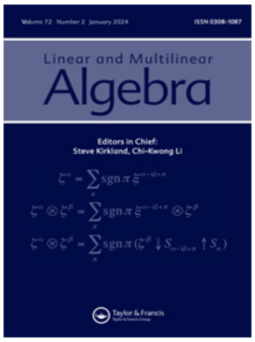

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Comparing eigenvector and degree dispersion with the principal ratio of a graph

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ABSTRACT

The principal ratio of a graph is the ratio of the greatest and least entry of its principal eigenvector. Since the principal ratio compares the extreme values of the principal eigenvector it is sensitive to outliers. This can be problematic for graphs (networks) drawn from empirical data. To account for this we consider the dispersion of the principal eigenvector (and degree vector). More precisely, we consider the coefficient of variation of the aforementioned vectors, that is, the ratio of the vector's standard deviation and mean. We show how both of these statistics are bounded above by the same function of the principal ratio. Further, this bound is sharp for regular graphs. The goal of this paper is to show that the coefficient of variation of the principal eigenvector (and degree vector) can converge or diverge to the principal ratio in the limit. In doing so, we find an example of a graph family (the complete split graph) whose principal ratio converges to the golden ratio. We conclude with conjectures concerning extremal graphs of the aforementioned statistics.

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1. Introduction

There are several measures of graph irregularity which are used to determine how 'close' a given graph is to being regular. One such measure, the *principal ratio*, is the ratio of the greatest and least entry of the principal eigenvector of a graph G. Throughout we assume that graphs are connected, simple, and undirected. We reserve (λ, x) to denote the principal eigenpair of the adjacency matrix of G. The principal ratio, then, is denoted $\gamma(G) = x_{\max}/x_{\min}$. A limitation of this statistic is its sensitivity to the position (and to an extent the degree) of individual vertices in the graph. For example, its applicability to empirical networks where the principal eigenvector is highly dispersed (e.g.scale-free networks [1–3]). This motivates the study of the underlying vector's dispersion.

Studying the distribution of vectors associated with graphs is not new. Notably, the variance of the degree vector was an early irregularity measure [4]. As such, we consider the coefficient of variation of the degree vector in addition to the principal eigenvector. Given a vector $x \in \mathbb{R}^n_+$ let μ denote its mean and σ its standard deviation. The coefficient of variation of x is the ratio σ/μ. For convenience, we will consider the square of the coefficient

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of variation which we denote

$$c_x := \left(\frac{\sigma}{\mu}\right)^2.$$

We reserve d to denote the degree vector of a graph G. We denote the square of the coefficient of variation of the principal eigenvector as c_e and the degree vector as c_d. The coefficient of variation and its square appear frequently across multiple disciplines: economic inequality [5], reliability of measures [6], and the efficiency of experimental designs [7]. Interestingly, the inverse of the coefficient of variation, μ/σ, is the signal-to-noise ratio (SNR). The SNR has found use in information theory [8], optics [9], internet topology [10], medical imaging [11], and nuclear engineering [12]. It is also used informally to measure the ratio of useful to irrelevant information being exchanged in a social network [13].

From the perspective of [13], we can think of the coefficient of variation as the noise-to-signal ratio. In this sense, 'noisy social networks' are resistant to novel information. Such networks are a topic of interest for researchers and practitioners alike. For example, echo chambers are social networks where individuals reject ideas which do not agree with their own (see [14, 15, 16]). Another example is an illicit trade network generated by an online digital black market. These networks feature structural properties which are distinct from their legal counterparts making them more resilient to external monitoring and intervention [17, 18]. This begs the question: which network structures are 'more noisy' than others? We show that the answer to this question depends on the underlying vector. To quantify this phenomenon we propose the normalized difference of c_d and c_e to measure how much more 'degree-noisy' or 'centrality-noisy' a given network is:

$$\Gamma(G) := \frac{c_d(G) - c_e(G)}{\gamma^2(G)} \in (-1, 1).$$

Our goal is to motivate the study of the dispersion of the principal eigenvector (and degree vector) in empirical settings by showing how they relate to the principal ratio and each other. We begin by showing that c_e and c_d are both bounded above by the same function of the principal ratio (namely $\gamma^2 - 1$). We then consider various graph families and compute the limit of the aforementioned statistics of said graphs. In particular, we present graph families for which the limit is 0, non-zero, or diverges to infinity. We summarize our results in Table 1 and note that all six cases for the limit of the principal ratio and the coefficient of variation (for the principal eigenvector or degree vector, respectively) are achieved. We provide conjectures for which graphs are extremal for the principal eigenvector and degree dispersion. We conclude with a conjecture that the star with n rays achieves the maximum of Γ for all n.

2. Background

Throughout we assume that graphs are connected, simple, and undirected. We consider the distribution of a vector so that the indices are often irrelevant. To better facilitate the discussion we will abuse notation and write

$$x = ((x_i, m_i))_{i\geq 1} \quad \text{for } x \in \mathbb{R}^n$$

to mean that x_i occurs multiplicity m_i in x. Let μ and σ denote the mean and standard deviation of x, then the *square of the coefficient of variation* is $c_x = (\sigma/\mu)^2$. With a slight

Table 1. The limit of $\gamma^2 - 1$, c_e, and c_d for various graph families including the complete graph with an edge removed; a particular complete triparite graph, a complete split graph (i.e. $S(n, m) = K_{n+m} - K_m$); the complete graph with a pendant edge, a kite whose head is an r-regular graph; the star; and the Cartesian product of a graph with itself.

G_n	$\lim \gamma^2 - 1$	$\lim c_e$	$\lim c_d$
$K_n - K_2$	0	0	0
$K_{1,n,n}$	3	0	0
$S(n, kn)$	$(\frac{\sqrt{4k+1}+1}{2})^2 - 1$	$\frac{k(\frac{\sqrt{4k+1}-1}{k}-2)^2}{(\sqrt{4k+1}+1)^2}$	$\frac{k^3}{(2k+1)^2}$
P_2K_{n-1}	∞	0	0
$P_nG_n^r$	∞	–	$(\frac{r-2}{r+2})^2$
$K_{1,n}$	∞	1	∞
$G^{\square n}$	∞	∞	0

abuse of notation, we write $c_e(G)$ and $c_d(G)$ to be the square of the coefficient of variation for the principal eigenvector and degree vector of G, respectively. When the context is clear, we will simply write c_e (respectively, c_d).

In some cases, we consider the difference between two graphs. Let $H \subseteq G$ be two graphs on the same vertex set. We write $G - H$ to be the graph formed by removing the edges of H from G. That is $E(G - H) = \{e \in G : e \notin H\}$ and $V(G - H) = V(G)$.

We begin with the following fact about the coefficient of variation of a positive vector.

Lemma 2.1: *Let* $x \in \mathbb{R}^n_+$ *then*

$$c_x = n\frac{\|x\|_2^2}{\|x\|_1^2} - 1. \tag{1}$$

Moreover,

$$c_x \leq \left(\frac{x_{\max}}{x_{\min}}\right)^2 - 1.$$

Proof: Let X to be the random variable which takes on x_i with probability $1/n$. Intuitively, X draws a coordinate-value of x uniformly at random. We have

$$\mathbb{E}[X] = \frac{\|x\|_1}{n} \quad \text{and} \quad \mathbb{E}[X^2] = \frac{\|x\|_2^2}{n}$$

so that

$$\|x\|_1^2 = n^2\mathbb{E}[X]^2 \quad \text{and} \quad \|x\|_2^2 = n\mathbb{E}[X^2].$$

It follows that

$$\frac{\|x\|_2^2}{\|x\|_1^2} = \frac{\mathbb{E}[X^2]}{n\mathbb{E}[X]^2}.$$

Whence $\mathrm{Var}(x) = \mathbb{E}[X^2] - \mathbb{E}[X]^2$ we have

$$\frac{\|x\|_2^2}{\|x\|_1^2} = \frac{\mathrm{Var}(X) + \mathbb{E}[X]^2}{n\mathbb{E}[X]^2}.$$

Indeed

$$n\left(\frac{\|x\|_2^2}{\|x\|_1^2}\right)-1=\frac{\mathrm{Var}(X)+\mathbb{E}[X]^2}{\mathbb{E}[X]^2}-1=\frac{\mathrm{Var}(X)}{\mathbb{E}[X]^2}=c_x.$$

Now assume that $\|x\|_2^2=1$. By an averaging argument, we have that $x_{\max}\geq n^{-1/2}$ so that

$$\|x\|_1^2\geq n^2x_{\min}^2=x_{\max}^2n^2\left(\frac{x_{\min}}{x_{\max}}\right)^2\geq n\left(\frac{x_{\min}}{x_{\max}}\right)^2.$$

The desired inequality follows by substitution into Equation (1). ■

This immediately implies the following.

Lemma 2.2: $c_e(G)\leq\gamma^2(G)-1$.

Consider $c_d(G)$ and note that Lemma 2.1 yields $c_d\leq(\Delta/\delta)^2-1$. Since $c_d(G)$ is a function of the degree vector and $\gamma(G)$ is a function of the principal eigenvector it is natural to think that they are incomparable, *a priori*. Surprisingly $c_d(G)$ is similarly bounded above and the bound is sharp for regular graphs.

Lemma 2.3: $c_d(G)\leq\gamma^2(G)-1$.

Proof: We have

$$\|D\|_1^2=(2|E|)^2\quad\text{and}\quad\|d\|_2^2=\sum_{uv\in E(G)}\deg(u)+\deg(v)\leq 2|E|\Delta$$

so that by Equation (1),

$$c_d\leq n\left(\frac{2|E|\Delta}{4|E|^2}\right)-1=\frac{n\Delta}{2|E|}-1=\frac{\Delta}{\bar{d}}-1\leq\frac{\Delta}{\delta}-1.$$

From [19, 20] we have $\sqrt{\Delta/\delta}\leq\gamma$ yielding $c_d\leq\gamma^2-1$ as desired. ■

The coefficient of variation is invariant under normalization. When considering c_e it can be useful to specify a given normalization. In some cases, we will assume that $\|x\|_2^2=1$ or we will assume $x_{\max}$ (or similarly $x_{\min}$) is 1.

We have further shown the following.

Lemma 2.4: $c_e\leq\frac{n}{\lambda+1}-1$.

Proof: Let (λ,x) be the principal eigenpair of G so that $\|x\|_2^2=1$. Appealing to the Rayleigh quotient definition of the principal eigenvector we have

$$\|x\|_1^2=\sum_{u,v\in V}x_ux_v\geq\left(2\sum_{uv\in E}x_ux_v\right)+\sum_{u\in V}x_u^2+=\lambda+1.$$

The result follows by Equation (1). ■

The following was shown in the proof of Lemma 2.3.

Lemma 2.5: $c_d(G)\leq(\Delta/\bar{d})-1$ *where* $\bar{d}$ *is the average degree.*

3. Dispersion of various graph families

We now prove the statements made in Table 1 by considering the graph families provided therein. The purpose is to show that the principal ratio and the dispersion of the principal eigenvector (resp. degree vector) of a graph family can converge or diverge.

3.1. The complete graph with an edge removed

In this section, we consider $K_n - K_2$, the complete graph with an edge removed.

Theorem 3.1: *Let $G_n = K_n - \{1, 2\}$ with $n > 2$. Then*

$$\lim_{n\to\infty} \gamma(G_n) = 1, \ \lim_{n\to\infty} c_e(G_n) = 0, \quad \text{and} \quad \lim_{n\to\infty} c_d(G_n) = 0.$$

Proof: Let $G_n = K_n - \{1, 2\}$ with $n > 2$ and let (λ, x) be its principal eigenpair.

By symmetry, we have $a := x_i$ for $i > 2$ and $b := x_1, x_2$ so that the eigenequations satisfy

$$\lambda a = (n-3)a + 2b$$
$$\lambda b = (n-2)a.$$

Setting $b = 1$ and solving for a yields

$$a = \frac{(n-3) + \sqrt{n^2 + 2n - 7}}{2(n-2)}.$$

We have that $\lim_n \gamma(K_n - K_2) = \lim_n a = 1$. As $\lambda = (n-2)a$ we appeal to Lemma 2.4 to conclude $\lim_{n\to\infty} c_e = 0$ Finally, whence $\Delta = n - 1$ and $\delta = n - 2$ we have from Lemma 2.5 $\lim_{n\to\infty} c_d = 0$ ■

3.2. The complete tripartite graph

Let $K_{a,b,c}$ be the complete tripartite graph with clouds of size a, b, c.

Theorem 3.2: *We have*

$$\lim \gamma(K_{1,n,n}) = 2, \lim c_e(K_{1,n,n}) = 0, \quad \text{and} \quad \lim c_d(K_{1,n,n}) = 0.$$

Proof: Consider $K_{1,n,n}$ and let (λ, x) be its principal eigenpair. By symmetry we have that $a := x_1$ and $b := x_i$ for $i > 1$ so that

$$x = ((a, 1), (b, 2n)) \quad \text{and} \quad d = ((2n, 1), (n + 1, 2n)).$$

The eigenequations of $K_{1,n,n}$ are

$$\lambda a = 2nb$$
$$\lambda b = 1 + nb.$$

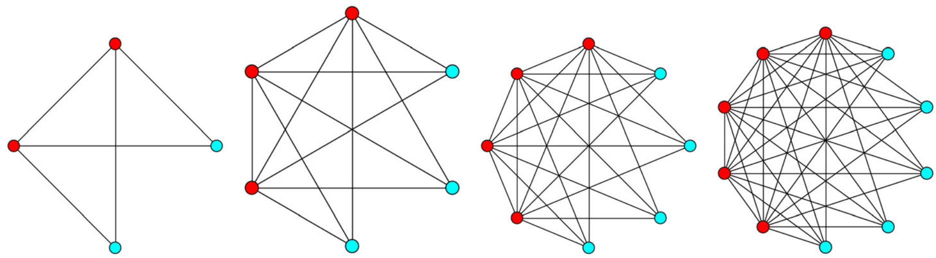

Figure 1. The complete split graph $S(n, n)$ for $2 \le n \le 5$.

Setting $a = 1$ and solving for b yields

$$b = \frac{n + \sqrt{n^2 + 8n}}{4n}$$

We have $\lim_{n\to\infty} \gamma(K_{1,n,n}) = 2$. Moreover, by Equation (1), we have $\lim_{n\to\infty} c_e(K_{1,n,n}) = 0$ and $\lim_{n\to\infty} c_d(K_{1,n,n}) = 0$. ■

3.3. The complete split graph

We define the complete split graph to be a clique on n vertices an independent set with m vertices, $S(n, m) = K_{n+m} - K_m$ [21–23]. A drawing of $S(n, n)$ is given in Figure 1.

Lemma 3.3: *Let (λ, x) be the principal eigenpair of $S(n, m)$ then*

$$x_v = \begin{cases} 1 & : v \le n \\ \frac{1-n+\sqrt{(n-1)^2+4nm}}{2m} & : v > n. \end{cases}$$

Furthermore, under this normalization $x_{\max} = 1$.

Proof: We have by symmetry that $a = x_v$ for $v \le n$ and $b = x_v$ for $v > n$. The eigenequations are of the form

$$\lambda a = (n-1)a + mb$$
$$\lambda b = na.$$

Setting $a = 1$, substituting the first eigenequation into the second, and solving for b gives the desired result. By straight forward computation, we find that $b \le a$ if and only if $m(m-1) \ge 0$. Since $m \ge 1$, the inequality is always satisfied. ■

Theorem 3.4: *Fix $k \ge 1$,*

$$\lim_{n\to\infty} \gamma(S(n, k \cdot n)) = \frac{\sqrt{4k+1}+1}{2}.$$

Proof: From Lemma 3.3 we have that the principal ratio of $S(n, m)$ is

$$\gamma(S(n, kn)) = \frac{1}{b} = \frac{2kn}{1 - n + \sqrt{(n-1)^2 + 4kn^2}}.$$

The conclusion follows naturally. ■

Corollary 3.5: *We have* $\lim_{n\to\infty} \gamma(S(n, n)) = \varphi$ *is the golden ratio.*

Theorem 3.6: *Fix* $k \geq 1$,

$$\lim_{n\to\infty} c_e(S(n, kn)) = \frac{k\left(\frac{\sqrt{4k+1}-1}{k} - 2\right)^2}{(\sqrt{4k+1}+1)^2}.$$

Proof: Let (λ, x) be the principal eigenpair of $S(n, m)$ as in Lemma 3.3. We have

$$c_e = \frac{\sigma^2}{\mu^2} = \frac{(b-1)^2(nm^2 + n^2m)}{(n+m)(n+mb)^2}.$$

Substituting $m = kn$ and appealing to the proof of Theorem 3.4, we have

$$\lim_{n\to\infty} c_e(S(n, kn)) = \lim_{n\to\infty} \frac{(b-1)^2 k}{(kb+1)^2} = \frac{k\left(\frac{\sqrt{4k+1}-1}{k} - 2\right)^2}{(\sqrt{4k+1}+1)^2}.$$ ■

Theorem 3.7: *Fix k then*

$$\lim_{n\to\infty} c_d(S(n, kn)) = \frac{k^3}{(2k+1)^2}.$$

Proof: Let d be the degree vector of $S(n, m)$ so that $d = ((n + m - 1, n), (n, m))$. We equate

$$c_d(S(n, m) = \frac{\sigma^2}{\mu^2} = \frac{(m-1)^2(nm^2 + n^2m)}{(n+m)(n^2 + 2nm - n)^2}.$$

Substituting $m = kn$, we find

$$\lim_{n\to\infty} c_d(S(n, kn) = \lim_{n\to\infty} \frac{kn^2(kn-1)^2}{(n^2(2k+1) - n)^2} = \frac{k^3}{(2k+1)^2}.$$ ■

3.4. The kite graph

The kite graph (aka lollipop graph) $P_m K_s$ is formed by identifying the last vertex of a path on m vertices with a vertex from the complete graph on s vertices. Examples are given in Figure 2. Kite graphs appear frequently in the literature of the principal ratio [24, 25]. We begin with a bound on the spectral radius of the kite graph and an explicit formula for the principal eigenvector of the kite graph as provided in [19].

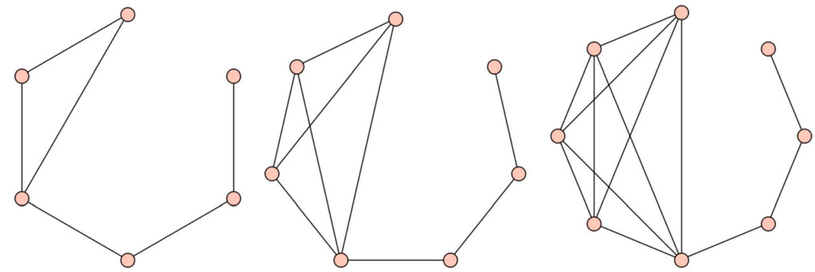

Figure 2. P_4K_3, P_4K_4 and P_4K_5.

Lemma 3.8 ([19]): *For $m \geq 2$ and $s \geq 3$,*

$$s - 1 + \frac{1}{s(s-1)} < \lambda(P_m \cdot K_s) < s - 1 + \frac{1}{(s-1)^2}.$$

We now show how the entries of the principal eigenvector of P_mK_s can be expressed in terms of the spectral radius.

Lemma 3.9 ([19]): *Let λ be the greatest eigenvalue of P_mK_s and let x be its principal eigenvector. Let $\zeta = (\lambda + \sqrt{\lambda - 4})/2$ and $\tau = \zeta^{-1}$ then*

$$x_k = \frac{\zeta^k - \tau^k}{\zeta - \tau} x_1 \quad \text{for } 1 \leq k \leq m,$$

and

$$x_k = \frac{1}{s-1} \frac{\zeta^{m+1} - \tau^{m+1}}{\zeta - \tau} x_1 \quad \text{for } m + 1 \leq k \leq n.$$

For simplicity, we consider the kite whose path is of length 2 (i.e. K_n with a pendant edge).

Theorem 3.10: *Consider P_2K_{n-1}. We have*

$$\lim_{n\to\infty} \gamma(P_2K_{n-1}) = \infty, \lim_{n\to\infty} c_e(P_2K_{n-1}) = 0, \lim_{n\to\infty} c_d(P_2K_{n-1}) = 0.$$

Proof: From Lemma 3.9 we have $\gamma(P_2K_{n-1}) == \zeta + \tau > \zeta$. Appealing to Lemma 3.8, we find $\lambda > n - 2$ so that $\zeta > (n-2)/2$ hence $\lim \gamma(P_2K_{n-1}) = \infty$. Similarly, we have from Lemma 2.4 that $\lim c_e(P_2K_{n-1}) = 0$. Finally, since $\Delta(P_2K_{n-1}) = n - 1$ and $\overline{d} = (n^2 - 3n + 4)/n$, we have $\lim c_d(P_2K_{n-1}) = 0$ by Lemma 2.5. ■

3.5. A kite whose head is a regular graph

Let G_n^r be an r-regular connected graph on n labelled vertices. Consider the graph $P_mG_n^r$ which is formed from identifying the m-vertex of P_m with the 1-vertex in G_n^r. Two examples are given in Figure 3.

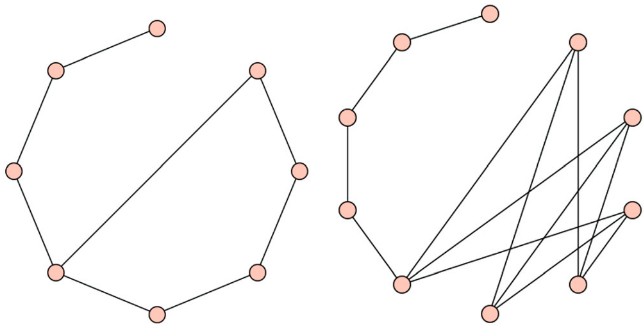

Figure 3. P_4C_5 and $P_5K_{3,3}$.

Theorem 3.11: *We have*

$$\lim_{n\to\infty} c_d(P_nG_n^r) = \left(\frac{r-2}{r+2}\right)^2.$$

Proof: By construction $d = ((1,1),(2,n-2),(r,n-1),(r+1,1))$. We have by Equation (1)

$$\lim_{n\to\infty} c_d(P_nG_n^r) = \lim_{n\to\infty} \frac{(2n-1)(r^2n+4n+2r-6)}{r^2n^2+4rn^2+4n^2-4rn-8n+4} - 1 = \left(\frac{r-2}{r+2}\right)^2. \qquad \blacksquare$$

We make use of the following Theorem.

Theorem 3.12 ([19]): *Let G be a connected graph of order n with spectral radius $\lambda > 2$ and principal eigenvector x. Let d be the shortest distance from a vertex on which x is maximum to a vertex on which it is minimum. Then*

$$\gamma(G) \le \frac{\zeta^{d+1} - \tau^{d+1}}{\zeta - \tau}$$

where $\zeta = \frac{1}{2}(\lambda + \sqrt{\lambda^2 - 4})$ and $\tau = \zeta^{-1}$. Equality is attained if and only if G is regular or there is an induced path of length $d > 0$ whose endpoints index $x_{\min}$ and $x_{\max}$ and the degrees of the endpoints are 1 and 3 or more, respectively, while all other vertices of the path have degree 2 in G.

Theorem 3.13: *Fix $r \ge 4$. Then*

$$\lim_{n\to\infty} \gamma(P_nG_n^r) = \infty.$$

Proof: Let (λ, x) be the principal eigenpair of $P_nG_n^r$. Since G_n^r is an induced subgraph of $P_nG_n^r$ we have that $\lambda \ge r-1$. Clearly $x_{\min} = x_1$ and $x_{\max} = x_n$. As $P_nG_n^r$ satisfies the conditions of Theorem 3.12, we have that

$$\gamma(P_nG_n^r) = \frac{\zeta^{n+1} - \tau^{n+1}}{\zeta - \tau} \ge \zeta^n.$$

Whence $r \ge 4$ we have that $\zeta > 1$ so that

$$\lim_{n\to\infty} \gamma(P_nG_n^r) = \infty. \qquad \blacksquare$$

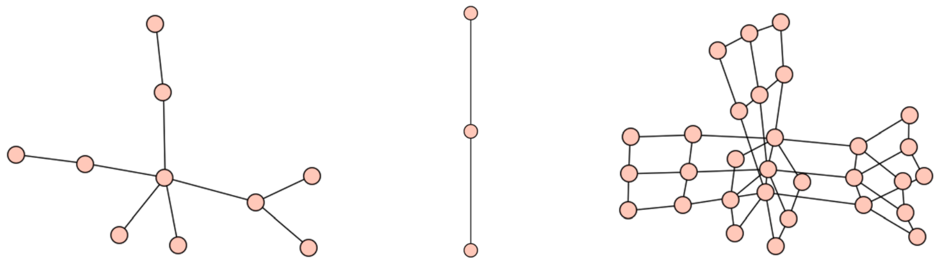

Figure 4. A randomly generated BA(10,1) graph (see [26]), P_3, and their Cartesian product, respectively.

3.6. The star

We now consider the star graph $K_{1,n}$.

Theorem 3.14: *We have*

$$\lim_{n\to\infty} \gamma(K_{1,n})^2 - 1 = \infty, \quad \lim_{n\to\infty} c_e(K_{1,n}) = 1, \quad \text{and} \quad \lim_{n\to\infty} c_d(K_{1,n}) = \infty.$$

Proof: Let $K_{1,n}$ denote the star with n rays. It is well known that

$$x = ((1,1),(n^{-1/2},n)) \quad \text{and} \quad d = ((n,1),(1,n)).$$

Clearly $\lim_{n\to\infty} \gamma(K_{1,n})^2 - 1 = \infty$. The remaining limits follow by Equation (1). ■

3.7. Cartesian powers of a graph

Given two graphs A and B, the Cartesian product $A\square B$ is the graph where

$$V(A\square B) = V(A) \times V(B) = \{(a,b) : a \in V(A), b \in V(B)\}$$

and (a,b) is incident to (a',b') if and only if $(a,a') \in E(A)$ and $b = b'$ or $(b,b') \in E(B)$ and $a = a'$. An example is given in Figure 4. We begin by presenting a folkloric result.

Lemma 3.15: *Let (λ, x) and (ρ, y) be the principal eigenvectors of A and B, respectively. Let $z \in \mathbb{R}^{|A||B|}$ where $z = x \otimes y$ that is $z_{ab} = x_a y_b$. Then $(\lambda+\rho, z)$ is the principal eigenpair of $A\square B$.*

Proof: We have

$$\begin{aligned}(A\square B)z_{ab} &= \left(\sum_{a'\in N_A(a)} z_{a'b} + \sum_{b'\in N_B(b)} z_{ab'}\right) z_{ab} = \sum_{a'\in N_A(a)} z_{a'b}z_{ab} + \sum_{b'\in N_B(b)} z_{ab'}z_{ab}\\ &= y_b\left(\sum_{a'\in N_A(a)} x_{a'}\right) x_a + x_a\left(\sum_{b'\in N_B(b)} y_{b'}\right) y_b = y_bAx_a + x_aBy_b\\ &= y_b(\lambda x_a) + x_a(\rho y_b) = (\lambda+\rho)x_ay_b = (\lambda+\rho)z_{ab}.\end{aligned}$$

■

We show that $c_e(G^{\square k})$ has the following form.

Lemma 3.16: *We have*

$$c_e(A\square B) = c_e(A)c_e(B) + c_e(A) + c_e(B).$$

Proof: Let (λ, x) and (ρ, y) be the principal eigenpair of A and B, respectively. From Lemma 3.15, we have that $z = x \otimes y$ is the principal eigenvector of $A\square B$. Note that

$$\frac{\|z\|_2^2}{\|z\|_1^2} = \frac{\sum (x_a y_b)^2}{(\sum x_a y_b)^2} = \frac{(\sum x_a^2)(\sum y_b^2)}{(\sum x_a)^2(\sum y_b)^2} = \frac{\|x\|_2^2\|y\|_2^2}{\|x\|_1^2\|y\|_1^2}.$$

So that

$$\begin{aligned} c_e(A\square B) &= |V(A)||V(B)|\left(\frac{\|x\|_2^2\|y\|_2^2}{\|x\|_1^2\|y\|_1^2}\right) - 1 \\ &= \left(|V(A)|\frac{\|x\|_2^2}{\|x\|_1^2}\right)\left(|V(B)|\frac{\|y\|_2^2}{\|y\|_1^2}\right) - 1 \\ &= (c_e(A)+1)(c_e(B)+1) - 1 \\ &= c_e(A)c_e(B) + c_e(A) + c_e(B). \end{aligned}$$

■

We turn our attention to $c_d(G^{\square k})$. Consider vectors $x \in \mathbb{R}^n, y \in \mathbb{R}^m$. We write $z = x \oplus y \in \mathbb{R}^{nm}$ such that $z_{ij} = x_i + y_j$. For convenience, we write

$$\bigoplus_{i=1}^{k} x_i = ((\cdots((x_1 \oplus x_2) \oplus x_3) \oplus \cdots) \oplus x_k).$$

Note that the degree vector of $G^{\square k}$ is $\bigoplus_{i=1}^{k} d$ where d is the degree vector of G.

Lemma 3.17: *Let $x \in \mathbb{Z}_+^n$. Then*

$$\left\|\bigoplus_{i=1}^{k} x\right\|_1 = kn^{k-1}\|x\|_1.$$

Proof: The case of $k = 1$ is trivial. Proceeding by induction, we find

$$\begin{aligned} \left\|\bigoplus_{i=1}^{k} x\right\|_1 &= \sum_{i_1}\ldots\sum_{i_k}(x_{i_1} + \cdots + x_{i_k}) \quad \text{where } i_j \in [n] \\ &= \sum_{i_1}\ldots\sum_{i_{k-1}}\left(n(x_{i_1} + \cdots + x_{k-1}) + \|x\|_1\right) \end{aligned}$$

$$= n\left(\sum_{i_1}\dots\sum_{i_{k-1}}(x_{i_1}+\dots+x_{k-1})\right)+n^{k-1}\|x\|_1$$
$$= n((k-1)n^{k-2}\|x\|_1)+n^{k-1}\|x\|_1 = kn^{k-1}\|x\|_1. \quad \blacksquare$$

Lemma 3.18: *Let $x \in \mathbb{Z}_+^n$. Then*

$$\left\|\bigoplus_{i=1}^{k} x\right\|_2^2 = kn^{k-2}(n\|x\|_2^2+(k-1)\|x\|_1^2)$$

Proof: The case of $k = 1, 2, 3$ are clear. We further have that

$$\left\|\bigoplus_{i=1}^{k} x\right\|_2^2 = \sum_{i_1}\dots\sum_{i_k}(x_{i_1}+\dots+x_{i_k})^2 \text{ where } i_j \in [n]$$
$$= \sum_{i_1}\dots\sum_{i_k}\Big((x_{i_1}+\dots+x_{i_{k-1}})^2+x_{i_k}(2(x_{i_1}+\dots+x_{i_{k-1}})+x_{i_k}^2)\Big)$$
$$= \left(\sum_{i_1}\dots\sum_{i_k}(x_{i_1}+\dots+x_{i_{k-1}})^2\right)$$
$$+\left(\sum_{i_1}\dots\sum_{i_k}x_{i_k}(2(x_{i_1}+\dots+x_{i_{k-1}})+x_{i_k}^2)\right)$$
$$= n\cdot\left\|\bigoplus_{i=1}^{k-1} x\right\|_2^2+\left(2\|x\|_1\cdot\left\|\bigoplus_{i=1}^{k-1} x\right\|_1+n^{k-1}\|x\|_2^2\right)$$
$$= n\big((k-1)n^{k-3}(n\|x\|_2^2+(k-2)\|x\|_1^2\big)$$
$$+2\|x\|_1((k-1)n^{k-2}\|x\|_1)+n^{k-1}\|x\|_2^2$$
$$= kn^{k-1}\|x\|_2^2+k(k-1)n^{k-2}\|x\|_1^2$$
$$= kn^{k-2}(n\|x\|_2^2+(k-1)\|x\|_1^2).$$

$\blacksquare$

We now find a simple equation for $c_d(G^{\square k})$.

Lemma 3.19: *For a graph G,*

$$c_d(G^{\square k}) = \frac{c_d(G)}{k}.$$

Proof: For simplicity let $D = \bigoplus_{i=1}^{k} d$. We have that

$$c_d(G^{\square k}) = |D|\frac{\|D\|_2^2}{\|D\|_1^2}-1$$

$$= |d|^k \left(\frac{k|d|^{k-2}(|d| \cdot \|d\|_2^2 + (k-1)\|d\|_1^2)}{(k|d|^{k-1}\|d\|_1)^2} \right) - 1$$

$$= \frac{|d| \cdot \|d\|_2^2 + (k-1)\|d\|_1^2}{k\|d\|_1^2} - 1$$

$$= \frac{|d| \cdot \|d\|_2^2 - \|d\|_1^2}{k\|d\|_1^2} = \frac{1}{k}\left(|d|\frac{\|d\|_2^2}{\|d\|_1^2} - 1\right)$$

$$= \frac{c_d(G)}{k}.$$

■

Theorem 3.20: *Let G be a non-regular graph. Then*

$$\lim_{k\to\infty} \gamma^2(G^{\square k}) - 1 = \infty, \lim_{k\to\infty} c_e(G^{\square k}) = \infty, \quad \text{and} \quad \lim_{k\to\infty} c_d(G^{\square k}) = 0.$$

Proof: Let (λ, x) be the principal eigenpair of G. By Lemma 3.15, $\gamma = x_{\max}/x_{\min}$ and $\gamma(G^{\square k}) = (x_{\max}/x_{\min})^k$. Further since G is non-regular we have that $\gamma(G) > 1$ from which it follows

$$\lim_{k\to\infty} \gamma^2(G^{\square k}) - 1 = \infty.$$

The remaining two limits follow from Lemmas 3.16 and 3.19, respectively. ■

4. Extremal graphs

We conclude with conjectures and questions concerning the extremal graphs of c_e and c_d.

The kite graph (aka lollipop graph) is the extremal graph for the maximum hitting time of a graph as well as the maximum principal ratio for graphs on n vertices [24, 25, 27]. In each case, the head size (i.e. s in P_mK_s) is a function of n. The maximum hitting time occurs when $s \approx (2n+1)/3$ while maximizing the principal ratio requires $s \approx n/\log n$. We conjecture that a kite graph maximizes c_e when the head size is precisely $s = 4$. This conjecture was previously observed in the context of molecular graphs [28].

Conjecture 4.1 ('Four's a Crowd', [28]): The connected graph which achieves the maximum of c_e on $n \geq 6$ vertices is $P_{n-3}K_4$.

The extremal graph for c_d was proved in [29].

Theorem 4.2 ([29]): *The connected graph which achieves the maximum of c_d on n vertices is the star $S_{n-1} = K_{1,n-1}$.*

Consider again the irregularity measure

$$\Gamma(G) := \frac{c_d(G) - c_e(G)}{\gamma^2(G)}.$$

From Lemmas 2.2 and 2.3, we have that $|\Gamma| < 1$ (n.b., strict inequality follows from the fact that the bounds are sharp only for regular graphs). Consider the following.

Theorem 4.3:

$$\lim_{n\to\infty} \Gamma(K_{1,n}) = 1/4 \quad \text{and} \quad \lim_{k\to\infty}\lim_{n\to\infty} \Gamma(S(k,nk)) = 1/4.$$

Proof: Let (λ, x) be the principal eigenpair of $K_{1,n}$. Recall from Lemma 3.14 that $\gamma = \sqrt{n}$. We have then

$$\lim_{n\to\infty} \Gamma(K_{1,n}) = \lim_{n\to\infty} \frac{\left(\frac{n^3}{4n^2} - 1\right) - \left(\frac{2n}{n} - 1\right)}{n} = 1/4.$$

Moreover, we have

$$\lim_{k\to\infty}\lim_{n\to\infty} \Gamma(S(k,nk) = \lim_{k\to\infty} \frac{\frac{k^3}{(2k+1)^2} - \frac{k\left(\frac{\sqrt{4k+1}-1}{k}-2\right)^2}{(\sqrt{4k+1}+1)^2}}{\left(\frac{\sqrt{4k+1}+1}{2}\right)^2} = 1/4. \qquad \blacksquare$$

Based on experimental evidence we make the following conjecture.

Conjecture 4.4: $\Gamma(G) \le 1/4$ and the star is extremal.

We leave the following questions for the interested reader. Are there constants $\varepsilon_1, \varepsilon_2 > 0$ such that $-1 + \varepsilon_1 \le \Gamma \le 1 - \varepsilon_2$? It is not clear that $\varepsilon_1 = \varepsilon_2$ in view of the following question: does there exist a graph family such that $c_e(G_n) \downarrow 0$ but $c_d(G_n) \uparrow \infty$?

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