline{G}^b)$, which implies $h_1(\overline{G}^b)\cdot \mathrm{Tr}(X) \ge \langle C, X\rangle$ and $h_1(\overline{G}^b)\cdot\mathrm{Tr}(X') \ge \langle C, X'\rangle$. Summing up and using $\mathrm{Tr}(X) + \mathrm{Tr}(X') = \mathrm{Tr}(Y) = 1$, we get $h_1(\overline{G}^b) \ge \langle C, X\rangle + \langle C, X'\rangle = \langle \tilde{C}, Y\rangle = h_1(B_0(\overline{G}))$.

Assume now G is bipartite r-regular, $\lambda_2 = \lambda_2(A_G)$, and $n := |V_1| = |V_2|$; we show (64). First, we compute the parameter $\widehat{h}(\overline{G}^b)$. For this, note that $\overline{G}^b$ is $(n-r)$-regular. Moreover, if M_G denotes the incidence matrix of G, then the incidence matrix of $\overline{G}^b$ is $J - M_G$, whose second-largest singular value is equal to the second-largest singular value of M_G and thus to λ_2. Hence, using Relation (48), we obtain $\widehat{h}(\overline{G}^b) = \frac{n}{2}\frac{\lambda_2}{n-r+\lambda_2}$, as desired. Next, we compute the parameter $\varphi_H(\overline{G})$. For this, note that $\overline{G}$ is $(2n-1-r)$-regular, the second-largest eigenvalue of $A_{\overline{G}}$ is $-1 - \lambda_{\min}(A_G) = r - 1$, and its smallest eigenvalue is $-1 - \lambda_2(A_G) = -1 - \lambda_2$. In view of (61), we get $\varphi_H(\overline{G}) = n\frac{r+\lambda_2}{2n-r+\lambda_2}$, as desired. One can then easily check that the inequality in (64) is equivalent to $(r - \lambda_2)(n - r) \ge 0$, which holds because $\lambda_2 \le r \le n$. Hence, the inequality in (64) is strict precisely when $\lambda_2 < r < n$, that is, when G is connected and $G \ne K_{n,n}$. □

We summarize the various bounds obtained for the parameter $g_{\rm bc}(G)$ when G is an arbitrary r-regular graph (Figure 3(a)) and when G is bipartite r-regular (Figure 3(b)). As before, let $\lambda_1 = r \ge \lambda_2 \ge \cdots \ge \lambda_n$ denote the eigenvalues of A_G. Then, $\overline{G}$ is $(n-1-r)$-regular, with $\lambda_2(A_{\overline{G}}) = -1 - \lambda_n$ and $\lambda_n(A_{\overline{G}}) = -1 - \lambda_2$.

Figure 3. Bounds on $g_{\mathrm{bc}}(G)$; recall $h_1(B_0(\overline{G})) \leq \widehat{h}(B_0(\overline{G}))$, with equality if $B_0(\overline{G})$ is edge-transitive (Proposition 3).

(a)

$$\frac{1}{2}\sqrt{g_{\mathrm{bc}}(G)} \leq \overbrace{h_1(B_0(\overline{G})) \leq \tfrac{1}{2}\varphi_H(\overline{G})}^{\substack{\text{with equality if } \overline{G} \text{ is vertex-}\\ \text{and edge-transitive}\\ \textbf{Prop. 6}}} \underbrace{\leq \widehat{h}(B_0(\overline{G}))}_{\substack{\text{with equality if and only if}\\ \lambda_n = r-n \text{ or } \lambda_2+\lambda_n=0\\ \textbf{Prop. 7}}}$$

(b)

$$\frac{1}{2}\sqrt{g_{\mathrm{bc}}(G)} \leq \underbrace{h_1(B_0(\overline{G})) = h_1(\overline{G}^b)}_{\textbf{Prop. 8}} \overbrace{\leq \widehat{h}(\overline{G}^b)}^{\substack{\text{with equality if and only if}\\ \lambda_2 = r \text{ or } r=n\\ \textbf{Prop 8}}} \leq \underbrace{\tfrac{1}{2}\varphi_H(\overline{G}) \leq \widehat{h}(B_0(\overline{G}))}_{\substack{\text{with equality if and only if}\\ \lambda_n = r-n \text{ or } \lambda_2+\lambda_n=0\\ \textbf{Prop. 7}}}$$

Notes. (a) Bounds on $g_{\mathrm{bc}}(G)$ for G r-regular. (b) Bounds on $g_{\mathrm{bc}}(G)$ for G bipartite r-regular.

5. Examples

We now illustrate the behavior of the various parameters discussed earlier on some classes of regular graphs. Recall the definition of the matrix M_G in Lemma 7.

5.1. The Perfect Matching

For $n \geq 2$, let G be a perfect matching on $2n$ vertices. Then, $M_G = I$, $r = 1$, $\lambda_2 = 1$, and G is vertex- and edge-transitive. Using Proposition 2, we obtain

$$h_1(G) = \widehat{h}(G) = \frac{n}{2}\frac{\lambda_2}{r+\lambda_2} = \frac{n}{4} \quad \text{and} \quad g_1(G) = \widehat{g}(G) = \frac{n^2}{4}.$$

We have $g(G) = \lfloor n/2 \rfloor \lceil n/2 \rceil$ and $h(G) = \frac{1}{n}\lfloor n/2 \rfloor \lceil n/2 \rceil$ (obtained by maximizing ab and $\frac{ab}{a+b}$ with $a, b \geq 0$ integers and $a + b \leq n$). Hence, $h_1(G) = \frac{1}{2}\sqrt{g_1(G)}$ and $h_1(G)$, $g_1(G)$ give tight bounds for $h(G)$ and $g(G)$ (with equality for n even and up to rounding for n odd).

5.2. The Complete Bipartite Graph $K_{n,n}$ Minus a Perfect Matching

For $n \geq 2$, let G be the complete bipartite graph $K_{n,n}$ with a deleted perfect matching (also known as the *crown graph* on $2n$ vertices). Then, G is vertex- and edge-transitive, $(n-1)$-regular, $M_G = J_n - I_n$, and $\lambda_2 = 1$. We have $h(G) = \frac{1}{2}$ and $g(G) = 1$. Using Proposition 2, we obtain

$$h_1(G) = \widehat{h}(G) = \frac{n}{2}\frac{\lambda_2}{r+\lambda_2} = \frac{1}{2}, \text{ and } g_1(G) = \widehat{g}(G) = \begin{cases} \dfrac{n^2}{8(n-2)} & n \geq 4, \\ 1 & n \leq 4. \end{cases}$$

Hence, the bound $h_1(G)$ is tight for both $h(G)$ and $\frac{1}{2}\sqrt{g(G)}$, whereas the ratio $g_1(G)/g(G)$ grows linearly in n. Note that $h_1(G) < \frac{1}{2}\sqrt{g_1(G)}$ for $n \geq 5$, which gives an example with strict separation between the parameters h_1 and $\frac{1}{2}\sqrt{g_1}$ (and thus, $\widehat{h}$ and $\frac{1}{2}\sqrt{\widehat{g}}$). In view of (63), the parameter $g_{\mathrm{bc}}(G)$ is upper bounded by $4\widehat{h}(\overline{G}^b)^2$ and by $\varphi_H(\overline{G})^2$. Note that $4\widehat{h}(\overline{G}^b)^2 = 4\left(\frac{n}{4}\right)^2 = \frac{n^2}{4}$, which improves on Haemers's bound $\varphi_H(\overline{G})^2 = \left(\frac{n^2}{n+2}\right)^2$ for $n \geq 3$. This thus gives a class of graphs for which strict inequality holds in (64).

5.3. The Cycle Graph C_n

Let G be the cycle C_n on $n \geq 3$ vertices, which is vertex- and edge-transitive and two-regular. The eigenvalues of the adjacency matrix A_{C_n} are $2\cos(2\pi j/n)$, where $j = 0, \ldots, n-1$ (see, e.g., Brouwer and Haemers [3]), so $\lambda_2(A_{C_n}) = 2\cos(2\pi/n)$, and $\lambda_n(A_{C_n}) = -2$ if n is even and $\lambda_n(A_{C_n}) = -2\cos(\pi/n)$ if n is odd.

First, we compute the parameters for the extended bipartite double graph $B_0(C_n)$. Using Proposition 6 and Relations (61) and (62), we get

$$h_1(B_0(C_n)) = \frac{1}{2}\varphi_H(C_n) = \begin{cases} \dfrac{n}{4}\cos(\pi/n)^2 & \text{if } n \text{ even,} \\ \dfrac{n}{4}(2\cos(\pi/n) - 1) & \text{if } n \text{ odd,} \end{cases} \quad \widehat{h}(B_0(C_n)) = \frac{n}{4}\frac{2\cos(2\pi/n)+1}{\cos(2\pi/n)+2}.$$

Hence, we have $h_1(B_0(C_n)) = \widehat{h}(B_0(C_n)) (= 0)$ for $n = 3$ (in which case, $B_0(C_3) = K_{3,3}$) and strict inequality $h_1(B_0(C_n)) < \widehat{h}(B_0(C_n))$ for $n \geq 4$ (as expected from Proposition 7). Note also that $B_0(C_n)$ is not edge-transitive if $n \geq 4$. One can also show that

$$h(B_0(C_n)) = \begin{cases} \dfrac{1}{4}(n-2) & \text{if } n \text{ even,} \\ \dfrac{(n-1)(n-3)}{4(n-2)} & \text{if } n \text{ odd,} \end{cases} \quad g(B_0(C_n)) = \begin{cases} \dfrac{1}{4}(n-2)^2 & \text{if } n \text{ even,} \\ \dfrac{1}{4}(n-1)(n-3) & \text{if } n \text{ odd.} \end{cases}$$

Therefore, $h(B_0(C_n)) \le \frac{1}{2}\sqrt{g(B_0(C_n))}$, with equality for n even. Moreover, the ratio $\widehat{h}(B_0(C_n))/h(B_0(C_n))$ tends to one as $n \to \infty$, so the bound $\widehat{h}(B_0(C_n))$ (and thus, $h_1(B_0(C_n))$, too) is asymptotically tight for $h(B_0(C_n))$ and $\frac{1}{2}\sqrt{g(B_0(C_n))}$.

For n, even the graph $G = C_n$ is bipartite. Then, we have

$$h(C_n) \le h_1(C_n) = \widehat{h}(C_n) = \frac{n}{4}\frac{\lambda_2}{\lambda_2 + r} = \frac{n}{4}\frac{\cos(2\pi/n)}{\cos(2\pi/n)+1} \le \frac{\alpha(C_n)}{4} = \frac{n}{8}.$$

Therefore, $h_1(C_n) = \Theta(n/8) = \Theta(\alpha(C_n)/4)$. Moreover, one can construct a bipartite bi-independent pair (A, B) showing $h(C_n) = \Theta(n/8)$ (see also Chen et al. [5]). Namely, for $n \equiv 0 \pmod 4$, set $A = \{1,3,\dots,\frac{n}{2}-1\}$, $B = \{\frac{n}{2}+2, \frac{n}{2}+4, \dots, n-2\}$ with $|A| = \frac{n}{4}$, $|B| = \frac{n}{4} - 1$, and, for $n \equiv 2 \pmod 4$, set $A = \{1,3,\dots,\frac{n}{2}-2\}$, $B = \{\frac{n}{2}+1, \frac{n}{2}+3, \dots, n-2\}$ with $|A| = |B| = \frac{n-2}{4}$.

5.4. The Hypercube Graph Q_r

The hypercube graph Q_r is the bipartite graph with vertex set $V = \{0,1\}^r$, where two vertices are adjacent when their Hamming distance is one. Therefore, the bipartition is $V = V_1 \cup V_2$, where V_1 (resp., V_2) consists of all $x \in V$ with an even (resp., odd) Hamming weight $|x|$. The graph Q_r is vertex- and edge-transitive and r-regular. The eigenvalues of A_{Q_r} are $r - 2k$ for $k = 0, \dots, r$, where the eigenvalue $r - 2k$ has multiplicity $\binom{r}{k}$. Therefore, $\lambda_2(A_{Q_r}) = r - 2$. Thus, the parameter $h_1(Q_r)$ is given by

$$h_1(Q_r) = \widehat{h}(Q_r) = 2^{r-3}\frac{r-2}{r-1}.$$

One can show that $\lim_{r\to\infty} h_1(Q_r)/h(Q_r) = 1$. For this, we will show that $h(Q_r) \ge \frac{a(r-1)}{4}$, where the sequence $(a(r))_{r\ge 0}$ is defined recursively by

$$a(2r) := 2^{2r} - \binom{2r}{r},\ a(2r+1) := 2 \cdot a(2r) \text{ if } r \ge 1, \text{ and } a(0) = 0. \tag{65}$$

Using the fact that $\binom{2r}{r} \sim \frac{2^{2r}}{\sqrt{\pi r}}$, one obtains $a(r-1) \sim 2^{r-1}$ and $h(Q_r) \ge 2^{r-3}(1 - c/\sqrt{r})$ (for some constant $c > 0$), and thus, $h_1(Q_r)/h(Q_r)$ tends to one as $r \to \infty$. Note that the bound $h(Q_r) \le \alpha(Q_r)/4 = 2^{r-1}/4 = 2^{r-3}$ from Lemma 1 is slightly weaker than $h(Q_r) \le h_1(Q_r)$, but already strong enough to exhibit $h(Q_r) \sim 2^{r-3}$ (when combined with the lower bound $h(Q_r) \ge \frac{a(r-1)}{4}$).

We now show that $h(Q_r) \ge \frac{a(r-1)}{4}$. For this, it is useful to observe that the graph Q_r is isomorphic to $B_0(Q_{r-1})$, the extended bipartite double of Q_{r-1} (the bipartition of Q_r provides the bipartition of $B_0(Q_{r-1})$ by simply deleting the last coordinate in all vertices of Q_r). Thus, we have $h(Q_r) = h(B_0(Q_{r-1})) = h_{\text{bi}}(Q_{r-1})$, where the last equality follows from (5). Hence, instead of searching for bipartite bi-independent pairs in Q_r, we may as well search for (general) bi-independent pairs in Q_{r-1}, which is a simpler task. We show that $h_{\text{bi}}(Q_r) \ge \frac{1}{4}a(r)$ for all $r \ge 1$. First, consider the case of Q_{2r}. Define the sets

$$L := \{x \in \{0,1\}^{2r} : |x| \le r-1\}, \quad U := \{x \in \{0,1\}^{2r} : |x| \ge r+1\}.$$

Then, (L, U) is a (balanced) bi-independent pair in Q_{2r}, with $|L| = |U| = \frac{1}{2}\left(2^{2r} - \binom{2r}{r}\right) = \frac{1}{2}a(2r)$, which implies $h_{\text{bi}}(Q_r) \ge \frac{1}{4}a(2r)$. Consider now the case of Q_{2r+1}. Define $L' := L \times \{0,1\}$ and $U' := U \times \{0,1\} \subseteq \{0,1\}^{2r+1}$. Then, the pair (L', U') is (balanced) bi-independent in Q_{2r+1}, with $|L'| = |U'| = a(2r) = \frac{1}{2}a(2r+1)$, which implies $h_{\text{bi}}(Q_{2r+1}) \ge \frac{1}{4}a(2r+1)$.

This construction can be used to show that $\alpha_{\text{bal}}(Q_r) \ge a(r-1)$ for all $r \ge 1$. For this, given $A \subseteq \{0,1\}^r$, define the following subsets of $\{0,1\}^{r+1}$ obtained by adding a parity bit,

$$A_{\text{even}} := \{(x, |x| \bmod 2) : x \in A\} \subseteq \{0,1\}^{r+1},\ A_{\text{odd}} := \{(x, |x|+1 \bmod 2) : x \in A\} \subseteq \{0,1\}^{r+1}.$$

Applying this to the sets $L, U \subseteq \{0,1\}^{2r}$, we obtain $L_{\text{even}}, U_{\text{odd}} \subseteq \{0,1\}^{2r+1}$ such that $(L_{\text{even}}, U_{\text{odd}})$ is balanced bipartite bi-independent in Q_{2r+1} with $|L_{\text{even}}| = |U_{\text{odd}}| = |L| = a(2r)/2$, which implies $\alpha_{\text{bal}}(Q_{2r+1}) \ge a(2r)$. Similarly, using the sets $L', U' \subseteq \{0,1\}^{2r+1}$, we obtain $L'_{\text{even}}, U'_{\text{odd}} \subseteq \{0,1\}^{2r+2}$ that provide a balanced bipartite bi-independent pair in Q_{2r+2} with $|L'_{\text{even}}| = |U'_{\text{odd}}| = |L'| = a(2r+1)/2$, which implies $\alpha_{\text{bal}}(Q_{2r+2}) \ge a(2r+1)$.

Conjecture 1. *We conjecture that equality $\alpha_{\text{bal}}(Q_r) = a(r-1)$ holds for all $r \geq 1$.*

We have verified numerically that Conjecture 1 indeed holds for any $r \leq 13$. For $r \leq 8$, this can be verified using an integer programming solver (like Gurobi [20]). For larger values, $r \leq 13$, we show this in an indirect manner. We consider the semidefinite upper bound on $\alpha_{\text{bal}}(Q_r)$ that is obtained from the Lasserre relaxation of order 2. After applying a symmetry reduction (as done in Gijswijt et al. [17] and Litjens et al. [32]), we solve the resulting semidefinite program numerically and obtain an upper bound that coincides with $a(r-1)$ for $r \leq 13$. In addition, $\alpha_{\text{bal}}(Q_r)/a(r-1) \to 1$ as $r \to \infty$ because $\alpha_{\text{bal}}(Q_r) \leq \alpha(Q_r) = 2^{r-1}$ and $a(r-1) \sim 2^{r-1}$.

Observe that $\alpha_{\text{bal}}(Q_{r+1}) \geq 2 \cdot \alpha_{\text{bal}}(Q_r)$. For this, for $x \in \{0,1\}^r$, let $x' \in \{0,1\}^r$ be obtained by switching the last bit of x so that the weights of x, x' have distinct parities, and for a set $A \subseteq \{0,1\}^r$ and $b \in \{0,1\}$, define $Ab := \{(x,b) : x \in A\} \subseteq \{0,1\}^{r+1}$. The claim now follows from the fact that if (A, B) is a balanced bipartite bi-independent pair in Q_r, then the pair $(B1 \cup B'0, A1 \cup A'0)$ is balanced bipartite bi-independent in Q_{r+1} with size $2|A \cup B|$. Hence, Conjecture 1 implies equality $\alpha_{\text{bal}}(Q_{r+1}) = 2 \cdot \alpha_{\text{bal}}(Q_r)$ for r odd.

Interestingly, the sequence $a(r)$ in (65) corresponds to the sequence A307768 in OEIS Foundation Inc. [37], which counts the number of heads-or-tails games of length r during which, at some point, there are as many heads as tails. It is also related to several other well-known combinatorial counting problems; see, for example, Eğecioğlu and King [10] or Feller [12, chapter III] for an overview. It is interesting to understand the exact relationship of this sequence with the parameter $\alpha_{\text{bal}}(Q_r)$.

6. Lasserre Bounds for the Balanced Parameters

In this section, we turn our attention to the "balanced" parameters $\alpha_{\text{bal}}(G)$, $g_{\text{bal}}(G)$ and $h_{\text{bal}}(G)$ that are obtained by restricting the optimization to balanced bipartite bi-independent pairs in the definition of $\alpha(G)$, $g(G)$, and $h(G)$. Recall from (3) that $\frac{1}{4}\alpha_{\text{bal}}(G) = \frac{1}{2}\sqrt{g_{\text{bal}}(G)} = h_{\text{bal}}(G)$. As these are NP-hard parameters, one is interested in finding efficient bounds for them, strengthening those for the original parameters $g(G)$ and $h(G)$.

Let $G = (V = V_1 \cup V_2, E)$ be a bipartite graph. Following the approach in Section 3.1, each of the parameters $\alpha_{\text{bal}}(G)$, $g_{\text{bal}}(G)$ and $h_{\text{bal}}(G)$ has a natural polynomial optimization formulation, which offers the starting point to define several hierarchies of semidefinite relaxations. For this, define the vector $f := \chi^{V_1} - \chi^{V_2}$. Let $I_{G,\text{bal}}$ denote the ideal in $\mathbb{R}[x]$ that is generated by the ideal I_G (itself generated by $x_i^2 - x_i$ for $i \in V$ and $x_i x_j$ for $\{i,j\} \in E$) and the polynomial $f^{\mathsf{T}}x$. For an integer t, let $I_{G,\text{ bal},t}$ denote its truncation at degree t, where all summands are restricted to have degree at most t. Then, the formulation for $\alpha_{\text{bal}}(G)$ follows by replacing the ideal I_G (resp., $I_{G,2\alpha(G)}$) by the ideal $I_{G,\text{bal}}$ (resp., $I_{G,\text{ bal},2\alpha(G)}$) in (19) (resp., (20)). Similarly, $g_{\text{bal}}(G)$ (resp., $h_{\text{bal}}(G)$) is obtained by adding the "balancing" constraint $f^{\mathsf{T}}x = 0$ to the program (27) defining $g(G)$ (resp., to the program (28) defining $h(G)$). Now, each of these polynomial optimization formulations can be used to define a Lasserre-type hierarchy. In this way, one obtains the hierarchies $\text{las}_{\text{bal},r}(G)$, $g_{\text{bal},r}(G)$, and $h_{\text{bal},r}(G)$ for $r \in \mathbb{N}$ that converge to $\alpha_{\text{bal}}(G)$, $g_{\text{bal}}(G)$, and $h_{\text{bal}}(G)$, respectively, after $r \geq \alpha(G)$ steps. They are obtained, respectively, from Programs (22) (defining $\text{las}_r(G)$), (29) (defining $g_r(G)$), and (30) (defining $h_r(G)$) by replacing the truncated ideal $I_{G,2r}$ by its balanced analog $I_{G,\text{ bal},2r}$; that is,

$$\text{las}_{\text{bal},r}(G) = \min\{\lambda : \lambda - x^{\mathsf{T}}x \in \Sigma_2 + I_{G,\text{bal},2\text{r}}\},$$

$$g_{\text{bal},r}(G) = \min\{\lambda : \lambda - x^{\mathsf{T}}Cx \in \Sigma_2 + I_{G,\text{bal},2\text{r}}\},$$

$$h_{\text{bal},r} = \min\{\lambda : x^{\mathsf{T}}(\lambda I - C)x \in \Sigma_2 + I_{G,\text{bal},2\text{r}}\}.$$

We will now focus on the Lasserre bounds of order $r = 1$. We will give explicit semidefinite formulations and show relationships between the various parameters. The parameter $\text{las}_{\text{bal},1}(G)$ is the analog of $\text{las}_1(G) = \vartheta(G)$ obtained by adding a balancing constraint to Program (23). However, adding a balancing constraint to the formulation of $\vartheta(G)$ in (24) leads to another parameter $\vartheta_{\text{bal}}(G)$ that is, in general, weaker than $\text{las}_{\text{bal},1}(G)$. The parameters $g_{\text{bal},1}(G)$ and $h_{\text{bal},1}(G)$ are obtained by adding a balancing constraint to the respective programs, defining $g_1(G)$ and $h_1(G)$. Moreover, they can be shown to be nested between $\text{las}_{\text{bal},1}(G)$ and $\vartheta_{\text{bal}}(G)$; see Proposition 9. For bipartite regular graphs, we will investigate some natural symmetric variations of these parameters, with the hope of obtaining a new closed-form parameter strengthening $\widehat{h}(G)$. However, as we will show, it turns out that in all cases, one recovers the parameter $\widehat{h}(G)$; see Propositions 11 and 12. Therefore, the refined formulations taking into account the balancing constraints do not yet lead to stronger eigenvalue bounds for the parameter $\alpha_{\text{bal}}(\cdot)$.

6.1. The Lasserre Bounds of Order $r = 1$ for the Balanced Parameters

We begin with semidefinite reformulations for the parameter $\text{las}_{\text{bal},1}(G)$.

Lemma 10. *For any bipartite graph $G = (V, E)$, we have*

$$\text{las}_{\text{bal},1}(G) = \max_{X \in \mathcal{S}^{|V|}} \left\{ \langle I, X \rangle : \begin{pmatrix} 1 & \text{diag}(X)^{\mathsf{T}} \\ \text{diag}(X) & X \end{pmatrix} \succeq 0,\ X_{ij} = 0 \text{ if } \{i,j\} \in E,\ \langle ff^{\mathsf{T}}, X \rangle = 0 \right\}, \tag{66}$$

$$= \min_{Z \in \mathcal{S}^{|V|}, u \in \mathbb{R}^{|V|}, s \in \mathbb{R}} \left\{ \lambda : \begin{pmatrix} \lambda & -u^{\mathsf{T}}/2 \\ -u/2 & \text{Diag}(u) - I + Z + sff^{\mathsf{T}} \end{pmatrix} \succeq 0,\ Z \in \mathcal{S}_G \right\}. \tag{67}$$

Proof. As in Section 3.2,the proof uses Lemma 4. By definition, $\text{las}_{\text{bal},1}(G)$ is the smallest scalar λ for which $\lambda - x^{\mathsf{T}} I x \in \Sigma_2 + I_{G,\text{bal},2}$, that is, $\lambda - x^{\mathsf{T}} I x - (a_0 + a^{\mathsf{T}} x) f^{\mathsf{T}} x \in \Sigma_2 + I_{G,2}$ for some $a_0 \in \mathbb{R}, a \in \mathbb{R}^n$. Thus, $\text{las}_{\text{bal},1}(G)$ is the smallest λ such that $[x]_1^{\mathsf{T}} \left(Q - \begin{pmatrix} \lambda & a_0 f^{\mathsf{T}}/2 \\ a_0 f/2 & -I + \frac{af^{\mathsf{T}} + fa^{\mathsf{T}}}{2} \end{pmatrix} \right) [x]_1 \in I_{G,2}$ for some $a_0 \in \mathbb{R}, a \in \mathbb{R}^n$. Applying Lemma 4, we arrive at the program

$$\text{las}_{\text{bal},1}(G) = \min_{Z \in \mathcal{S}^{|V|}, u, a \in \mathbb{R}^{|V|}, a_0 \in \mathbb{R}} \left\{ \lambda : \begin{pmatrix} \lambda & \frac{1}{2}(-u + a_0 f)^{\mathsf{T}} \\ \frac{1}{2}(-u + a_0 f) & \text{Diag}(u) - I + Z + \frac{af^{\mathsf{T}} + fa^{\mathsf{T}}}{2} \end{pmatrix} \succeq 0, Z \in \mathcal{S}_G \right\}.$$

Now, we take the dual of this semidefinite program. We also apply some simplifications, such as observing that $Xf = 0$ is equivalent to $\langle ff^{\mathsf{T}}, X \rangle = 0$ when $X \succeq 0$, which, in turn, implies $f^{\mathsf{T}} \text{diag}(X) = 0$ when $\begin{pmatrix} 1 & \text{diag}(X)^{\mathsf{T}} \\ \text{diag}(X) & X \end{pmatrix} \succeq 0$. In this way, we arrive at Program (66). Taking the dual of (66) gives the (simplified) program (67). Note that strong duality holds because Program (67) is strictly feasible (e.g., take $s = 0$, $Z = 0$, $u = \mu e$ with $\mu > 1$, and $\lambda > \frac{n}{4} \frac{\mu^2}{\mu - 1}$). □

Hence, Program (66) is the analog of Program (23) defining $\text{las}_1(G) = \vartheta(G)$, to which we add the balancing condition $\langle ff^{\mathsf{T}}, X \rangle = 0$. Next, we consider the analog of Program (24) to which we add the balancing conditions $\langle ff^{\mathsf{T}}, X \rangle = 0$ and $f^{\mathsf{T}} \text{diag}(X) = 0$, giving the parameter

$$\vartheta_{\text{bal}}(G) := \max_{X \in \mathcal{S}^{|V|}} \{ \langle J, X \rangle : X \succeq 0,\ \text{Tr}(X) = 1,\ X_{ij} = 0 \text{ if } \{i,j\} \in E,$$
$$\langle ff^{\mathsf{T}}, X \rangle = 0,\ \langle \text{Diag}(f), X \rangle = 0 \}, \tag{68}$$

$$= \min_{Z \in \mathcal{S}^{|V|}, \lambda, s, v \in \mathbb{R}} \{ \lambda : \lambda I - J + Z + v\, \text{Diag}(f) + sff^{\mathsf{T}} \succeq 0,\ Z \in \mathcal{S}_G \}, \tag{69}$$

where the second formulation (69) follows by taking the dual of (68) (and observing that (69) is strictly feasible). We will see in Proposition 9 that $\vartheta_{\text{bal}}(G)$ provides a weaker bound for $\alpha_{\text{bal}}(G)$ than $\text{las}_{\text{bal},1}(G)$.

We now consider the parameter $g_{\text{bal},1}(G)$. By definition, $g_{\text{bal},1}(G)$ is the smallest scalar λ for which $\lambda - x^{\mathsf{T}} C x \in \Sigma_2 + I_{G,\text{bal},2}$. Comparing with the definition of $\text{las}_{\text{bal},1}(G)$, we see that it suffices to exchange the matrices C and I to get the semidefinite formulations of $g_{\text{bal},1}(G)$ in the next lemma (recall also Remark 3).

Lemma 11. *For any bipartite graph $G = (V, E)$, we have*

$$g_{\text{bal},1}(G) = \max_{X \in \mathcal{S}^{|V|}} \left\{ \langle C, X \rangle : \begin{pmatrix} 1 & \text{diag}(X)^{\mathsf{T}} \\ \text{diag}(X) & X \end{pmatrix} \succeq 0,\ X_{ij} = 0 \text{ if } \{i,j\} \in E,\ \langle ff^{\mathsf{T}}, X \rangle = 0 \right\}, \tag{70}$$

$$= \min_{\lambda, s \in \mathbb{R}, u \in \mathbb{R}^{|V|}, Z \in \mathcal{S}^{|V|}} \left\{ \lambda : \begin{pmatrix} \lambda & -u^{\mathsf{T}}/2 \\ -u/2 & \text{Diag}(u) - C + Z + sff^{\mathsf{T}} \end{pmatrix} \succeq 0,\ Z \in \mathcal{S}_G \right\}. \tag{71}$$

Finally, we give semidefinite formulations for the parameter $h_{\text{bal},1}(G)$.

Lemma 12. *Let $G=(V,E)$ be a bipartite graph. Then, we have*

$$h_{\mathrm{bal},1}(G)=\max_{X\in\mathcal{S}^{|V|}}\{\langle C,X\rangle : X\succeq 0,\ \mathrm{Tr}(X)=1,\ X_{ij}=0\ \text{ if } \{i,j\}\in E,$$
$$\langle ff^{\mathsf{T}},X\rangle=0,\ \langle \mathrm{Diag}(f),X\rangle=0\},\tag{72}$$

$$h_{\mathrm{bal},1}(G)=\min_{\lambda,v,s\in\mathbb{R},Z\in\mathcal{S}^{|V|}}\{\lambda:\lambda I-C+Z+v\,\mathrm{Diag}(f)+sff^{\mathsf{T}}\succeq 0,\ Z\in\mathcal{S}_G\}.\tag{73}$$

Proof. The argument is similar to the one used to show Lemma 10. Namely, one starts with the definition of $h_{\mathrm{bal},1}(G)$ as the smallest λ for which $x^{\mathsf{T}}(\lambda I-C)x\in\Sigma_2+I_{G,\mathrm{bal},2}$. Using Lemma 4, one arrives at a semidefinite program whose dual can be shown (after some simplifications) to take the form (72). Then, one takes the dual of Program (72), which has the form (73). □

We now compare the parameters $\mathrm{las}_{\mathrm{bal},1}(G)$, $\vartheta_{\mathrm{bal}}(G)$, $g_{\mathrm{bal},1}(G)$ and $h_{\mathrm{bal},1}(G)$.

Proposition 9. *For any bipartite graph G, we have the inequalities*

$$\frac{1}{4}\mathrm{las}_{\mathrm{bal},1}(G)\le\frac{1}{2}\sqrt{g_{\mathrm{bal},1}(G)}\le h_{\mathrm{bal},1}(G)=\frac{1}{4}\vartheta_{\mathrm{bal}}(G).$$

Moreover, we have $\frac{1}{2}\sqrt{g_{\mathrm{bal},1}(G)}=\frac{1}{4}\vartheta_{\mathrm{bal}}(G)\iff \mathrm{las}_{\mathrm{bal},1}(G)=\vartheta_{\mathrm{bal}}(G)$.

Proof. The equality $\vartheta_{\mathrm{bal}}(G)=4h_{\mathrm{bal},1}(G)$ follows from the fact that Programs (68) (defining $\vartheta_{\mathrm{bal}}(G)$) and (72) (defining $h_{\mathrm{bal},1}(G)$) differ only in their objective functions that are, respectively, $\langle J,X\rangle$ and $\langle C,X\rangle$, combined with the identity $J-4C=ff^{\mathsf{T}}$.

The inequality $\mathrm{las}_{\mathrm{bal},1}(G)\le\vartheta_{\mathrm{bal}}(G)$ follows using Formulations (66) and (68) and a classic argument (repeated for convenience). If X is optimal for (66) with $x:=\mathrm{diag}(X)$, then $X-xx^{\mathsf{T}}\succeq 0$, $f^{\mathsf{T}}x=0$, $\mathrm{Tr}(X)=e^{\mathsf{T}}x$, so $X/\mathrm{Tr}(X)=X/e^{\mathsf{T}}x$ is feasible for (68), and thus, we have $\vartheta_{\mathrm{bal}}(G)\ge\frac{1}{e^{\mathsf{T}}x}\langle J,X\rangle\ge\frac{1}{e^{\mathsf{T}}x}\langle J,xx^{\mathsf{T}}\rangle=e^{\mathsf{T}}x=\mathrm{las}_{\mathrm{bal},1}(G)$.

For the inequality $\mathrm{las}_{\mathrm{bal},1}(G)^2\le 4\cdot g_{\mathrm{bal},1}(G)$, pick an optimal solution X for (66) with $x:=\mathrm{diag}(X)$ so that $X-xx^{\mathsf{T}}\succeq 0$, and use again the fact that $4C=J-ff^{\mathsf{T}}$. Then, we have $4\cdot g_{\mathrm{bal},1}(G)\ge\langle 4C,X\rangle=\langle J,X\rangle\ge\langle J,xx^{\mathsf{T}}\rangle=(e^{\mathsf{T}}x)^2=\langle I,X\rangle^2=\mathrm{las}_{\mathrm{bal},1}(G)^2$.

We now show the inequality $4\cdot g_{\mathrm{bal},1}(G)\le\vartheta_{\mathrm{bal}}(G)^2$. For this, let X be optimal for Program (70) defining $g_{\mathrm{bal},1}(G)$. Then, X is feasible for (66), and thus, $\mathrm{las}_{\mathrm{bal},1}(G)\ge\mathrm{Tr}(X)$. In addition, $X/\mathrm{Tr}(X)$ is feasible for (68), and thus, $\vartheta_{\mathrm{bal}}(G)\ge\frac{1}{\mathrm{Tr}(X)}\langle J,X\rangle$. Using $4C=J-ff^{\mathsf{T}}$, we obtain $4\cdot g_{\mathrm{bal},1}(G)=\langle 4C,X\rangle=\langle J,X\rangle=\mathrm{Tr}(X)\cdot\langle J,X/\mathrm{Tr}(X)\rangle\le\mathrm{las}_{\mathrm{bal},1}(G)\cdot\vartheta_{\mathrm{bal}}(G)\le\vartheta_{\mathrm{bal}}(G)^2$. Finally, this argument also shows that equality $4\cdot g_{\mathrm{bal},1}(G)=\vartheta_{\mathrm{bal}}(G)^2$ implies $\mathrm{las}_{\mathrm{bal},1}(G)=\vartheta_{\mathrm{bal}}(G)$, which concludes the proof. □

Quite surprisingly, whereas we had the inequality $h_1(G)\le\frac{1}{2}\sqrt{g_1(G)}$ (recall Proposition 1), we now have the reverse inequality $\frac{1}{2}\sqrt{g_{\mathrm{bal},1}(G)}\le h_{\mathrm{bal},1}(G)$ for the balanced analogs. We next give an example where this inequality is strict.

Example 2. Let G be the bipartite graph from Figure 2. One can check that $h_{\mathrm{bal},1}(G)=2/3$, $g_{\mathrm{bal},1}(G)=4/3$ and $\mathrm{las}_{\mathrm{bal},1}(G)=9/4$, which shows that the strict inequalities $\frac{1}{4}\mathrm{las}_{\mathrm{bal},1}(G)<\frac{1}{2}\sqrt{g_{\mathrm{bal},1}(G)}<h_{\mathrm{bal},1}(G)$ hold. To see this, consider the matrices

$$X_1=\frac{1}{12}\begin{pmatrix}1&1&0&2\\1&5&2&4\\0&2&1&1\\2&4&1&5\end{pmatrix},\quad X_2=\frac{1}{9}\begin{pmatrix}3&1&0&4\\1&7&4&4\\0&4&3&1\\4&4&1&7\end{pmatrix},\quad X_3=\frac{1}{32}\begin{pmatrix}12&3&0&15\\3&24&15&12\\0&15&12&3\\15&12&3&24\end{pmatrix}.$$

Then, X_1 is feasible for (72) with $\langle C,X_1\rangle=2/3$, X_2 is feasible for (70) with $\langle C,X_2\rangle=4/3$, and X_3 is feasible for (66) with $\langle I,X_3\rangle=9/4$. One can check optimality of these solutions for the respective programs (for this, use the constraint $\langle ff^{\mathsf{T}},X\rangle=0$ to reduce the semidefinite program to an equivalent semidefinite program involving smaller matrices, and then construct a solution of the dual program with the same objective value).

6.2. Symmetric Versions of the Parameters $\text{las}_{\text{bal},1}(G)$, $\vartheta_{\text{bal}}(G)$ and $g_{\text{bal},1}(G)$

Here, we address the question whether it is possible to obtain closed-form eigenvalue-based upper bounds for $\alpha_{\text{bal}}(G)$ that improve on the spectral parameter $\widehat{h}(G)$ from (48). For this, a natural approach is to restrict the optimization in the programs (67), (69), and (71) to matrices $Z = tA_G$ for some $t \in \mathbb{R}$ and, for (67) and (71), to vectors $u = \mu e$ for some $\mu \in \mathbb{R}$. Moreover, we add a term $v\text{Diag}(f)$ to the matrix involved in (67) and (71), which amounts to adding the redundant constraint $\langle \text{Diag}(f), X\rangle = 0$ to the programs (66) and (70). The motivation for this is to get possibly sharper bounds. In addition, the bounds obtained in this way are easier to compare (see Proposition 10). However, as we will show in Proposition 11, these additional constraints will turn out to be redundant for bipartite regular graphs.

Therefore, we consider the parameters

$$\widehat{\text{las}_{\text{bal}}}(G) := \min_{\lambda,\mu,t,s,v\in\mathbb{R}} \left\{ \lambda : \begin{pmatrix} \lambda & -\mu e^{\mathsf{T}}/2 \\ -\mu e/2 & (\mu-1)I + tA_G + sff^{\mathsf{T}} + v\,\text{Diag}(f) \end{pmatrix} \succeq 0 \right\}, \tag{74}$$

$$= \max_{X\in\mathcal{S}^{|V|},\, x\in\mathbb{R}^{|V|}} \left\{ \langle I, X\rangle : \begin{pmatrix} 1 & x^{\mathsf{T}} \\ x & X \end{pmatrix} \succeq 0, \text{Tr}(X) = e^{\mathsf{T}}x, \langle A_G, X\rangle = 0, \langle ff^{\mathsf{T}}, X\rangle = 0, \langle \text{Diag}(f), X\rangle = 0 \right\}, \tag{75}$$

$$\widehat{\vartheta_{\text{bal}}}(G) := \min_{\lambda,t,v,s\in\mathbb{R}} \{\lambda : \lambda I - J + tA_G + v\,\text{Diag}(f) + sff^{\mathsf{T}} \succeq 0\}, \tag{76}$$

$$= \max\{\langle J, X\rangle : X \succeq 0, \text{Tr}(X) = 1, \langle A_G, X\rangle = 0, \langle ff^{\mathsf{T}}, X\rangle = 0, \langle \text{Diag}(f), X\rangle = 0\}, \tag{77}$$

$$\widehat{g_{\text{bal}}}(G) := \min_{\lambda,\mu,t,s,v\in\mathbb{R}} \left\{ \lambda : \begin{pmatrix} \lambda & -\mu e^{\mathsf{T}}/2 \\ -\mu e/2 & \mu I - C + tA_G + sff^{\mathsf{T}} + v\,\text{Diag}(f) \end{pmatrix} \succeq 0 \right\}, \tag{78}$$

$$= \max_{X\in\mathcal{S}^{|V|},\, x\in\mathbb{R}^{|V|}} \left\{ \langle C, X\rangle : \begin{pmatrix} 1 & x^{\mathsf{T}} \\ x & X \end{pmatrix} \succeq 0, \text{Tr}(X) = e^{\mathsf{T}}x, \langle X, A_G\rangle = 0, \langle ff^{\mathsf{T}}, X\rangle = 0, \langle \text{Diag}(f), X\rangle = 0 \right\}. \tag{79}$$

(Because each of the programs (74), (76), and (78) is strictly feasible, strong duality holds as claimed earlier.) We begin with comparing the parameters given and show the analog of Proposition 9.

Proposition 10. *For any bipartite graph G, we have*

$$\frac{1}{4}\widehat{\text{las}_{\text{bal}}}(G) \le \frac{1}{2}\sqrt{\widehat{g_{\text{bal}}}(G)} \le \frac{1}{4}\widehat{\vartheta_{\text{bal}}}(G).$$

Proof. We use the formulations (75), (77), and (79) for the parameters $\widehat{\text{las}_{\text{bal}}}(G)$, $\widehat{\vartheta_{\text{bal}}}(G)$, $\widehat{g_{\text{bal}}}(G)$, respectively. Then, the inequalities follow in the same way as in the proof of Proposition 9. □

Next, we compute the parameter $\widehat{\vartheta_{\text{bal}}}(G)$ and show its relation to $\widehat{h}(G)$.

Proposition 11. *Assume $G = (V_1 \cup V_2, E)$ is bipartite r-regular, set $n := |V_1| = |V_2|$, and let λ_2 denote the second-largest eigenvalue of A_G. Then, we have*

$$\widehat{\vartheta_{\text{bal}}}(G) = \frac{2n\lambda_2}{r+\lambda_2} = 4\cdot\widehat{h}(G).$$

We delay the proof, which is a bit technical, to Appendix D. As the proof will show, Program (76), defining $\widehat{\vartheta_{\text{bal}}}(G)$, admits an optimal solution with $v = 0$. Hence, when G is bipartite regular, the constraint $\langle \text{Diag}(f), X\rangle = 0$ is redundant in program (76), and one can set $v = 0$ in Program (76); the same observation applies to the programs defining $\widehat{g_{\text{bal}}}(G)$ and $\widehat{\text{las}_{\text{bal}}}(G)$.

We can now compute the parameters $\widehat{\text{las}_{\text{bal}}}(G)$ and $\widehat{g_{\text{bal}}}(G)$ and show their relation to $\widehat{h}(G)$.

Proposition 12. *For any regular bipartite graph G, we have*

$$\frac{1}{4}\widehat{\text{las}_{\text{bal}}}(G) = \frac{1}{2}\sqrt{\widehat{g_{\text{bal}}}(G)} = \frac{1}{4}\vartheta_{\text{bal}}(G) = \widehat{h}(G).$$

Proof. Assume G is bipartite regular, and set $n := |V_1| = |V_2|$. If G is complete bipartite, then $\alpha_{\text{bal}}(G) = 0$ and, using (77) and Proposition 10, one can check that $\widehat{\vartheta_{\text{bal}}}(G) = 0$, so the result holds. We now assume that G is not complete bipartite. In view of Propositions 10 and 11, it suffices to show $\widehat{\text{las}_{\text{bal}}}(G) \geq \widehat{\vartheta_{\text{bal}}}(G)$. Assume that (λ, μ, t, s, v) is feasible for the Program (74) defining $\widehat{\text{las}_{\text{bal}}}(G)$; we construct a feasible solution for Program (76) defining $\widehat{\vartheta_{\text{bal}}}(G)$ with the same objective value λ. Call $Q \in \mathcal{S}^{1+|V_1|+|V_2|}$ the matrix appearing in Program (74). By taking a Schur complement with respect to its upper left corner entry λ, we obtain

$$\lambda((\mu-1)I + tA_G + sff^{\mathsf{T}} + v\,\text{Diag}(f)) - \frac{\mu^2}{4}J \succeq 0.$$

We now claim that $\mu > 1$. For this, observe that the submatrices of Q indexed by V_1 and V_2 read $(\mu-1)I_n + sJ_n \pm vI_n$. Because they are both positive semidefinite, this implies $(\mu-1)I_n + sJ_n \succeq 0$, and thus, $\mu \geq 1$. Assume that $\mu = 1$. Then, the conditions $sJ_n \pm vI_n \succeq 0$ imply $v = 0$. Let $i \in V_1$ and $j \in V_2$ that are not adjacent (they exist because $G \neq K_{n,n}$). Then, the principal submatrix of Q indexed by $\{0, i, j\}$ takes the form $\begin{pmatrix} \lambda & -1/2 & -1/2 \\ -1/2 & s & -s \\ -1/2 & -s & s \end{pmatrix}$, and it must be positive semidefinite, so we reach a contradiction. Hence, we have $\mu > 1$. Thus, we can scale the matrix and obtain

$$\lambda I + \frac{\lambda t}{\mu-1}A_G + \frac{\lambda s}{\mu-1}ff^{\mathsf{T}} + \frac{\lambda v}{\mu-1}\text{Diag}(f) - \frac{\mu^2}{4(\mu-1)}J \succeq 0.$$

Note that $\frac{\mu^2}{4(\mu-1)} - 1 = \frac{(\mu-2)^2}{4(\mu-1)} \geq 0$, and add $\left(\frac{\mu^2}{4(\mu-1)} - 1\right)J \succeq 0$ to the matrix. Therefore, we obtain

$$\lambda I + \frac{\lambda t}{\mu-1}A_G + \frac{\lambda s}{\mu-1}ff^{\mathsf{T}} + \frac{\lambda v}{\mu-1}\text{Diag}(f) - J \succeq 0,$$

which gives a feasible solution to Formulation (76) of $\widehat{\vartheta_{\text{bal}}}(G)$ and thus shows $\widehat{\vartheta_{\text{bal}}}(G) \leq \lambda = \widehat{\text{las}_{\text{bal}}}(G)$. □

Remark 7. One idea for trying to get a stronger closed-form bound for $\alpha_{\text{bal}}(G)$ could be to consider a possibly weaker symmetrization of the parameter $\text{las}_{\text{bal},1}(G)$, where we now allow a vector u taking distinct values for nodes in V_1 and in V_2 instead of restricting to $u = \mu e$ for some $\mu \in \mathbb{R}$. Therefore, we consider the following variation $\widetilde{\text{las}_{\text{bal}}}(G)$ of the parameter $\widehat{\text{las}_{\text{bal}}}(G)$, defined by

$$\min_{\lambda,\mu_1,\mu_2,t,s,v\in\mathbb{R}} \left\{\lambda : \begin{pmatrix} \lambda & -u^{\mathsf{T}}/2 \\ -u/2 & \text{Diag}(u) - I + tA_G + sff^{\mathsf{T}} + v\,\text{Diag}(f) \end{pmatrix} \succeq 0,\ u = \mu_1\chi^{V_1} + \mu_2\chi^{V_2}\right\}. \tag{80}$$

By its definition, the parameter $\widetilde{\text{las}_{\text{bal}}}(G)$ lower bounds $\widehat{\text{las}_{\text{bal}}}(G)$, for which the optimization is restricted to the case $\mu_1 = \mu_2$. Nevertheless, it turns out that the two parameters are, in fact, equal. To see this, let us use the dual semidefinite program of (80), which reads

$$\widetilde{\text{las}_{\text{bal}}}(G) = \max\left\{\langle I, X\rangle : \begin{pmatrix} 1 & x^{\mathsf{T}} \\ x & X \end{pmatrix} \succeq 0,\ \langle A_G, X\rangle = 0,\ \langle ff^{\mathsf{T}}, X\rangle = 0,\right.$$
$$\left.\langle \text{Diag}(f), X\rangle = 0,\ \langle \text{Diag}(\chi^{V_k}), X\rangle = x^{\mathsf{T}}\chi^{V_k} \text{ for } k = 1,2\right\}. \tag{81}$$

Assume (x, X) is optimal for Program (75) defining $\widehat{\text{las}_{\text{bal}}}(G)$. In order to show that (x, X) is feasible for (81), we only need to check that $\langle \text{Diag}(\chi^{V_k}), X\rangle = x^{\mathsf{T}}\chi^{V_k}$ for $k = 1, 2$. For this, note that feasibility for (75) implies $x^{\mathsf{T}}f = 0$, and thus, $x^{\mathsf{T}}\chi^{V_1} = x^{\mathsf{T}}\chi^{V_2}$. Moreover, $\langle \text{Diag}(f), X\rangle = 0$ gives $\langle \text{Diag}(\chi^{V_1}), X\rangle = \langle \text{Diag}(\chi^{V_2}), X\rangle$, and $\text{Tr}(X) = e^{\mathsf{T}}x$ gives $\langle \text{Diag}(\chi^{V_1}), X\rangle + \langle \text{Diag}(\chi^{V_2}), X\rangle = x^{\mathsf{T}}\chi^{V_1} + x^{\mathsf{T}}\chi^{V_2}$. Combining these facts, we get $\langle \text{Diag}(\chi^{V_k}), X\rangle = x^{\mathsf{T}}\chi^{V_k}$ for $k = 1, 2$, as desired. This shows $\widehat{\text{las}_{\text{bal}}}(G) \leq \widetilde{\text{las}_{\text{bal}}}(G)$, and thus, equality $\widehat{\text{las}_{\text{bal}}}(G) = \widetilde{\text{las}_{\text{bal}}}(G)$ holds.

7. Concluding Remarks

In this paper, we investigate the parameters $g(G)$, $h(G)$, $\alpha_{\text{bal}}(G)$ (and other related parameters) dealing with (balanced) bipartite bi-independent pairs in a bipartite graph G. We show that deciding whether $\alpha_{\text{bal}}(G) = \alpha(G)$ is an NP-complete problem and that this implies NP-hardness of the parameters $\alpha_{\text{bal}}(G), h(G), g(G)$. We offer a systematic study of the basic semidefinite bounds that are obtained at the first level of sums-of-squares (Lasserre) hierarchies. In particular, we introduce the semidefinite bounds $h_1(G), g_1(G)$ (for $g(G), h(G)$) and $\text{las}_{\text{bal},1}(G)$, $\vartheta_{\text{bal}}(G)$ (for $\alpha_{\text{bal}}(G)$). These semidefinite bounds can be seen as natural variations of the celebrated theta number $\vartheta(G)$ of Lovász [33], allowing a quadratic objective (for $h_1(G)$, $g_1(G)$) or adding a balancing constraint (for $\text{las}_{\text{bal},1}(G)$, $\vartheta_{\text{bal}}(G)$). However, whereas $\vartheta(G) = \alpha(G)$ when G is bipartite, the parameters $h_1(G)$, $g_1(G)$, $\text{las}_{\text{bal},1}(G)$, $\vartheta_{\text{bal}}(G)$ give only upper bounds for the respective combinatorial graph parameters. An interesting fact is that $h_1(G)$, in fact, provides a better bound for $g(G)$ than $g_1(G)$ (recall Proposition 1). Another interesting fact is that $\text{las}_{\text{bal},1}(G) \le \vartheta_{\text{bal}}(G)$ and that the inequality may be strict, whereas the unbalanced analogs both coincide with $\vartheta(G)$ (recall Proposition 9 and Relation (25)). We also show that deciding whether $h(G) = h_1(G)$ is an NP-hard problem. An object of further study will be to investigate the numerical behavior of the various bounds introduced in this paper.

When G is an r-regular bipartite graph, we give closed-form eigenvalue-based bounds that are obtained by restricting to symmetric solutions in the definitions of $h_1(G)$, $g_1(G)$, $\text{las}_{\text{bal},1}(G)$, and $\vartheta_{\text{bal}}(G)$. In this way, we obtain the parameter $\widehat{h}(G) = \frac{n}{2}\frac{\lambda_2}{r+\lambda_2}$, where λ_2 is the second-largest eigenvalue of A_G, and G has n vertices on each side of its bipartition. Then, $h(G) \le h_1(G) \le \widehat{h}(G)$ holds, and it turns out that $\widehat{h}(G)$ provides a better bound for $g(G)$ than its corresponding eigenvalue-bound $\widehat{g}(G)$. Moreover, only edge-transitivity is required to show equality $h_1(G) = \widehat{h}(G)$, whereas one needs vertex- and edge-transitivity to show $g_1(G) = \widehat{g}(G)$. Bipartite regular graphs that are edge-transitive but not vertex-transitive are known as semisymmetric graphs; the smallest such graph, constructed by Folkman [15], is four-regular with 20 vertices. We show that the natural eigenvalue bounds corresponding to the various semidefinite relaxations of $\alpha_{\text{bal}}(G)$ all coincide (up to simple transformation) with the parameter $\widehat{h}(G)$ and that the same holds for a natural strengthening of $h_1(G)$ (recall Proposition 4). Hence, finding a stronger closed-form bound for $\alpha_{\text{bal}}(G)$ that is able to take advantage of the restriction to balanced independent sets remains an open problem.

We have considered the parameter $\widehat{h}(G)$ (in Relation (49)) and gave a closed-form expression for it in the case when G is a r-regular bipartite graph. More generally, one can consider the case when G is a bipartite (r_1, r_2)-regular graph, which means that every vertex in V_1 has degree r_1 and every vertex in V_2 has degree r_2. Then, along the same lines as for Proposition 3, one can also compute a closed-form expression for $\widehat{h}(G)$. It will be interesting to compute this parameter for the graphs $G^n_{k,\ell}$ and $G^{n,q}_{k,\ell}$ that are related to cross-intersecting subset and subspace families, as mentioned in the introduction, and to check their relationship with the bounds by Pyber [39] and Suda and Tanaka [41].

Therefore, we see, in this paper, an application of the second-largest eigenvalue λ_2 to the study of parameters involving (balanced) independent sets in bipartite graphs. The second-largest eigenvalue λ_2 has been widely studied and has well-known applications to various graph properties. For instance, there is a classical upper bound on λ_2 for any r-regular graph in terms of r and its diameter [36], and large r-regular graphs with small second eigenvalue are shown to be Hamiltonian [29]. A notable application of λ_2 is for bounding the edge expansion (or isoperimetric number), sometimes denoted h_G, and defined as the minimum value of $E(S, V \setminus S)/|S|$ taken over all $S \subseteq V$ with $1 \le |S| \le |V|/2$. Namely, if G is r-regular, then $(r - \lambda_2)/2 \le h_G \le \sqrt{r^2 - \lambda_2^2}$ (see [34]). We refer, for example, to Brouwer and Haemers [3] and Cvetković and Simić [6] and further references therein for more information.

Among other examples, we have considered the hypercube $G = Q_r$ on $\{0,1\}^r$. We show that $\alpha_{\text{bal}}(Q_r) \ge a(r-1)$ for all $r \ge 1$, where $a(r)$ is as defined in (65). Computational experiments suggest that this is the exact value. Showing $\alpha_{\text{bal}}(Q_r) = a(r-1)$ for all r is an interesting open problem that would offer a new link from balanced bi-independent sets to other combinatorial counting problems such as the number of r-steps random walks on a line starting from the origin and returning to it at least once.

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Appendix A. Application to Product-Free Sets in Finite Groups

Let Γ be a finite group. A subset $A \subseteq \Gamma$ is called *product-free* if $uv \notin A$ for all $u, v \in A$. A problem of interest is to find the maximum cardinality of a product-free set in Γ; see, for example, Kedlaya [27] and Gowers [18] for background and an overview of results on this problem. As in Kedlaya [27], let $\beta(\Gamma)$ denote the maximum density $|A|/|\Gamma|$ of a product-free set $A \subseteq \Gamma$. Clearly, $\beta(\Gamma) \le 1/2$ (because, for any $x \in A$, the sets A and xA are disjoint subsets of Γ). It is known that any finite abelian group satisfies $1/7 \le \beta(\Gamma) \le 1/2$. Moreover, any finite group satisfies $\beta(\Gamma) = \Omega(1/n^{3/14})$, and the question arose whether $\beta(\Gamma) = \Omega(1/n^{\epsilon})$ for all $\epsilon > 0$. Gowers [18] answered in the negative by showing that $\beta(\mathrm{PSL}_2(q)) = O(1/n^{1/9})$ (see Example A.1).

As a crucial ingredient in his proof (which applies, in fact, to a more general setting), Gowers [18] introduces an upper bound on the product-free set density of Γ in terms of the second eigenvalue of an associated bipartite Cayley graph. We follow the exposition by Kedlaya [27] and Vallentin [45], which relies on using (a variation of) the parameter $\widehat{h}$ applied to this bipartite Cayley graph.

Let us fix a product-free set $A \subseteq \Gamma$ and define the bipartite Cayley graph $G_{\Gamma,A} = (V_1 \cup V_2, E)$, where V_1 and V_2 are two disjoint copies of Γ, where $u \in V_1$, $v \in V_2$ are adjacent in $G_{\Gamma,A}$ if $uv \in A$. Note that the graph $G_{\Gamma,A}$ is $|A|$-regular. Let A_k denote the copy of A within the set V_k for $k = 1, 2$. Then, by construction, (A_1, A_2) is a bi-independent pair in $G_{\Gamma,A}$ because A is product-free.

The next result relates the size of $|A|$ to the second-largest eigenvalue of the adjacency matrix of $G_{\Gamma,A}$. It is essentially based on Gowers [18, lemma 3.2] and Kedlaya [27, lemma 5.3] (and Vallentin's presentation [45]).

Lemma A.1. *Let Γ be a finite group, $n := |\Gamma|$, and let k denote the minimum dimension of a nontrivial representation of Γ. Let $A \subseteq \Gamma$ be a product-free set, and let λ_2 denote the second-largest eigenvalue of the adjacency matrix of the bipartite Cayley graph $G_{\Gamma,A}$. Then, we have*

$$\lambda_2 \le \sqrt{\frac{|A|(n-|A|)}{k}}. \tag{A.1}$$

Proof. Set $G := G_{\Gamma,A}$, and write its adjacency matrix as in (47). By Lemma 7, λ_2^2 is the second-largest eigenvalue of $M_G M_G^{\mathsf{T}}$; let k_2 denote its multiplicity. As G is $|A|$-regular, G has $n|A|$ edges, and thus, $\mathrm{Tr}(M_G M_G^{\mathsf{T}}) = n|A|$. On the other hand, by considering the spectral decomposition of $M_G M_G^{\mathsf{T}}$, we obtain $\mathrm{Tr}(M_G M_G^{\mathsf{T}}) \ge |A|^2 + \lambda_2^2 k_2$. By combining both facts, we deduce $n|A| \ge |A|^2 + \lambda_2^2 k_2$, and thus, $\lambda_2 \le \sqrt{|A|(n-|A|)/k_2}$.

We now show that $k_2 \ge k$, which, combined with the inequality for λ_2, gives the desired inequality (A.1). For this, let W denote the eigenspace of $M_G M_G^{\mathsf{T}}$ corresponding to the eigenvalue λ_2^2 so that W has dimension k_2. One can easily check that

$$W = \{x \in \mathbb{R}^{|V_1|} : x^{\mathsf{T}} e = 0,\ x^{\mathsf{T}} M_G M_G^{\mathsf{T}} x = \lambda_2^2 \|x\|^2\}.$$

We show that W is invariant under some nontrivial action of Γ. For this, consider the action of Γ on the space $\mathbb{R}^{|V_1|}$ defined by right multiplication; that is, for $\gamma \in \Gamma$ and $x = (x_u)_{u\in\Gamma}$, define $x^{\gamma} := (x_{u\gamma})_{u\in\Gamma}$. We claim that $(M_G^{\mathsf{T}} x^{\gamma})_v = (M_G^{\mathsf{T}} x)_{\gamma^{-1}v}$ for any $v \in \Gamma$. Indeed,

$$(M_G^{\mathsf{T}} x^{\gamma})_v = \sum_{u\in\Gamma} M_G(u,v) x_u^{\gamma} = \sum_{u\in\Gamma: uv\in A} x_{u\gamma} = \sum_{w\in\Gamma: w\gamma^{-1}v\in A} x_w = \sum_{w\in\Gamma} M_G(w, \gamma^{-1}v) x_w = (M_G^{\mathsf{T}} x)_{\gamma^{-1}v}.$$

From this follows that $x^{\mathsf{T}} M_G M_G^{\mathsf{T}} x = (x^{\gamma})^{\mathsf{T}} M_G M_G^{\mathsf{T}} x^{\gamma}$ and $e^{\mathsf{T}} x = e^{\mathsf{T}} x^{\gamma}$. Hence, $x \in W$ implies $x^{\gamma} \in W$, and thus, the space W is invariant under this action of Γ. This action is nontrivial because a nonzero vector $x \in W$ is not a multiple of the all-ones vector, and thus, $x^{\gamma} \ne x$ for some $\gamma \in \Gamma$. Therefore, we can conclude that $k_2 = \dim W \ge k$, and the proof is complete. □

We can now show the following bound on the product-free set density, which is essentially theorem 3.3 of Gowers [18] (see Remark A.1).

Theorem A.1. *Let Γ be a finite group, and let k denote the minimum dimension of a nontrivial representation of Γ. If A is a product-free set in Γ, then we have $|A| \le \frac{|\Gamma|}{1+k^{1/3}}$.*

Proof. As (A_1, A_2) is a bipartite bi-independent pair in $G_{\Gamma,A}$, we have $\frac{|A|}{2} \le h(G_{\Gamma,A})$, and thus, $\frac{|A|}{2} \le \widehat{h}(G_{\Gamma,A}) = \frac{n}{2}\frac{\lambda_2}{|A|+\lambda_2}$, which implies $|A|^2 \le \lambda_2(n-|A|) \le (n-|A|)\sqrt{|A|(n-|A|)/k}$, using (A.1). This implies

$$\left(\frac{|A|}{n-|A|}\right)^{3/2} \le \frac{1}{k^{1/2}},$$

and thus,

$$|A| \le \frac{n}{1+k^{1/3}}$$

as desired. □

Remark A.1. The upper estimates in (A.1) and Theorem A.1 offer a slight sharpening of the known results. Indeed, Gowers shows $\lambda_2 := \lambda_2(A_{G_{\Gamma,A}}) \le \sqrt{n|A|/k}$ (lemma 3.2 in Gowers [18]), a bound that is a bit weaker than the one in (A.1), which he then uses to show $|A| \le \frac{n}{k^{1/3}}$ (theorem 3.3 in Gowers [18]). Vallentin [45] uses his eigenvalue bound to conclude $\frac{|A|}{2} \le h(G_{\Gamma,A}) \le \frac{n}{|A|}\lambda_2 \le \frac{n}{|A|}\sqrt{n|A|/k}$, and thus, $|A| \le 2^{2/3}\frac{n}{k^{1/3}}$. Our slightly sharper estimate $|A| \le \frac{n}{1+k^{1/3}}$ follows using the sharper bound in (A.1) and the sharper eigenvalue bound $h(G_{\Gamma,A}) \le \widehat{h}(G_{\Gamma,A}) = \frac{n}{2}\frac{\lambda_2}{|A|+\lambda_2}$.

One recovers the known bound $\beta(\Gamma) \le 1/2$ using Theorem A.1. This bound is tight, for instance, when Γ is the symmetric group S_n (in which case, $k = 1$ because the sign representation is a nontrivial representation of dimension 1). Because the set $S_n \setminus A_n$ consisting of all permutations with an odd sign is product-free with size $n!/2$, one gets $\beta(S_n) \ge 1/2$, and thus, the bound is tight: $\beta(S_n) = 1/2$. In contrast, it has been a long-standing open problem to determine the product-free density of the alternating group A_n; it was shown recently in Keevash et al. [28] that $\beta(A_n) = \Theta(1/\sqrt{n})$.

Example A.1 (Gowers [18]). Consider the group $\Gamma = \mathrm{PSL}_2(q)$, which is the group of all 2×2 matrices over $\mathbb{F}_q$ with determinant one, quotiented by the subgroup $\{I, -I\}$. As Gowers notes, it is one of the simplest infinite families of finite simple groups (i.e., nontrivial groups whose only normal subgroups are the trivial group and the group itself). It is natural to consider *simple* finite groups because any product-free subset in a quotient of a finite group lifts to a product-free subset in the group itself.

The order of $\mathrm{PSL}_2(q)$ is $n = q(q^2-1)/2$. Frobenius proved that every nontrivial representation of $\mathrm{PSL}_2(q)$ has dimension at least $k = (q-1)/2$, which is at least $n^{1/3}/4$. Applying Theorem A.1, one obtains that the maximum size of a product-free subset in Γ is at most $4^{1/3} n^{8/9}$, and thus, $\beta(\mathrm{PSL}_2(q)) = O(1/n^{1/9})$.

Appendix B. Proof of Lemma 8

We use the fact that $\begin{pmatrix} 1 & x^\top \\ x & X \end{pmatrix} \succeq 0 \Longleftrightarrow X - xx^\top \succeq 0$.

The "only if" part in Lemma 8 is easy: if $X - xx^\top \succeq 0$ and $e^\top x = 1$, then $\langle J, X\rangle \ge e^\top x x^\top e = 1$. We now show the "if" part. Therefore, assume $X \in \mathcal{S}^n$ satisfies $X \succeq 0$, Tr(X) = 1 and $\langle J, X \rangle \ge 1$; we construct $x \in \mathbb{R}^n$ such that $e^\top x = 1$ and $X - xx^\top \succeq 0$. For this, consider the spectral decomposition $X = \sum_{i=1}^n \beta_i u_i u_i^\top$, where the u_i's form an orthonormal basis of eigenvectors, $\beta_i \ge 0$, and $\sum_{i=1}^n \beta_i = \mathrm{Tr}(X) = 1$. Define the vectors

$$a := (\sqrt{\beta_i} \cdot e^\top u_i)_{i=1}^n \quad \text{and} \quad x := \sum_{i=1}^n \frac{\beta_i \cdot e^\top u_i}{\|a\|^2} u_i.$$

Then, we have $\|a\|^2 = \sum_{i=1}^n \beta_i (e^\top u_i)^2 = \langle J, X\rangle \ge 1$ and $e^\top x = 1$. We now show $X - xx^\top \succeq 0$. For this, let $z \in \mathbb{R}^n$ be any vector; we show that $z^\top (X - xx^\top) z \ge 0$. Indeed, we have

$$\begin{aligned} z^\top (X - xx^\top) z = z^\top X z - (z^\top x)^2 &= \sum_{i=1}^n \beta_i (z^\top u_i)^2 - \frac{1}{\|a\|^4} \left(\sum_{i=1}^n \beta_i \cdot e^\top u_i \cdot z^\top u_i \right)^2 \\ &= \sum_{i=1}^n \beta_i (z^\top u_i)^2 - \frac{1}{\|a\|^4} \left(\sum_{i=1}^n \sqrt{\beta_i}(e^\top u_i) \cdot \sqrt{\beta_i}(z^\top u_i) \right)^2 \\ &\ge \sum_{i=1}^n \beta_i (z^\top u_i)^2 - \frac{1}{\|a\|^4} \left(\sum_{i=1}^n \beta_i (e^\top u_i)^2 \right) \left(\sum_{i=1}^n \beta_i (z^\top u_i)^2 \right) \\ &= \sum_{i=1}^n \beta_i (z^\top u_i)^2 \left(1 - \frac{1}{\|a\|^2} \right) \ge 0, \end{aligned}$$

using Cauchy-Schwartz inequality for the first inequality and $\|a\| \ge 1$ for the last one. □

Appendix C. Proof of Proposition 5

Here, we show the result of Proposition 5. As starting point, we use the formulation of $g_1(G)$ from (35), where we restrict the optimization to matrices Z of the form $Z = tA_G$ for some scalar $t \in \mathbb{R}$ and to vectors u of the form $u = \mu e$ for some $\mu \in \mathbb{R}$. Note that when G is vertex- and edge-transitive, this restriction can be made without loss of generality. Then, we consider the equivalent reformulation obtained by taking the Schur complement with respect to the upper left corner λ of the matrix in (35). Therefore, we aim to compute the optimum value of the program

$$\widehat{g}(G) := \min_{\lambda, \mu, t \in \mathbb{R}} \left\{ \lambda \mid \lambda(\mu I - C + tA_G) - \frac{\mu^2}{4} J \succeq 0, \lambda \ge 0 \right\}, \tag{C.1}$$

which upper bounds $g_1(G)$ and is equal to it when G is vertex- and edge-transitive; we will show that this optimum value has the form claimed in Proposition 5. For this, we need to express the condition that the eigenvalues of the matrix $\lambda(\mu I - C + tA_G) - \frac{\mu^2}{4} J$ are nonnegative. By considering the eigenvalue of this matrix for the all-ones vector, we get the condition

$$\lambda\left(\mu - \frac{n}{2} + tr\right) - \frac{\mu^2}{2} n \ge 0. \tag{C.2}$$

In addition to this, we need to ensure that $\mu I - C + tA_G \succeq 0$. Note that the matrix $A := tA_G - C$ has the block-form (10), with $M := tM_G - \frac{1}{2} J_n$. We have $MM^\top = t^2 M_G M_G^\top + (n/4 - tr) J_n$. Hence, the eigenvalue of $MM^\top$ at the all-ones vector is equal to

$t^2r^2 + n(n/4 - tr) = (tr - n/2)^2$, and its second-largest eigenvalue is $t^2\lambda_2(M_GM_G^{\mathsf{T}}) = t^2\lambda_2^2$. Therefore, we obtain that

$$\mu I - C + tA_G \succeq 0 \Longleftrightarrow \mu \geq |tr - n/2| \ \text{ and } \ \mu \geq |t\lambda_2| = |t|\lambda_2. \tag{C.3}$$

Again, we assume G is not complete bipartite, and thus, $\lambda > 0$. Then, it follows from (C.2) that $\mu - \frac{n}{2} + tr \geq 0$, and combined with (C.3), we must have $\mu - \frac{n}{2} + tr > 0$. Set

$$\mu(t) := \max\{|tr - n/2|, |t|\lambda_2\}. \tag{C.4}$$

Then, we can conclude that $\widehat{g_1}(G)$ can be reformulated as

$$\widehat{g}(G) = \min_{\mu, t\in\mathbb{R}} \left\{ F(\mu) := \frac{n}{2}\frac{\mu^2}{\mu + tr - n/2} : \mu + tr - n/2 > 0,\, \mu \geq \mu(t) \right\}. \tag{C.5}$$

Our task is now to compute the minimum value of Program (C.5). It is useful to see the behavior of the function $F(\mu)$. For this, observe that its derivative is $F'(\mu) = \frac{n}{2}\frac{\mu^2 - \mu(n-2tr)}{(\mu+tr-n/2)^2}$. Hence, $F'(\mu) \leq 0$ (and thus $F(\mu)$ is monotone nonincreasing) when μ lies between zero and $n - 2tr$, and $F'(\mu) \geq 0$ (and thus, $F(\mu)$ is monotone nondecreasing) when μ lies outside the interval $[0, n-2tr]$ or $[n - 2tr, 0]$ (depending on the sign of $n - 2tr$). Note also that $F(\mu)$ has a vertical asymptote at $\mu = n/2 - tr$ (at which its denominator vanishes).

According to (C.5), we need to discuss according to the value of $\mu(t)$ in (C.4). Therefore, we partition the range of values taken by t into $\mathbb{R} = T_1 \cup T_2 \cup T_3$, where we set

$$T_1 := \{t \in \mathbb{R} : tr - n/2 \geq 0\}, \quad T_2 := \{t \in \mathbb{R} : tr - n/2 < 0,\, t \geq 0\}, \quad T_3 := \{t \in \mathbb{R} : t < 0\}.$$

Then, for $\ell \in \{1,2,3\}$ and for $t \in T_\ell$, set

$$F_\ell(t) := \min_\mu \{F(\mu) : \mu + tr - n/2 > 0,\, \mu \geq \mu(t)\},$$

so that we have

$$\widehat{g}(G) = \min_{\ell\in\{1,2,3\}} \ \min_{t\in T_\ell} \ F_\ell(t). \tag{C.6}$$

We thus need to compute the value of $\min_{t\in T_\ell} F_\ell(t)$ for each $\ell = 1,2,3$. Therefore, we distinguish the three cases $\ell = 1,2,3$.

Case 1: $\ell = 1$. Assume $t \in T_1$. Then, $t > 0$, and $\mu(t) = \max\{tr - n/2, t\lambda_2\}$. Then, we have

$$F_1(t) = \min_\mu \{F(\mu) : \mu \geq \mu(t)\} = F(\mu(t)),$$

where the last equality follows because the function $F(\mu)$ is monotone nondecreasing on $[0, \infty)$. We have two cases.

- Either $tr - n/2 \geq t\lambda_2$, which implies $\mu(t) = tr - n/2$, and thus, $F_1(t) = F(tr - n/2) = \frac{n}{4}(tr - n/2)$. Note that in this case, we have $r > \lambda_2$. Then, we obtain

$$\min_{t\in T_1}\{F_1(t) : tr - n/2 \geq t\lambda_2\} = \min\left\{\frac{n}{4}(tr - n/2) : t \geq \frac{n}{2(r-\lambda_2)}\right\} = \frac{n^2}{8}\frac{\lambda_2}{r - \lambda_2}. \tag{C.7}$$

- Or $tr - n/2 \leq t\lambda_2$ so that $t \leq \frac{n}{2(r-\lambda_2)}$ if $\lambda_2 < r$, and $\mu(t) = t\lambda_2$. Then, we have

$$\min_{t\in T_1}\{F_1(t) : tr - n/2 \leq t\lambda_2\} = \min\left\{F(t\lambda_2) = \frac{n}{2}\frac{t^2\lambda_2^2}{t(\lambda_2 + r) - n/2} : \frac{n}{2r} \leq t \leq \frac{n}{2(r-\lambda_2)}\right\},$$

setting $\frac{n}{2(r-\lambda_2)} = \infty$ if $r = \lambda_2$. Consider the function $\psi(t) := F(t\lambda_2)$, whose derivative is

$$\psi'(t) = \frac{n\lambda_2^2}{2}\frac{t(t(\lambda_2 + r) - n)}{(t(\lambda_2 + r) - n/2)^2}$$

Note that $\frac{n}{2(\lambda_2+r)} \leq \frac{n}{2r} \leq \frac{n}{\lambda_2+r}$, where $\frac{n}{2(\lambda_2+r)}$ is an aymptote of $\psi(t)$ (as it is a zero of its denominator). We also need to compare the relative positions of $\frac{n}{\lambda_2+r}$ (zero of $\psi'(t)$) and $\frac{n}{2(r-\lambda_2)}$ (upper bound of the range for t); note that $\frac{n}{\lambda_2+r} \leq \frac{n}{2(r-\lambda_2)}$ if and only if $r \leq 3\lambda_2$. We can now compute the minimum value taken by the function $\psi(t)$ for $\frac{n}{2r} \leq t \leq \frac{n}{2(r-\lambda_2)}$. When $r \leq 3\lambda_2$, it is attained at $\frac{n}{\lambda_2+r}$ with value $\psi\left(\frac{n}{\lambda_2+r}\right) = \frac{n^2\lambda_2^2}{(\lambda_2+r)^2}$, and when $r \geq 3\lambda_2$ (so that $\lambda_2 < r$), it is attained at $\frac{n}{2(r-\lambda_2)}$ with value $\psi\left(\frac{n}{2(r-\lambda_2)}\right) = \frac{n^2\lambda_2}{8(r-\lambda_2)}$. In summary, we have shown that

$$\min_{t\in T_1}\{F_1(t) : tr - n/2 \leq t\lambda_2\} = \frac{n^2\lambda_2^2}{(\lambda_2 + r)^2} \qquad \text{if } r \leq 3\lambda_2, \tag{C.8}$$

$$= \frac{n^2\lambda_2}{8(r - \lambda_2)} \qquad \text{if } r \geq 3\lambda_2. \tag{C.9}$$

We can now compute $\min_{t\in T_1} F_1(t)$ by comparing (C.7) and (C.8), (C.9). We obtain

$$\min_{t\in T_1} F_1(t) = \min\left\{\frac{n^2}{8}\frac{\lambda_2}{r-\lambda_2}, \frac{n^2\lambda_2^2}{(\lambda_2+r)^2}\right\} = \frac{n^2\lambda_2^2}{(\lambda_2+r)^2} \qquad \text{if } r \le 3\lambda_2, \tag{C.10}$$

$$\min_{t\in T_1} F_1(t) = \frac{n^2}{8}\frac{\lambda_2}{r-\lambda_2} \qquad \text{if } r \ge 3\lambda_2. \tag{C.11}$$

Case 2: $\ell = 2$. Assume $t \in T_2$, then $tr - n/2 \le 0$, and $t \ge 0$. In this case, $\mu(t) = \max\{n/2 - tr, t\lambda_2\}$. We now have $0 \le n/2 - tr \le \mu(t)$. Moreover, one can verify that

$$F_2(t) = \min_{\mu\ge\mu(t)} F(\mu) = F(n-2tr) \qquad \text{if } \mu(t) \le n - 2tr, \tag{C.12}$$

$$= F(\mu(t)) \ge F(n-2tr) \qquad \text{if } \mu(t) \ge n-2tr. \tag{C.13}$$

Hence, the minimum value of $F_2(t)$ for $t \in T_2$ is equal to $F(n-2tr) = n(n-2tr)$, which is obtained when $\mu(t) \le n - 2tr$. We now proceed to compute the minimum value taken by $F(n-2tr)$ for $t \in T_2$ and $\mu(t) \le n-2tr$. For this, we distinguish two cases depending on the value of $\mu(t)$.

- Either $n/2 - tr \ge t\lambda_2$, that is, $t \le \frac{n}{2(r+\lambda_2)}$, and thus, $\mu(t) = n/2 - tr \le n - 2tr$. Then, we have

$$\min_{t\in T_2}\left\{F_2(t) : t \le \frac{n}{2(r+\lambda_2)}\right\} = \min\left\{n(n-2tr) : 0 \le t \le \frac{n}{2(r+\lambda_2)}\right\} = \frac{n^2\lambda_2}{r+\lambda_2}. \tag{C.14}$$

- Or $n/2 - tr \le t\lambda_2$, that is, $t \ge \frac{n}{2(r+\lambda_2)}$, and thus, $\mu(t) = t\lambda_2$. Then, $\mu(t) = t\lambda_2 \le n - 2tr$ is equivalent to $t \le \frac{n}{\lambda_2+2r}$ $(\le \frac{n}{2r})$. Then, we have

$$\min_{t\in T_2}\left\{F_2(t) : \frac{n}{2(r+\lambda_2)} \le t \le \frac{n}{\lambda_2+2r}\right\} = \min\left\{n(n-2tr) : \frac{n}{2(r+\lambda_2)} \le t \le \frac{n}{\lambda_2+2r}\right\} \tag{C.15}$$

$$= \frac{n^2\lambda_2}{\lambda_2+2r}. \tag{C.16}$$

Comparing the values in (C.14) and (C.16), we obtain that

$$\min_{t\in T_2} F_2(t) = \frac{n^2\lambda_2}{\lambda_2+2r}. \tag{C.17}$$

Case 3: $\ell = 3$. Assume $t \in T_3$, that is, $t<0$, and thus, $tr - n/2 < 0$ and $\mu(t) = \max\{n/2 - tr, -t\lambda_2\}$. Then, $F_3(t) = \min_{\mu\ge\mu(t)} F(\mu)$ (because $\mu + tr - n/2 > 0$). If $-t\lambda_2 \le n/2 - tr$, then $\mu(t) = n/2 - tr$, and we find that $F_3(t) = F(n-2tr)$. Or else, if $-t\lambda_2 \le n/2 - tr$, then $\mu(t) = -t\lambda_2 \le n - 2tr$, and we have again $F_3(t) = F(n-2tr)$. Hence, $F_3(t) = F(n-2tr) = n(n-2tr)$ for all $t \in T_3$. Then, we have

$$\min_{t\in T_3} F_3(t) = \min\{n(n-2tr) : t < 0\} = n^2. \tag{C.18}$$

We can now finally compute the value of $\widehat{g}(G)$ as defined in (C.6) based on relations (C.10), (C.11), (C.17), and (C.18). Note that

$$n^2 \ge \frac{n^2\lambda_2}{\lambda_2+2r},$$

$$\frac{n^2\lambda_2^2}{(\lambda_2+r)^2} \le \frac{n^2\lambda_2}{\lambda_2+2r},$$

and

$$\frac{n^2\lambda_2}{\lambda_2+2r} \ge \frac{n^2}{8}\frac{\lambda_2}{r-\lambda_2}$$

if $r \ge 3\lambda_2$. Based on this, we obtain

$$\widehat{g}(G) = \begin{cases} \dfrac{n^2\lambda_2^2}{(\lambda_2+r)^2} & \text{if } r \le 3\lambda_2, \\ \dfrac{n^2\lambda_2}{8(r-\lambda_2)} & \text{if } r \ge 3\lambda_2, \end{cases}$$

which is the desired result. □

Appendix D. Proof of Proposition 11

We give here the proof of Proposition 11. For this, let $P := \lambda I - J + tA_G + v\,\mathrm{Diag}(f) + sff^\mathsf{T}$ denote the matrix appearing in Program (76). We need to find the smallest λ for which there exist $t, v, s \in \mathbb{R}$ such that $P \succeq 0$. Note that $A_G e = re$, $(\mathrm{Diag}\, f)e = f$, $ff^\mathsf{T} e = 0$, $Je = 2ne$, $A_G f = -rf$, $(\mathrm{Diag}\, f)f = e$, $ff^\mathsf{T} f = 2nf$, and $Jf = 0$. Hence, P leaves the subspaces $\langle e, f\rangle$ and $\langle e, f\rangle^\perp$ invariant. Let u be an eigenvector of P for eigenvalue τ, and write $u = x + y$ with $x \in \langle e, f\rangle$ and $y \in \langle e, f\rangle^\perp$. Then, $Px + Py = \tau x + \tau y$, so $Px - \tau x = \tau y - Py$. The left-hand side is contained in $\langle e, f\rangle$, whereas the right-hand side is contained in $\langle e, f\rangle^\perp$, so both sides of the equality are zero. Therefore, τ is an eigenvalue corresponding to x (if $x \neq 0$) and also corresponding to y (if $y \neq 0$). Hence,

$$P \succeq 0 \iff \begin{cases} x^\mathsf{T} P x \geq 0 & \text{for all } x \in \langle e, f\rangle, \\ y^\mathsf{T} P y \geq 0 & \text{for all } y \in \langle e, f\rangle^\perp. \end{cases}$$

We now characterize when $x^\mathsf{T} P x \geq 0$ for all $x \in \langle e, f\rangle$ and when $y^\mathsf{T} P y \geq 0$ for all $y \in \langle e, f\rangle^\perp$.

(i) Let $x \in \langle e, f\rangle$ and write $x = ae + bf$ with $a, b \in \mathbb{R}$. Then,

$$\begin{aligned} Px &= a(\lambda e + tre + vf - 2ne) + b(\lambda f - trf + ve + 2nsf) \\ &= (a(\lambda + tr - 2n) + bv)e + (av + b(\lambda - tr + 2ns))f, \end{aligned}$$

so $x^\mathsf{T} P x = 2na(a(\lambda + tr - 2n) + bv)e + 2nb(av + b(\lambda - tr + 2ns))f$. Hence,

$$\begin{aligned} x^\mathsf{T} P x \geq 0 \quad \forall\, x \in \langle e, f\rangle &\iff a^2(\lambda + tr - 2n) + 2abv + b^2(\lambda - tr + 2ns) \geq 0 \quad \forall a, b \in \mathbb{R} \\ &\iff \begin{cases} v^2 \leq (\lambda + tr - 2n)(\lambda - tr + 2ns), \\ \lambda + tr - 2n \geq 0. \end{cases} \end{aligned} \tag{D.1}$$

Here, the first equivalence follows by rearranging terms in $x^\mathsf{T} P x$ and the second one by considering the expression in a and b as a quadratic equation in a and computing the discriminant.

(ii) Assume that $y = (c\ d)^\mathsf{T} \in \langle e, f\rangle^\perp$ is an eigenvector of P for eigenvalue τ, where $c, d \in \mathbb{R}^n$. Then, $c^\mathsf{T} e = d^\mathsf{T} e = 0$. Using the block-form of P, we obtain

$$Py = \begin{pmatrix} \lambda c + tM_G d + vc \\ \lambda d + tM_G^\mathsf{T} c - vd \end{pmatrix} = \tau \begin{pmatrix} c \\ d \end{pmatrix}.$$

Therefore, $(\tau - \lambda - v)c = tM_G d$ and $(\tau - \lambda + v)d = tM_G^\mathsf{T} c$. It follows that $t^2 M_G^\mathsf{T} M_G d = (\tau - \lambda - v)tM_G^\mathsf{T} c = (\tau - \lambda - v)(\tau - \lambda + v)d = ((\tau - \lambda)^2 - v^2)d$. Similarly, $t^2 M_G M_G^\mathsf{T} c = ((\tau - \lambda)^2 - v^2)c$. As $c \neq 0$ or $d \neq 0$, we have that $\frac{(\tau-\lambda)^2 - v^2}{t^2}$ is an eigenvalue of $M_G^\mathsf{T} M_G$ (if $t \neq 0$), which is distinct from its eigenvalue r^2 for eigenvector e, as $e^\mathsf{T} c = e^\mathsf{T} d = 0$. Therefore,

$$(\tau - \lambda)^2 - v^2 = t^2 \lambda_i(M_G^\mathsf{T} M_G) \quad (i \geq 2),$$

$$\text{and thus} \qquad \tau = \lambda \pm \sqrt{v^2 + t^2 \lambda_i(M_G^\mathsf{T} M_G)} \quad (i \geq 2).$$

We need to ensure $\tau \geq 0$. Hence, we obtain the condition

$$\lambda \geq \sqrt{v^2 + t^2 \lambda_2(M_G^\mathsf{T} M_G)} = \sqrt{v^2 + t^2 \lambda_2^2}.$$

Note this also holds if $t = 0$.

Summarizing, we obtain that $\widehat{\vartheta_{\mathrm{bal}}}(G)$ is the smallest λ such that there exist $t, s, v \in \mathbb{R}$, satisfying

$$\begin{cases} v^2 \leq (\lambda + tr - 2n)(\lambda - tr + 2ns), \\ \lambda + tr - 2n \geq 0, \\ \lambda \geq \sqrt{v^2 + t^2 \lambda_2^2}. \end{cases}$$

Without loss of generality, we may set $v = 0$ because if (λ, t, s, v) is feasible, then also $(\lambda, t, s, v = 0)$ is feasible. Hence, $\widehat{\vartheta_{\mathrm{bal}}}(G)$ is the minimum λ such that there exist $t, s \in \mathbb{R}$ satisfying

$$\begin{cases} \lambda + tr - 2n \geq 0, \\ \lambda - tr + 2ns \geq 0, \\ \lambda \geq |t|\lambda_2. \end{cases}$$

Now, we may eliminate the second equation, as we can choose s such that $\lambda - tr + 2ns = 0$. Therefore, $\widehat{\vartheta_{\mathrm{bal}}}(G)$ is the minimum λ such that there exists $t \in \mathbb{R}$ satisfying

$$\begin{cases} \lambda + tr - 2n \geq 0, \\ \lambda \geq |t|\lambda_2. \end{cases}$$

This implies $\lambda \geq 2n - tr$ and $\lambda \geq t\lambda_2$. Hence, λ is above the point of intersection, where $2n - tr = t\lambda_2$, that is, $t = \frac{2n}{\lambda_2 + r}$, which implies $\lambda \geq t\lambda_2 = \frac{2n\lambda_2}{\lambda_2 + r}$. Setting $t = \frac{2n}{\lambda_2 + r}$ and $\lambda = \lambda_2 t$ is feasible, so the optimum λ is $\frac{2n\lambda_2}{\lambda_2 + r}$, which completes the proof of Proposition 11. □

Let us point out that it follows from this proof that one may set $v = 0$ in Program (76) defining $\vartheta_{\text{bal}}(G)$; this observation was mentioned just after Proposition 11.

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