Optimization of eigenvalue bounds for the independence and chromatic number of graph powers

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Abstract

The k^{th} power of a graph $G = (V, E)$, G^k, is the graph whose vertex set is V and in which two distinct vertices are adjacent if and only if their distance in G is at most k. This article proves various eigenvalue bounds for the independence number and chromatic number of G^k which purely depend on the spectrum of G, together with a method to optimize them. Our bounds for the k-independence number also work for its quantum counterpart, which is not known to be a computable parameter in general, thus justifying the use of integer programming to optimize them. Some of the bounds previously known in the literature follow as a corollary of our main results. Infinite families of graphs where the bounds are sharp are presented as well.

1 Introduction

For a positive integer k, the k^{th} *power of a graph* $G = (V, E)$, denoted by G^k, is a graph with vertex set V in which two distinct elements of V are joined by an edge if there is a path in G of length at most k between them. For a nonnegative integer k, a *k-independent set* in a graph G is a vertex set such that the distance between any two distinct vertices on it is bigger than k. Note that the 0-independent set is $V(G)$ and an 1-independent set is an independent set. The *k-independence number* of a graph G, denoted by $\alpha_k(G)$, is the maximum size of a k-independent set in G. Note that $\alpha_k(G) = \alpha(G^k)$.

The k-independence number is an interesting graph-theoretic parameter that is closely related to coding theory, where codes relate to k-independent sets in Hamming graphs [45, Chapter 17]. The k-independence number of a graph is also directly related to the *k-distance chromatic number*, denoted by $\chi_k(G)$, which is just the chromatic number of G^k. Hence, $\chi_k(G) = \chi(G^k)$. It is well known that $\alpha_1(G) = \alpha(G) \geq n/\chi(G)$. Therefore, lower bounds on the k-distance chromatic number can be obtained by finding upper bounds on the corresponding k-independence number, and vice versa. The parameter α_k has also been studied in several other contexts (see [6, 13, 22, 23, 16, 48] for some examples) and it is related to other combinatorial parameters, such as the average distance [24], the packing chromatic number [26], the injective chromatic number [29], the strong chromatic index [47] and the d-diameter [9]. Recently, the k-independence number has also been related to the beans function of a connected graph [15].

The study of the k-independence number has attracted quite some attention. Firby and Haviland [24] proved an upper bound for $\alpha_k(G)$ in an n-vertex connected graph. In 2000, Kong and Zhao [38] showed that for every $k \geq 2$, determining $\alpha_k(G)$ is NP-complete for general graphs. They also showed that this problem remains NP-complete for regular bipartite graphs when $k \in \{2, 3, 4\}$ [39]. For each fixed integer $k \geq 2$ and $r \geq 3$, Beis, Duckworth and Zito [7] proved some upper bounds for $\alpha_k(G)$ in random r-regular graphs. O, Shi, and Taoqiu [49] showed sharp upper bounds for the k-independence number in an n-vertex r-regular graph for each positive integer $k \geq 2$ and $r \geq 3$. The case of $k = 2$ has also received some attention: Duckworth and Zito [13] showed a heuristic for finding a large 2-independent set of regular graphs, and Jou, Lin and Lin [35] presented a sharp upper bound for the 2-independence number of a tree.

Most of the existing algebraic work on bounding α_k is based on the following two classic results. Let G be a graph with n vertices and adjacency matrix eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. The first well-known spectral bound (or *'inertia bound'*) for the independence number $\alpha = \alpha_1$ of G is due to Cvetković [10]:

$$\alpha \leq \min\{|\{i : \lambda_i \geq 0\}|, |\{i : \lambda_i \leq 0\}|\}. \tag{1}$$

When G is regular, another well-known bound (*'ratio bound'*) is due to Hoffman (unpublished):

$$\alpha \leq \frac{n}{1 - \frac{\lambda_1}{\lambda_n}}. \tag{2}$$

Abiad, Cioabă, and Tait [1] obtained the first two spectral upper bounds for the k-independence number of a graph: an inertial-type bound and a ratio-type bound. They constructed graphs that attain equality for their first bound and showed that their second bound compares favorably to previous bounds on the k-independence number. Abiad, Coutinho, and Fiol [3] extended the spectral bounds from [1]. Wocjan, Elphick, and Abiad [52] showed that the inertial bound by Cvetković is also an upper bound for the quantum k-independence number. Recently, Fiol [20] introduced the minor polynomials in order to optimize, for k-partially walk-regular graphs, a ratio-type bound.

In this article we present several sharp inertial-type and ratio-type bounds for α_k and χ_k which depend purely on the eigenvalues of G, and we propose a method to optimize such bounds using Mixed Integer Programming (MILP). The fact that the inertial-type of bound that we consider is also valid to upper bound the quantum k-independence number [Theorem 7, [52]] justify the method we propose in this paper to optimize our bounds. It is not known whether quantum counterparts of α or χ are computable functions [46], and our bounds sandwich these parameters with the classical versions.

If one wants to use the classical spectral upper bounds on the independence number (1) and (2) to bound $\alpha(G^k) = \alpha_k(G)$, one needs to know how the spectrum of G^k relates to the spectrum of G. In the case when the spectrum of G and G^k are related, we show that previous work by Fiol [18] can be used to derive a sharp spectral bound for regular graphs which concerns the following problem posed by Alon and Mohar [5]: among all graphs G of maximum degree at most d and girth at least g, what is the largest possible value of $\chi(G^k)$?

In general, though, the spectra of G^k and G are not related. We also prove various eigenvalue bounds for α_k and χ_k which only depend on the spectrum of G. In particular, our bounds are functions of the eigenvalues of A and of certain counts of closed walks in G (which can be written as linear combinations of the eigenvalues and eigenvectors of A). Under some extra assumptions (for instance, that of partial walk-regularity), we improve the known spectral inertial-type bounds for the k-independence number. Our approach is based on a MILP implementation which finds the best polynomials that minimize the bounds. For some cases and some infinite families of graphs, we show that our bounds are sharp, and also in other cases that they coincide, in general, with the Lovász theta number.

2 A particular case: the spectrum of G^k and G are related

Our main motivation for this section comes from distance colorings, which have received a lot of attention in the literature. In particular, special efforts have been put on the following question of Alon and Mohar [5]:

Question 2.1. *What is the largest possible value of the chromatic number $\chi(G^k)$ of G^k, among all graphs G with maximum degree at most d and girth (the length of a shortest cycle contained in G) at least g?*

The main challenge in Question 2.1 is to provide examples with large distance chromatic number (under the condition of girth and maximum degree). For $k = 1$, this question was essentially a long-standing problem of Vizing, one that stimulated much of the work on the chromatic number of bounded degree triangle-free graphs, and was eventually settled asymptotically by Johansson [34] by using the probabilistic method. The case $k = 2$ was considered and settled asymptotically by Alon and Mohar [5].

The aim of this section is to show the first eigenvalue bounds on χ_k which concern Question 2.1 for regular graphs and when the spectrum of G^k is related to the one of G. The spectra of G and G^k are related when the adjacency matrix of G^k belongs to the algebra generated by the adjacency matrix of G, that is, there is a polynomial p such that $p(A(G)) = A(G^k)$. For instance, this happens when G is k-partially distance polynomial [11]. In this framework, and when $\deg p = k$ (or, in particular, when G is k-partially distance-regular [11]) we can use Proposition 2.2 from [18] to derive spectral bounds. Before stating the results, we need to introduce some concepts and notations.

Let $G = (V, E)$ be a graph with $n = |V|$ vertices, $m = |E|$ edges, and adjacency matrix A with spectrum $\operatorname{sp} G = \operatorname{sp} A = \{\theta_0^{m_0}, \theta_1^{m_1}, \dots, \theta_d^{m_d}\}$, where the different eigenvalues are in decreasing order, $\theta_0 > \theta_1 > \cdots > \theta_d$, and the superscripts stand for their multiplicities (since G is supposed to be connected, $m_0 = 1$). When the eigenvalues are presented with possible repetitions, we shall indicate them by $\operatorname{ev} G : \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. Let us consider the scalar product in $\mathbb{R}_d[x]$:

$$\langle f, g\rangle_G = \frac{1}{n}\operatorname{tr}(f(A)g(A)) = \frac{1}{n}\sum_{i=0}^{d} m_i f(\theta_i)g(\theta_i). \tag{3}$$

The so-called *predistance polynomials* $p_0(=1), p_1, \dots, p_d$, which were introduced by Fiol and Garriga in [21], are a sequence of orthogonal polynomials with respect to the above product, with $\operatorname{dgr} p_i = i$, and they are normalized in such a way that $\|p_i\|_G^2 = p_i(\theta_0)$ for $i = 0, \dots, d$. Therefore, they are uniquely determined, for instance, following the Gram-Schmidt process. These polynomials were used to prove the so-called 'spectral excess theorem' for distance-regular graphs, where $p_0(=1), p_1, \dots, p_d$ coincide with the so-called distance polynomials.

Proposition 2.2. *[18] Let $G = (V, E)$ be a regular graph with n vertices, spectrum $\operatorname{sp} G = \{\theta_0^{m_0}, \theta_1^{m_1}, \dots, \theta_d^{m_d}\}$, and predistance polynomials $p_0, \dots, p_d$. For a given integer $k \leq d$ and a vertex $u \in V$, let $s_k(u)$ be the number of vertices at distance at most k from u, and consider the sum polynomial $q_k = p_0 + \cdots + p_k$. Then, $q_k(\theta_0)$ is bounded above by the harmonic mean H_k of the numbers $s_k(u)$, that is*

$$q_k(\theta_0) \leq H_k = \frac{n}{\sum_{u\in V}\frac{1}{s_k(u)}},$$

and equality occurs if and only if $q_k(A) = I + A(G^k)$.

Since it is known that $q_k(\theta_0) \geq q_k(\theta_i)$ for $i = 1, \dots, d$, Proposition 2.2 and the bounds (1)–(2) yield the following bounds on α_k and χ_k:

Corollary 2.3. *Let G be a regular graph with eigenvalues $\lambda_1 \geq \cdots \geq \lambda_n$, satisfying $q_k(\lambda_1) = H_k$. Let $q_k' = q_k - 1$, so that $A(G^k) = q_k'(A)$. Then,*

$$\chi_k \geq \frac{n}{\min\{|\{i : q_k'(\lambda_i) \geq 0\}|, |\{i : q_k'(\lambda_i) \leq 0\}|\}}, \tag{4}$$

$$\chi_k \geq \frac{n}{1-\frac{q_k'(\lambda_1)}{\min\{q_k'(\lambda_i)\}}}, \tag{5}$$

and the corresponding upper bounds

$$\alpha_k \leq \min\{|\{i : q_k'(\lambda_i) \geq 0\}|, |\{i : q_k'(\lambda_i) \leq 0\}|\}, \tag{6}$$

$$\alpha_k \leq 1 - \frac{q_k'(\lambda_1)}{\min\{q_k'(\lambda_i)\}}. \tag{7}$$

Corollary 2.3 provides the first two spectral bounds to Question 2.1 for regular graphs. This is due to the fact that another case where $A(G^k) = q_k(A) - I$ (that is, the spectrum of G^k and G are related) is when G is δ-regular graph with girth g and $k = \lfloor \frac{g-1}{2} \rfloor$. In this situation, we know that G is k-partially distance-regular with $a_i = 0$ for $i \leq k$ [2] and hence $q_0 = 1$, $q_1 = 1 + x$, and $q_{i+1} = xq_i - (\delta - 1)q_{i-1}$ for $i = 1, \ldots, k-1$.

Regarding Question 2.1, Kang and Pirot [36] provide several upper and lower bounds for $k \geq 3$, all of which are sharp up to a constant factor as $d \to \infty$. While their upper bounds rely in part on the probabilistic method, their lower bounds are various direct constructions whose building blocks are incidence structures. Actually, some tight examples for our bound (5) can be constructed from the latter. In particular, from even cycles using the balanced bipartite product '$\bowtie$' introduced in [36, 37]. Let $G_1 = (V_1 = A_1 \cup B_1, E_1)$ and $G_2 = (V_2 = A_2 \cup B_2, E_2)$ be bipartite graphs with $|A_1| = |B_1|$ and $|A_2| = |B_2|$, also known as balanced bipartite graphs. Assume vertex sets $A_i = \{a^i_1, \ldots a^i_{n_i}\}$ and $B_i = \{b^i_1, \ldots b^i_{n_i}\}$ be ordered such that $(a^i_j, b^i_j) \in E_i$ for $j = 1, 2, \ldots, n_i$. Then the product $G_1 \bowtie G_2$ is defined as $(V_{G_1 \bowtie G_2}, E_{G_1 \bowtie G_2})$ with

$$\begin{aligned} V_{G_1 \bowtie G_2} &:= A_1 \times A_2 \cup B_1 \times B_2 \\ E_{G_1 \bowtie G_2} &:= \{((a^1_i, a^2), (b^1_i, b^2)) \mid i \in \{1, \ldots, n_1\}, (a^2, b^2) \in E_2\} \cup \\ &\quad\ \{((a^1, a^2_i), (b^1, b^2_i)) \mid i \in \{1, \ldots, n_2\}, (a^1, b^1) \in E_1\}, \end{aligned}$$

which is again a balanced bipartite graph. Moreover, if G_1 and G_2 are regular with degree d_1 and d_2, then $G_1 \bowtie G_2$ is regular with degree $d_1 + d_2 - 1$. The graphs $C_8 \bowtie C_8$, $C_8 \bowtie C_{12}$, $C_8 \bowtie C_{16}$ and $C_{12} \bowtie C_{12}$, where C_n denotes the cycle on n vertices, each have girth 6 and satisfy Equation (7) with equality for α_2. The bound (7) is also tight for several named Sage graphs, which are shown in Table 1.

Name	Girth	k	α_k
Moebius-Kantor Graph	6	2	4
Nauru Graph	6	2	6
Blanusa First Snark Graph	5	2	4
Blanusa Second Snark Graph	5	2	4
Brinkmann graph	5	2	3
Heawood graph	6	2	2
Sylvester Graph	5	2	6
Coxeter Graph	7	3	4
Dyck graph	6	2	8
F26A Graph	6	2	6
Flower Snark	5	2	5

Table 1: Named Sage graphs for which bound (7) from Corollary 2.3 is tight.

3 The general case: the spectrum of G^k and G are not related

In the general situation when the spectrum of G^k and G are not related, one can make use of the following recent spectral bounds for α_k given in [3]. Let G be a graph with eigenvalues $\lambda_1 \geq \cdots \geq \lambda_n$. Let $[2,n] = \{2,3,\ldots,n\}$. Given a polynomial $p \in \mathbb{R}_k[x]$, consider the following parameters:

- $W(p) = \max_{u\in V}\{(p(A))_{uu}\}$,
- $w(p) = \min_{u\in V}\{(p(A))_{uu}\}$,
- $\Lambda(p) = \max_{i\in[2,n]}\{p(\lambda_i)\}$,
- $\lambda(p) = \min_{i\in[2,n]}\{p(\lambda_i)\}$.

Theorem 3.1. (Abiad, Coutinho, Fiol [3]) . *Let G be a graph with n vertices and eigenvalues $\lambda_1 \geq \cdots \geq \lambda_n$.*

(*i*) **An inertial-type bound.** *Let $p \in \mathbb{R}_k[x]$ with corresponding parameters $W(p)$ and $\lambda(p)$. Then,*

$$\alpha_k \leq \min\{|i : p(\lambda_i) \geq w(p)|, |i : p(\lambda_i) \leq W(p)|\}. \tag{8}$$

(*ii*) **A ratio-type bound.** *Assume that G is regular. Let $p \in \mathbb{R}_k[x]$ such that $p(\lambda_1) > \lambda(p)$. Then,*

$$\alpha_k \leq n\frac{W(p)-\lambda(p)}{p(\lambda_1)-\lambda(p)}. \tag{9}$$

In Section 4 we shall prove new eigenvalue lower bounds for χ_k which only require the use of the spectrum of G, this also useful when the spectrum of G and G^k are not related.

3.1 Partially walk-regular graphs

A graph G is called *k-partially walk-regular*, for some integer $k \geq 0$, if the number of closed walks of a given length $l \leq k$, rooted at a vertex v, only depends on l. Thus, every (simple) graph is k-partially walk-regular for $k = 0, 1$, every regular graph is 2-partially walk-regular and, more generally, every k-partially distance-regular is $2k$-partially walk-regular. Moreover G is k-partially walk-regular for any k if and only if G is walk-regular, a concept introduced by Godsil and Mckay in [27]. For example, it is well-known that every distance-regular graph is walk-regular (but the converse does not hold). In other words, if G is k-partially walk-regular, for any polynomial $p \in \mathbb{R}_k[x]$ the diagonal of $p(A)$ is constant with entries

$$(p(A))_{uu} = w(p) = W(p) = \frac{1}{n} \operatorname{tr} p(A) = \frac{1}{n} \sum_{i=1}^{n} p(\lambda_i) \quad \forall u \in V.$$

Then, with $p \in \mathbb{R}_k[x]$, (8) and (9) become

$$\alpha_k \leq \min\{|i : p(\lambda_i) \geq \tfrac{1}{n} \textstyle\sum_{i=1}^{n} p(\lambda_i)|, |i : p(\lambda_i) \leq \tfrac{1}{n} \textstyle\sum_{i=1}^{n} p_k(\lambda_i)|\} \tag{10}$$

and

$$\alpha_k \leq \frac{\sum_{i=1}^{n} p(\lambda_i) - n \cdot \lambda(p)}{p(\lambda_1) - \lambda(p)}. \tag{11}$$

In particular, notice that if $\operatorname{tr} p(A) = \sum_{i=1}^{n} p(\lambda_i) = 0$, inequality (11) becomes

$$\alpha_k \leq \frac{n}{1 - \frac{p(\lambda_1)}{\lambda(p)}}. \tag{12}$$

This can be seen a generalization of Hoffman bound (2), since it is obtained when, in (12), we take $k = 1$ and $p_k(x) = x$ (in this case, note that $p(\lambda_1) = \lambda_1$ and $\lambda(p) = p(\lambda_n) = \lambda_n$). In fact, for this case of partially k-walk-regular graphs, Fiol [20] proved that the upper bound in (11) also applies for the Shannon capacity Θ [50] and the Lovász theta number ϑ [44] of G^k.

An alternative, and more direct proof of (12) is the following. Let G have adjacency matrix A, and let $U = \{1, 2, \ldots, \alpha_k\}$ be a maximal k-independent set in G, such that the first vertices of A correspond to U. Put $\boldsymbol{u} = (x\mathbf{1} \,|\, \mathbf{1})^\top$, where x is a variable such that the values of x correspond to the vertices in the maximal k-independent set U. Now consider the function

$$\phi(x) = \frac{\langle \boldsymbol{u}, p(A)\boldsymbol{u} \rangle}{||\boldsymbol{u}||^2} = \frac{2\alpha_k p(\lambda_1)x + (n - 2\alpha_k)p(\lambda_1)}{\alpha_k x^2 + n - \alpha_k},$$

which attains a minimum at $x_{\min} = 1 - \frac{n}{\alpha_k}$. Thus, $\phi(x_{\min})$ gives

$$\lambda(p) \leq \phi(x_{\min}) = \frac{p(\lambda_1)}{1 - \frac{n}{\alpha_k}},$$

whence (12) follows. The same proof idea was used to extend the ratio bound for oriented hypergraphs, but using the normalized Laplacian spectrum [4].

3.1.1 Optimizing the upper bounds for α_k

Notice that the bounds (10) and (11) are invariant under scaling and/or translating the polynomial p. Thus, when we are looking for the best polynomials, we can restrict ourselves to the following cases:

Bound (10)**:** upon changing the sign of an optimal solution p, we can always assume we are trying to find p that minimizes $|\{i : p(\lambda_i) \geq w(p)\}|$. Moreover, a constant can be added to p to make $w(p) = 0$. Thus, we get

$$\alpha_k \leq \min\{|i : p(\lambda_i) \geq 0|\}. \tag{13}$$

The optimization of this bound will be investigated in Section 4.1.

Bound (11)**:** we consider two simple possibilities:

(a) If $p = f \in \mathbb{R}[k]$ is a polynomial satisfying $\lambda(f) = 0$ and $f(\theta_0) = 1$, the best result is obtained with the so-called *minor polynomial* f_k that minimizes $\sum_{i=0}^{d} m_i f_k(\theta_i)$. This case was studied by Fiol in [20]. This polynomial can be found by solving the following linear programming problem (LP): Let f_k be defined by $f_k(\theta_0) = x_0 = 1$ and $f_k(\theta_i) = x_i$, for $i = 1, \ldots, d$, where the vector $(x_1, x_2, \ldots, x_d)$ is a solution of

$$\boxed{\begin{array}{rl} \texttt{minimize} & \sum_{i=0}^{d} m_i x_i \\ \texttt{subject to} & f[\theta_0, \ldots, \theta_m] = 0,\ m = k+1, \ldots, d \\ & x_i \geq 0,\ i = 1, \ldots, d \end{array}} \tag{14}$$

Here, $f[\theta_0, \ldots, \theta_m]$ denote the m-th divided differences of Newton interpolation, recursively defined by $f[\theta_i, \ldots, \theta_j] = \frac{f[\theta_{i+1}, \ldots, \theta_j] - f[\theta_i, \ldots, \theta_{j-1}]}{\theta_j - \theta_i}$, where $j > i$, starting with $f[\theta_i] = p(\theta_i) = x_i$, $0 \leq i \leq d$. Note that by equating these values to zero, we guarantee that $f_k \in \mathbb{R}_k[x]$. For more details about the minor polynomials, see [20]. Then, we get

$$\alpha_k \leq \sum_{i=0}^{d} m_i p_k(\theta_i) = \operatorname{tr} p_k(A), \qquad \text{and} \qquad \chi_k \geq \frac{n}{\sum_{i=0}^{d} m_i p_k(\theta_i)}. \tag{15}$$

(b) If $p = g \in \mathbb{R}_k[x]$ is the polynomial satisfying $\sum_{i=0}^{d} m_i g(\theta_i) = 0$ and $\lambda(g) = -1$, Eq. (12), with $\lambda_1 = \theta_0$, gives

$$\alpha_k \leq \frac{n}{1 + g(\theta_0)}, \qquad \text{and} \qquad \chi_k \geq 1 + g(\theta_0). \tag{16}$$

Hence, the best result is now obtained by maximizing $g(\theta_0)$. If $g(\theta_i) = x_i$ for $i = 0, \ldots, d$, this leads to the following LPP:

$$\boxed{\begin{array}{rl} \texttt{maximize} & x_0 \\ \texttt{subject to} & \sum_{i=0}^{d} m_i x_i = 0 \\ & f[\theta_0, \ldots, \theta_m] = 0,\ m = k+1, \ldots, d \\ & x_i = z_i - 1, z_i \geq 0,\ i = 1, \ldots, d \end{array}} \tag{17}$$

Consequently, both results (a) and (b) are equivalent in the sense that the best polynomial in (a) yields the same results as the best polynomial in (b). In the first case, f_k is the polynomial that minimizes $\sum_{i=0}^{d} m_i f_k(\theta_i)$, subject to $f_k(\theta_i) \geq 0$ for any $i = 1, \ldots, d$, and $f_k(\theta_0) = 1$. In the second case, g is the polynomial that maximizes $g(\lambda_0)$ under the conditions $g(\theta_i) \geq -1$ for any $i = 1, \ldots, d$ and $\sum_{i=0}^{d} m_i g(\theta_i) = 0$. Now, suppose that g satisfies the conditions in (b). Then, then the polynomial $f_k = \frac{g+1}{g(\theta_0)+1}$ satisfies the conditions in (a) and we get

$$\alpha_k \leq \textstyle\sum_{i=0}^{d} m_i f_k(\theta_i) = \frac{1}{g(\theta_0)+1}\left[\sum_{i=0}^{d} m_i g(\theta_i) + n\right] = \frac{n}{1+g(\theta_0)},$$

as expected. Similarly, if f_k satisfies the conditions in (a), then the polynomial $g = \frac{nf_k - \sum_{i=0}^{d} m_i f_k(\theta_i)}{\sum_{i=0}^{d} m_i f_k(\theta_i)}$ satisfies the conditions in (b), and yields the expected bound

$$\alpha_k \leq \tfrac{n}{1+g(\theta_0)} = \tfrac{1}{n}\textstyle\sum_{i=0}^{d} m_i f_k(\theta_i).$$

4 New spectral bounds for χ_k

In this section we prove several eigenvalue lower bounds for χ_k which only require the spectrum of G.

4.1 First inertial-type bound for χ_k

The first inertial-type bound is a consequence of the bound for α_k in (8) (for a general value of k, an infinite class of graphs which attain such a bound is shown in [1]):

$$\chi_k(G) \geq \frac{n}{\min\{|i : p_k(\lambda_i) \geq w(p_k)|, |i : p_k(\lambda_i) \leq W(p_k)|\}}. \tag{18}$$

In the case of k-partially walk-regular graphs, the optimization of such bounds has already been discussed in Section 3.1.

We should note that if one considers $p_2(A) = A^2$ the bound (18) becomes:

$$\chi_2(G) \geq \frac{n}{\min\{|i : \lambda_i^2 \geq \delta|, |i : \lambda_i^2 \leq \Delta|\}}, \tag{19}$$

and this bound is tight for an infinite family of graphs. Indeed, consider the incidence graph G of a projective plane $PG(2, q)$, then G^2 has two cliques of size $q^2 + q + 1$ (corresponding to the points and lines, since any two points are incident to a common line and any two lines are incident to a common point). Therefore, $\chi(G^2) \geq q^2 + q + 1$. This is an example that Alon and Mohar use in [5]. Note that (19) gives the same bound, as the eigenvalues of G are $q + 1, \sqrt{q}, 0, -\sqrt{q}$ and $-q - 1$. In particular, $w_2(G) = W_2(G) = q + 1$ (the degree of the graph), whereas there are only two eigenvalues $q + 1$ and $-q - 1$ whose square is $\geq +1$. So, as per the inertial-type bound from [1], $\alpha(G^2) \leq 2$, and hence $\chi(G^2) \geq \frac{2(q^2+q+1)}{2}$.

4.1.1 Optimization of the first inertial-type bound

Our goal is to introduce a mixed integer linear program (MILP) to compute the best polynomial giving the above bound in (8) (and hence the same for the bound in (18)). Since such a bound is also valid for the quantum k-independence number and this parameter is not computable in general, the use MILPs to find the best polynomial is justified.

Let G have spectrum $\operatorname{sp} G = \{\theta_0^{m_0}, \ldots, \theta_d^{m_d}\}$. Upon changing the sign of an optimal solution p, we can always assume we are trying to find $p \in \mathbb{R}_k[x]$, and minimizing $|\{i : p(\lambda_i) \geq w(p)\}|$ or, in term of multiplicities, $\min \sum_{j:p(\theta_j)\geq w(p)} m_j$. Moreover, assuming that $w(p) = p(A)_{uu}$ for some vertex $u \in V(G)$, a constant can be added to $p(x)$ making $w(p) = 0$.

Let $p(x) = a_k x^k + \cdots + a_0$, $\boldsymbol{b} = (b_0, \ldots, b_d) \in \{0,1\}^{d+1}$, and $\boldsymbol{m} = (m_0, \ldots, m_d)$. The following mixed integer linear program (MILP), with variables $a_0, \ldots, a_k$ and $b_1, \ldots, b_d$, finds the best polynomial for the bound (8):

$$\begin{array}{ll} \texttt{minimize} & \boldsymbol{m}^\top \boldsymbol{b} \\ \texttt{subject to} & \sum_{i=0}^k a_i (A^i)_{vv} \geq 0, \quad v \in V(G) \setminus \{u\} \\ & \sum_{i=0}^k a_i (A^i)_{uu} = 0 \\ & \sum_{i=0}^k a_i \theta_j^{\,i} - M b_j + \epsilon \leq 0, \quad j = 0, ..., d \quad (*) \\ & \boldsymbol{b} \in \{0,1\}^{d+1} \end{array} \tag{20}$$

Here M is set to be a large number, and ϵ small. The idea of this formulation is that each $b_j = 1$ represents an index j so that $p(\theta_j) \geq w(p) = 0$. In fact, condition $(*)$ gives that $p(\theta_j) \geq 0$ implies $b_j = 1$. So, upon minimizing the quantity of such indices j, we are optimizing $p(x)$ and the corresponding bound $\alpha_k \leq \boldsymbol{m}^\top \boldsymbol{b}$. For each $u \in V(G)$, we write one such MILP and find the best objective value of all. With respect to the choices for ϵ and M, note that we can always set $\epsilon = 1$ as scaling of the a_i's is allowed. If the M chosen is not large enough, the MILP will be unfeasible and we can repeat with a larger M.

In Table 2, the results of the MILP optimal bound (20) are shown for all named graphs in Sage with less than 100 vertices and diameter at least 3. We compare these to the Lovász theta number of G^k and the exact value of α_2. For regular graphs, the bound from Corollary 3.3 in [3] is also included. Observe that the bound in [3] generally outperforms our MILP for the graphs in Table 2. However, it should be noted that this bound requires regularity, whereas the MILP bound (20) is also applicable to irregular graphs. Table 3 shows for $n = 4, \ldots 9$ the proportion of irregular graphs on n vertices for which the optimal solution of our MILP matches the actual value of α_2.

In the case of k-partially walk-regular graphs, we only need to run the MILP (20) once, since all vertices have the same number of closed walks of length smaller of equal than k. Then, the problem can be formulated follows:

Let G be a k-partially walk-regular graph with diameter D and $\operatorname{sp} G = \{\theta_0^{m_0}, \theta_1^{m_1}, \ldots, \theta_d^{m_d}\}$. For a given $k < D$ $(\leq d)$, let $p(x) = a_k x^k + \cdots + a_0$, $\boldsymbol{b} = (b_0, \ldots, b_d) \in \{0,1\}^{d+1}$ and $\boldsymbol{m} = (m_0, \ldots, m_d)$. Now, the following MILP (21), with variables $a_1, \ldots, a_k$ and $b_0, \ldots, b_d$, finds the best polynomial and the corresponding bound for α_k:

Name	Bound in [3]	ϑ_2 [44]	Inertial-type bound MILP (20)	Inertial-type bound MILP (27)	α_2
Balaban 10-cage	17	17	19	19	17
Frucht graph	3	3	3	3	3
Meredith Graph	14	10	10	10	10
Moebius-Kantor Graph	4	4	6	4	4
Bidiakis cube	3	2	4	3	2
Gosset Graph	2	2	8	2	2
Gray graph	14	11	19	19	11
Nauru Graph	6	5	8	8	6
Blanusa First Snark Graph	4	4	4	4	4
Pappus Graph	4	3	7	6	3
Blanusa Second Snark Graph	4	4	4	4	4
Poussin Graph	-	2	4	-	2
Brinkmann graph	4	3	6	6	3
Harborth Graph	12	9	13	13	10
Perkel Graph	10	5	18	18	5
Harries Graph	17	17	18	18	17
Bucky Ball	16	12	16	16	12
Harries-Wong graph	17	17	18	18	17
Robertson Graph	3	3	5	5	3
Heawood graph	3	2	2	3	2
Herschel graph	-	2	3	-	2
Hoffman Graph	3	2	5	4	2
Sousselier Graph	-	3	5	-	3
Sylvester Graph	6	6	10	10	6
Coxeter Graph	7	7	7	7	7
Holt graph	6	3	7	8	3
Szekeres Snark Graph	12	10	13	14	9
Desargues Graph	5	5	6	6	4
Horton Graph	26	24	30	30	24
Kittell Graph	-	3	5	-	3
Tietze Graph	3	3	4	3	3
Double star snark	7	7	9	10	6
Krackhardt Kite Graph	-	2	4	-	2
Durer graph	3	2	3	3	2
Klein 3-regular Graph	13	13	19	19	12
Truncated Tetrahedron	3	3	4	4	3
Dyck graph	8	8	8	8	8
Klein 7-regular Graph	3	3	9	3	3
Ellingham-Horton 54-graph	14	12	20	20	11
Tutte-Coxeter graph	8	6	10	10	6
Ellingham-Horton 78-graph	21	19	27	27	18
Tutte Graph	11	10	13	13	10
Errera graph	-	2	4	-	2
F26A Graph	6	6	7	7	6
Watkins Snark Graph	14	9	13	13	9
Flower Snark	5	5	7	7	5
Markstroem Graph	6	6	7	7	6
Wells graph	6	3	9	10	2
Folkman Graph	4	3	5	5	3
Wiener-Araya Graph	-	8	12	-	8
Foster Graph	22	22	23	23	21
McGee graph	6	5	7	6	5
Franklin graph	3	2	4	3	2
Hexahedron	2	2	2	2	2
Dodecahedron	5	4	4	4	4
Icosahedron	2	2	4	2	2

Table 2: Comparison between different bounds for α_2.

Number of vertices	4	5	6	7	8	9
Proportion	0.86	0.84	0.76	0.62	0.46	0.27

Table 3: Proportion of small graphs for which the optimal value of the MILP coincides with α_2.

$$\begin{array}{ll} \texttt{minimize} & \boldsymbol{m}^{\mathsf{T}}\boldsymbol{b} \\ \texttt{subject to} & \sum_{i=0}^{d} m_i p(\theta_i) = 0 \\ & \sum_{i=0}^{k} a_i \theta_j^{\,i} - M b_j + \epsilon \leq 0, \quad j = 0, ..., d \\ & \boldsymbol{b} \in \{0,1\}^{d+1} \end{array} \tag{21}$$

Observe that the target polynomial p in (21) could be written as a linear combination of the predistance polynomials $p_1, \ldots, p_k$, since all of them are orthogonal to $p_0 = 1$ with respect to the scalar product in (3): $\langle p_j, 1\rangle_G = \frac{1}{n} \operatorname{tr} p_j(A) = w(p_j) = 0$, $j = 1, \ldots, k$, and, hence, so is p. This allows us to remove the first constraint in (20).

Next we illustrate how the MILP (21) can be used to find the best polynomials to upper bound α_k for an infinite family of Odd graphs. For every integer $\ell \geq 2$, the Odd graphs O_ℓ constitute a well-known family of distance-regular graphs with interactions between graph theory and other areas of combinatorics, such as coding theory and design theory. The vertices of O_ℓ correspond to the $\ell - 1$ subsets of a $(2\ell - 1)$-set, and adjacency is defined by void intersection. Note that O_3 is the Petersen graph. In general, O_ℓ is an ℓ-regular graph of order $n = \binom{2\ell-1}{\ell-1} = \frac{1}{2}\binom{2\ell}{\ell}$, diameter $D = \ell - 1$, and its eigenvalues and multiplicities are $\theta_i = (-1)^i(\ell - i)$ and $m(\theta_i) = m_i = \binom{2\ell-1}{i} - \binom{2\ell-1}{i-1}$ for $i = 0, 1, \ldots, \ell - 1$.

For the case $k = D - 1 = \ell - 2$, where α_k is the maximum number of vertices mutually at distance D, we have the following result:

Proposition 4.1. *For the Odd graph O_ℓ, with diameter $D = \ell - 1$, the $(D-1)$-independence number $\alpha_{D-1} = \alpha_{\ell-2}$ satisfies the bound*

$$\alpha_{\ell-2}(O_\ell) \leq \begin{cases} 2\ell - 2 & \text{for odd } \ell, \\ 2\ell - 1 & \text{for even } \ell. \end{cases} \tag{22}$$

Proof. We claim that, for such graphs, the polynomial $p \in \mathbb{R}_{\ell-2}[x]$ obtained from the MILP problem has zeros z_i for $i = 2, \ldots, \ell - 1$, where $z_i = \theta_i + (-1)^{\lceil \frac{i+1}{2} \rceil}\varepsilon$ for odd i, $z_i = \theta_i + (-1)^{\lfloor \frac{i-1}{2} \rfloor}\varepsilon$ for even i, and ε is the solution in $(0, 1)$ of the equation

$$\phi(\varepsilon) = \sum_{i=0}^{\ell} m_i p(\theta_i) = 0. \tag{23}$$

The reason is that this polynomial satisfies the main condition (23) of the MILP problem, and (p or $-p$) minimizes the number of 1's in the vector $\boldsymbol{b}$. More precisely, from the definition of p it is readily checked that

- If ℓ is odd, then $-p(\theta_1) > 0$ and $-p(\theta_i) < 0$ for $i = 0, 2, \dots, \ell$.
- If ℓ is even, then $p(\theta_i) > 0$ for $i = 0, 1$, and $p(\theta_i) < 0$ for $i = 2, \dots, \ell$.

In other words, in the first case $\boldsymbol{b} = (0, 1, 0, \dots, 0)$, and hence, $\alpha_{\ell-2} \le m_1 = 2\ell - 2$; whereas, in the second case, $\boldsymbol{b} = (1, 1, 0, \dots, 0)$, and hence, $\alpha_{\ell-2} \le m_0 + m_1 = 2\ell - 1$, as claimed. □

In Table 4 we show some examples of the results obtained for $\ell = 4, \dots, 8, 10, 12, 14$. For the first values, we also indicate the polynomial $\phi(\varepsilon)$, which is shown to be monic with a convenient scaling (obtained dividing (23) by $\pm\binom{2\ell-1}{\ell-1}$), together with its "key zero" $\varepsilon_0 \in (0, 1)$. Also, we compare the obtained MILP bound with the exact value of α_k.

$\alpha_2(O_4)$	Bound from the MILP Polynomial $\varepsilon^2 + 3\varepsilon - 2$ Exact value α_2	$7 = m_0 + m_1$ 0.561552813 7
$\alpha_3(O_5)$	Bound from the MILP Polynomial $\varepsilon^3 - 12\varepsilon + 4$ Exact value α_3	$8 = m_1$ 0.336508805 7
$\alpha_4(O_6)$	Bound from the MILP Polynomial $\varepsilon^4 + 4\varepsilon^3 - 46\varepsilon + 12$ Exact value α_4	$11 = m_0 + m_1$ 0.238605627 11
$\alpha_5(O_7)$	Bound from the MILP Polynomial $\varepsilon^5 - \varepsilon^4 - 41\varepsilon^3 + 41\varepsilon^2 + 246\varepsilon - 36$ Exact value α_5	$12 = m_1$ 0.1434068868 12
$\alpha_6(O_8)$	Bound from the MILP Polynomial $\varepsilon^6 + 7\varepsilon^5 - 45\varepsilon^4 - 287\varepsilon^3 + 256\varepsilon^2 + 1372\varepsilon - 144$ Exact value α_6	$15 = m_0 + m_1$ 0.1032025452 15
$\alpha_8(O_{10})$	Bound from the MILP Exact value α_b	$19 = m_0 + m_1$ 19
$\alpha_{10}(O_{12})$	Bound from the MILP Exact value α_{10}	$23 = m_0 + m_1$ 23
$\alpha_{12}(O_{14})$	Bound from the MILP Exact value α_{12}	$27 = m_0 + m_1$ 27

Table 4: Infinite family of Odd graphs for which the output from MILP (21) gives the best polynomials for upper bounding α_k.

Note that, when ℓ increases, ε tends to zero and hence the target polynomial p is closer and closer to the minor polynomial f_k up to a constant multiplicative factor. This gives an interesting view of the relationship between the inertial- and ratio-type methods. Moreover, the same result of Proposition 22 can also be proved by using only the minor polynomials, see [20]. Also, notice that, except for the Odd graph O_5, all the obtained bounds are tight. In fact, in the even case $\ell = 2k$, one can check that the vertices at maximum distance $2k-1$ from each other constitute a $2-(4k-1, 2k-1, k-1)$ symmetric design (see [30] for its

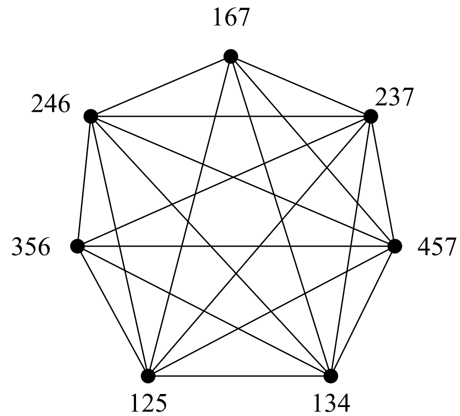

Figure 1: Maximal set of vertices in O_4 ($\alpha_2 = 7$) at mutual distance 3 (each pair of vertices—lines of the Fano plane F_7—has exactly one common digit—vertex of F_7).

definition). Such combinatorial structures exist, at least, for $k = 2, \dots, 7$ [51], which give the optimal values in Table 4 when $\ell = 2, 4, \dots, 14$. In particular, the 7 vertices of O_4 correspond to the lines (or the points) of the Fano plane (see Figure 1), and the 11 vertices of O_6 are the points of the Payley biplane.

Another infinite family of graphs for which (21) behaves nicely is a particular family of Cayley graphs. Let G be a finite group with identity element $\mathbf{1}$ and let $S \subseteq G$. The (directed) Cayley graph $\Gamma(G, S)$ is a graph with vertex set G and an arc for every pair $u, v \in G$ such that $uv^{-1} \in S$. If S is inverse-closed and does not contain $\mathbf{1}$, then $\Gamma(G, S)$ is symmetric and loopless, in which case we may view it as a simple undirected graph. Consider for each $n \geq 3$ the Cayley graph $\Gamma_n := \Gamma(D_{2n}, S_{2n})$ on the dihedral group $D_{2n} = \langle a, b \mid a^n = b^2 = (ab)^2 = \mathbf{1} \rangle$ and inverse-closed subset $S_{2n} = \{a, a^{-1}, b\} \subset D_{2n}$. Then $\{\Gamma_n\}_{n \geq 3}$ is a family of connected, 3-regular graphs on $2n$ vertices. The graph Γ_n is known as the *prism* graph [25] and the above construction as a Cayley graph is due to Biggs [8, pag. 126]. These graphs are vertex-transitive and, hence, walk-regular, but not distance-regular. Thus the Delsarte LP bound does not apply. Table 5 shows the behaviour of the MILP bound on Γ_n for $3 \leq n \leq 16$. Note that the optimal value equals exactly α_2 when $n \neq 2 \mod 4$. This trend continues if we solve the MILP for larger values of n. An easy way to prove that the exact values of α_2 are those expected from the table ($\alpha_2 = 2k$ if $n = 4k + i$ for $i = 0, 1, 2$, and $\alpha_2 = 2k + 1$ if $n = 4k + 3$) is to view Γ_n as the Cayley graph on the Abelian group $\mathbb{Z}_n \times \mathbb{Z}_2$ with generating set $S = \{\pm(1, 0), \pm(0, 1)\}$. Then the graph can be represented by a plane tessellation with rectangles $n \times 2$ [54] (or embedding on the torus) which allows us a neat identification of the maximum 2-independent vertex sets.

n	3	4	5	6	7	8	9	10	11	12	13	14	15	16
MILP bound	1	2	2	4	3	4	4	6	5	6	6	8	7	8
α_2	1	2	2	2	3	4	4	4	5	6	6	6	7	8

Table 5: An infinite family of Cayley graphs Γ_n for which the MILP bound equals α_2 when $n \neq 2 \mod 4$.

4.2 Second inertial-type bound for χ_k

The bound (18) can be strengthened when $k = 1$ and $p_k(A) = A$ as follows (see Elphick and Wokjan [14, Th. 1]). Let $n^+ = |i : \lambda_i > 0|$, $n^0 = |i : \lambda_i = 0|$, and $n^- = |i : \lambda_i < 0|$. Then,

$$\chi(G) \geq 1 + \max\left(\frac{n^+}{n^-}, \frac{n^-}{n^+}\right) \geq \frac{n}{n^0 + \min\{n^+, n^-\}}, \tag{24}$$

with equality for the two bounds only if $n^0 = 0$, since

$$1 + \max\left(\frac{n^+}{n^-}, \frac{n^-}{n^+}\right) = \frac{n^+ + n^-}{\min\{n^+, n^-\}}.$$

The goal of this section is to extend the inertial-type bound (24) to the distance chromatic number $\chi_k(G)$ in the case when G is k-partially walk-regular.

Theorem 4.2. *Let G be a k-partially walk-regular graph with adjacency matrix eigenvalues $\lambda_1 \geq \cdots \geq \lambda_n$. Let $p_k \in \mathbb{R}_k[x]$ such that $\sum_{i=1}^n p_k(\lambda_i) = 0$. Then,*

$$\chi_k \geq 1 + \max\left(\frac{|j : p_k(\lambda_j) < 0|}{|j : p_k(\lambda_j) > 0|}\right). \tag{25}$$

Proof. An analogous argument as it is used in [14, Th. 1] applies here by using $p_k(A)$ instead of A. The proof in [14] relies on the fact that there exist χ unitary matrices U_i such that:

$$\sum_{i=1}^{\chi-1} U_i A U_i^* = -A.$$

Now we consider $p_k(A)$ instead of A and a k-partially walk-regular graph G with $\sum_{i=1}^n p_k(\lambda_i) = 0$ (recall that $p_k(A)$ has constant zero diagonal if and only if $\mathrm{tr} p_k(A) = 0$, or equivalently, $\sum_{i=1}^n p_k(\lambda_i) = 0$)). Then it follows that

$$\sum_{i=1}^{\chi_k-1} U_i p_k(A) U_i^* = -p_k(A). \tag{26}$$

Observe that the above holds because Theorem 6 in [53] is also valid for weighted adjacency matrices with zero diagonal. Let $v_1, \ldots, v_n$ be the eigenvectors of unit length corresponding to the eigenvalues $p_k(\lambda_1) \geq \cdots \geq p_k(\lambda_n)$. Let $p_k(A) = p_k(B) - p_k(C)$, where

$$p_k(B) = \sum_{i=1}^{|j:p_k(\lambda_j)>0|} p_k(\lambda_i) v_i v_i^*, \qquad p_k(C) = \sum_{i=n-|j:p_k(\lambda_j)<0|+1}^{n} -p_k(\lambda_i) v_i v_i^*.$$

Observe that $p_k(B)$ and $p_k(C)$ are positive semidefinite matrices, and we also know that $\mathrm{rank}(p_k(B)) = |j : p_k(\lambda_j) > 0|$ and $\mathrm{rank}(p_k(C)) = |j : p_k(\lambda_j) < 0|$. Denote by P^+ and P^- the orthogonal projectors onto the subspaces spanned by the eigenvectors corresponding to the positive and negative eigenvalues of $p_k(A)$, respectively:

$$P^+ = \sum_{i=1}^{\mathrm{rank}(p_k(B))} v_i v_i^* \qquad \text{and} \qquad P^- = \sum_{i=n-\mathrm{rank}(p_k(C))+1}^{n} v_i v_i^*.$$

Note that

$$p_k(B) = P^+ p_k(A) P^+ \qquad \text{and} \qquad p_k(C) = -P^- p_k(A) P^-.$$

Then, equation (26) can be rewritten as follows

$$\sum_{i=1}^{\chi_k-1} U_i p_k(B) U_i^* - \sum_{i=1}^{\chi_k-1} U_i p_k(C) U_i^* = p_k(C) - p_k(B),$$

and, if we multiply both sides by P^-, we obtain

$$P^- \sum_{i=1}^{\chi_k-1} U_i p_k(B) U_i^* P^- - P^- \sum_{i=1}^{\chi_k-1} U_i p_k(C) U_i^* P^- = p_k(C).$$

Now, since we know that $P^- \sum_{i=1}^{\chi_k-1} U_i p_k(C) U_i^* P^-$ is positive semidefinite, we obtain

$$P^- \sum_{i=1}^{\chi_k-1} U_i p_k(B) U_i^* P^- \succeq p_k(C)$$

(where, with X, Y being matrices, $X \succeq Y$ means that $X - Y$ is positive semidefinite). Finally, using the fact that the rank of a sum is less or equal than the sum of the ranks of the summands, that the rank of a product is less than or equal to the minimum of the ranks of the factors, and Lemma 2 in [14] (if $X, Y \in \mathbb{C}^{n \times n}$ are positive semidefinite and $X \succeq Y$, then $\mathrm{rank}(X) \geq \mathrm{rank}(Y)$), we obtain the desired inequality

$$(\chi_k - 1)\,|j : p(\lambda_j) > 0| \geq |j : p(\lambda_j) < 0|.$$

□

Note that the bound from Theorem 4.2 is equivalent to

$$\chi_k \geq 1 + \max\left(\frac{|j : p_k(\lambda_j) > 0|}{|j : p_k(\lambda_j) < 0|}, \frac{|j : p_k(\lambda_j) < 0|}{|j : p_k(\lambda_j) > 0|}\right).$$

Observe also that the maximum is taken over all polynomials p_k.

Regarding the second inertial-type bound (25), we note that not all graphs allow for an improvement of such bound due to the presence of zeros, and in that case one can better use the inertial-type bound (8) which we optimize for α_k (and hence also for χ_k) in Section 4.1.1.

4.2.1 Optimization of the second inertial-type bound

Similarly to our discussion in Section 4.1.1 for the optimization of the first inertial-type bound, we can use MILPs to optimize the polynomials appearing in the second inertial-type bound (25). For this bound, however, we must solve n MILPs to obtain the best possible bound. The procedure goes as follows: for each $\ell \in \{1, ..., n-1\}$, we solve the following MILP:

$$\begin{array}{ll} \texttt{maximize} & 1 + \frac{n - \mathbf{1}^\intercal \boldsymbol{b}}{\ell} \\ \texttt{subject to} & \sum_{j=1}^{n} \sum_{i=0}^{k} a_i \lambda_j^i = 0 \\ & \sum_{i=0}^{k} a_i \lambda_j^i - M b_j + \epsilon \leq 0, \quad j = 1, ..., n \\ & \sum_{i=0}^{k} a_i \lambda_j^i - M c_j \leq 0, \qquad\quad j = 1, ..., n \\ & \sum_{i=1}^{n} c_i = \ell \\ & \boldsymbol{b} \in \{0,1\}^n, \quad \boldsymbol{c} \in \{0,1\}^n \end{array} \tag{27}$$

Unlike the previous MILP (20), which optimized the first inertial-type bound for χ_k, for the above MILP we require $\boldsymbol{b} \in \{0,1\}^n$, $\boldsymbol{c} \in \{0,1\}^n$ since here we look at all eigenvalues, including the repeated ones. As before, the a_i are the coefficients of the polynomial of degree at most k, say $p(x) = a_k x^k + \cdots + a_0$, and the first restriction is the hypothesis of the theorem, that is $\operatorname{tr} p(A) = 0$. The second restriction implies that if $p(\lambda_j) \geq 0$, then $b_j = 1$, whereas the third restriction implies that if $p(\lambda_j) > 0$, then $c_j = 1$. Thus, we have:

- $|j : p_k(\lambda_j) > 0| = \mathbf{1}^\intercal \boldsymbol{c} = \sum_{i=1}^{n} c_i = \ell$ (fourth restriction),
- $|j : p_k(\lambda_j) = 0| = \mathbf{1}^\intercal (\boldsymbol{b} - \boldsymbol{c})$, and
- $|j : p_k(\lambda_j) < 0| = n - \mathbf{1}^\intercal \boldsymbol{b}$,

from where we set the function to maximize.

In theory, this MILP is a sound way to approximate Theorem 4.2. However, in practice the limited precision of MILP solvers leads to implementation problems for certain graphs. Consider for example the prism graph Γ_4, for which MILP (20) was tight. Solving MILP

(27) with Gurobi for $k = 2$, we find optimal value 7. This is clearly not a valid lower bound, as $\chi_2(\Gamma_4) = 4$. The corresponding optimal parameters are $p_2(x) = 833.3249999999999x^2 - 1666.6499999999999x - 2499.975$ and $b = (1, 0, 0, 0, 0, 0, 0, 1)$, $c = (0, 0, 0, 0, 0, 0, 0, 1)$. In other words, eigenvalue 3 is supposedly a root of p_2 and the other eigenvalues are not. However, due to rounding this is not exactly true: 3 is not a root of p_2, but it is a root of the polynomial $833\frac{1}{3}x^2 - 1666\frac{2}{3}x - 2500$ (or its monic equivalent $x^2 - 2x + 3$), which has eigenvalue -1 as a second root. Eigenvalue 1 with multiplicity 3 is then the only eigenvalue such that this polynomial is negative, so the bound becomes $1 + \frac{3}{1} = 4$, which is tight.

In general, it is hard to prevent these types of errors, as no MILP solver has perfect accuracy. For $k = 2$, we will consider a restriction of MILP (27), where this can be detected and prevented. For a regular graph G with eigenvalues $d = \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$, consider the polynomial $p_2(x) = x^2 + bx - d$. This polynomial has two distinct roots $x_1 < 0 < x_2$ such that $x_1x_2 = -d$ and $b = -(x_1 + x_2)$. Moreover, note that for any choice of b, it satisfies the trace condition $\sum_{i=1}^{n} p_2(\lambda_i) = 0$. Therefore, it corresponds to a valid solution of MILP (27). Since the optimal polynomial is fixed up to the coefficient b, we can now calculate which eigenvalues are root pairs of p_2 and fix the bound accordingly.

To find an optimal value of b we do not need to solve an MILP. Instead, the following greedy strategy suffices. Suppose λ is the smallest negative eigenvalue such that $p_2(\lambda) < 0$. To maximize the numerator of Equation (25), it is better to choose x_1 close to λ, as this will increase the value of x_2. For every negative eigenvalue λ, we therefore compute the bound for $x_1 = \lambda - \varepsilon$ with $\varepsilon > 0$ small. By placing x_1 or x_2 close to 0, we also cover the cases where exactly all negative or all positive eigenvalues lie in the negative range of p_2. Finally, we set every eigenvalue as a root of p_2 and compute the corresponding lower bound. Observe that this strategy can easily be adapted for the polynomial $-p_2$, which also satisfies the trace condition. To obtain the best value bound, we consider all above cases for p_2 and $-p_2$ and take the maximum.

In Table 2, we compute the corresponding upper bound on α_2 for the named Sage graphs and compare it to previous results. Note that these values are an upper bound for the actual optimum of MILP (27), as we restricted the optimal polynomial. On this particular set of graphs, the bound generally performs better than MILP (20), most notably on the Gosset graph and Klein 7-regular graph. Like MILP (20), MILP (27) is tight for the incidence graphs of projective planes $PG(2, q)$ with q a prime power and the prism graphs Γ_n with $n \neq 2 \mod 4$. Note that the latter are generalized Petersen graphs with parameters $(n, 1)$. The bound is also tight for (generalised) Petersen graphs with $(n, k) \in \{(5, 2), (8, 3), (10, 2)\}$. The second graph is also known as the Möbius-Kantor graph and is walk-regular, but not distance-regular.

4.3 First ratio-type bound for χ_k

Let G be a graph with eigenvalues $\lambda_1 \geq \cdots \geq \lambda_n$ and let $[2, n] = \{2, 3, \ldots, n\}$. Given a polynomial $p_k \in \mathbb{R}_k[x]$, recall the following parameters: $W(p_k) = \max_{u \in V}\{(p_k(A))_{uu}\}$, $w(p_k) = \min_{u \in V}\{(p_k(A))_{uu}\}$, $\Lambda(p_k) = \max_{i \in [2,n]}\{p_k(\lambda_i)\}$, $\lambda(p_k) = \min_{i \in [2,n]}\{p_k(\lambda_i)\}$.

Then notice that, for a regular graph, the upper bound (9) for α_k of Theorem 3.1(ii)[3]

becomes (28). In the next theorem we show that such inequality also holds for a general graph.

Theorem 4.3. *Let G be a graph with n vertices, adjacency matrix A, and eigenvalues $\lambda_1 \geq \cdots \geq \lambda_n$. Let $p_k \in \mathbb{R}_k[x]$ such that $p_k(\lambda_1) > p_k(\lambda_i)$ for $i = 2, \ldots, n$. Then,*

$$\chi_k \geq \frac{p_k(\lambda_1) - \lambda(p_k)}{W(p_k) - \lambda(p_k)}. \tag{28}$$

Proof. The proof uses an argument which follows the main lines of reasoning as Haemers does for deriving a lower bound for χ of any graph in [28, Th. 4.1 (i)]. However, as the last steps are different, we include the complete proof. Let $\boldsymbol{\nu} = (\nu_1, \ldots, \nu_n)$ be the (positive) Perron (column) λ_1-eigenvector of A. Let $V_1, \ldots, V_{\chi_k}$ be the color classes of G^k. Let $\tilde{S}$ be the $n \times \chi_k$ matrix with entries

$$(\tilde{S})_{uj} = \begin{cases} \nu_u, & \text{if } u \in V_j, \\ 0, & \text{otherwise.} \end{cases}$$

Notice that, with the appropriate length of the vector $\mathbf{1}$, we have

$$\tilde{S}\mathbf{1} = \boldsymbol{\nu} \quad \text{and} \quad \tilde{S}^\top \boldsymbol{\nu} = (\textstyle\sum_{u \in V_1} \nu_u^2, \ldots, \sum_{u \in V_{\chi_k}} \nu_u^2)^\top.$$

Let S be the matrix $\tilde{S}$ with all its normalized column vector. That is, $S = \tilde{S}D^{\frac{1}{2}}$ where $D = \tilde{S}^\top \tilde{S} = \operatorname{diag}(\sum_{u \in V_1} \nu_u^2, \ldots, \sum_{u \in V_{\chi_k}} \nu_u^2)$. Now consider the $\chi_k \times \chi_k$ matrix $B = S^\top p_k(A) S$ which, as it is readily checked by using the above, has eigenvalue $p_k(\lambda_1)$ with eigenvector $D^{\frac{1}{2}}\mathbf{1}$. Moreover, since each principal submatrix of B corresponding to a color class has all its off-diagonal entries equal to zero, we have

$$\begin{aligned}(B)_{ii} &= \sum_{u \in V_i} (S^\top)_{iu} (p_k(A))_{uu} (S)_{ui} = \sum_{u \in V_i} (p_k(A))_{uu} \frac{\nu_u^2}{\sum_{v \in V_i} \nu_v^2} \\ &\leq W(p_k) \frac{1}{\sum_{v \in V_i} \nu_v^2} \sum_{u \in V_i} \nu_u^2 = W(p_k), \qquad i = 1, \ldots, \chi_k.\end{aligned}$$

Besides, by using interlacing, all the eigenvalues of B must be between $\lambda(p_k)$ and $p_k(\lambda_1)$. Hence,

$$\chi_k W(p_k) \geq \sum_{i=1}^{\chi_k} (B)_{ii} = \operatorname{tr}(B) \geq p_k(\lambda_1) + (\chi_k - 1)\lambda(p_k)$$

and the result follows. □

4.4 Second ratio-type bound for χ_k

In this section we extend the algebraic bound for χ by Haemers [28, Th. 4.1(*ii*)] to the distance chromatic number.

Theorem 4.4. *Let G be a k-partially walk-regular graph with adjacency matrix eigenvalues $\lambda_1 \geq \cdots \geq \lambda_n$. Let $p_k \in \mathbb{R}_k[x]$ such that $\sum_{i=1}^n p_k(\lambda_i) = 0$, and let $\Phi_1 \geq \Phi_2 \geq \cdots \geq \Phi_n$ be the eigenvalues of $p_k(A)$. If $\Phi_2 > 0$, then*

$$\chi_k \geq 1 - \frac{\Phi_{n-\chi_k+1}}{\Phi_2}. \tag{29}$$

Proof. An analogous interlacing argument as the one used in as in [28, Th. 4.1 (ii)] applies here, where instead of the adjacency matrix A and the quotient matrix B, now we consider linear combinations of both matrices, $p_k(A)$ and $p_k(B)$. □

5 Concluding remarks

We should note that computing our eigenvalue bounds (using the MILPs) is significantly faster than solving the SDP of the Lovász theta bound, and in many cases our bounds perform fairly good, as shown in Table 2.

The optimization of the first inertial-type bound (8) using the MILP (20) has special interest since our first inertial-type bound (8) provide an upper bound for the quantum k-independence number [Theorem 7, [52]], which is, in general, not known to be a computable parameter.

While for distance-regular graphs one can use the celebrated linear programming bound by Delsarte [12] on G^k in order to bound α_k, our inertial-type bound (8) and its MILP (20) are more general since they can also be applied to vertex-transitive graphs which are not distance-regular, or in general, to walk-regular graphs which are not distance-regular.

For walk-regular graphs, it is expected that our first inertial bound implementation (21) does not outperform the ratio-type bound implemented using the so-called minor polynomials [20]. This is due to the fact that our MILP (21) uses a linear combination of the eigenvalue multiplicities which is more restrictive than the multiplicity linear combination used with the minor polynomials. However, our first inertial-type bound implementation with the MILP (20) is more general than the ratio-type bound implementation from [20], since the latter requires walk-regularity while our first inertial-type bound (8) and its MILP (20) apply to general graphs.

We end with two open problems that we feel are most natural to try next. The same MILP method as we use in Sections 4.1.1 and 4.2.1 could be useful to find the target polynomial in other graphs and/or for other values of k. Some graph candidates would be vertex-transitive graphs which are not distance-regular (since otherwise one can just use Delsarte LP bound). Finally, note that our MILP formulations to optimize the spectral bounds for α_k and χ_k have a polynomial number of input variables, hence it would be interesting to study whether these formulations admit an algorithm in polynomial time [43].

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