Extremal Graphs for Weights

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Given a graph $G = (V, E)$ and $\alpha \in \mathbb{R}$, we write $w_\alpha(G) = \sum_{xy \in E} d_G(x)^\alpha d_G(y)^\alpha$, and study the function $w_\alpha(m) = \max\{w_\alpha(G) : e(G) = m\}$. Answering a question from [1], we determine $w_1(m)$ for every m, and we also give bounds for the case $\alpha \neq 1$.

1. Introduction

The aim of this note is to continue the work started by Bollobás and Erdős [1] on the α-weight of a graph with a given number of edges. For $\alpha \in \mathbb{R}$, the *α-weight* $w_\alpha(xy)$ of an edge xy of a graph G is defined as $w_\alpha(xy) = d(x)^\alpha d(y)^\alpha$, where $d(x)$ and $d(y)$ are the degrees of the vertices x and y. The *α-weight* $w_\alpha(G)$ of G is the sum of the α-weights of its edges.

In [1], Bollobás and Erdős studied the extremal α-weights of graphs with a given number of edges, with emphasis on the case $\alpha = -\frac{1}{2}$, when the weights are the so called *Randić weights*, as defined in [3]. They also proved that the Randić weight of a graph G of order n with no isolated vertices is at least $\sqrt{n-1}$, with equality if and only if $G \cong K_{1,n-1}$. Concerning the case $\alpha = 1$, in [1] it was proved that if $m = \binom{k}{2}$ then the maximum 1-weight of a graph of size m is $m(k-1)^2$, with equality iff G is the union of K_k and isolated vertices. In [1] it was also conjectured that if $\binom{k}{2} < m \leq \binom{k+1}{2}$ then the maximum is attained on a graph of order $k+1$ which contains a complete graph of order k. One of our aims is to prove this conjecture. We do this in §2.

Our second main aim is to consider α-weights with $\alpha \neq 1$. What is the maximum α-weight of a graph with m edges, and what is the minimum? Rather trivially, for $\alpha \leq 0$ the maximum is attained on m independent edges, and for $\alpha \geq 0$ the minimum is attained on m independent edges, so for $\alpha < 0$ and $\alpha > 0$ we are interested in graphs of minimum α-weight and maximum α-weight respectively. For positive values of α, considered in §3, it is convenient to distinguish three cases. When $0 \le \alpha \le 1$, as shown in [1], Hölder's inequality together with our result for $\alpha = 1$ shows that among graphs of fixed size $\binom{k}{2}$, K_k has largest α-weight. When $\alpha > 1$, we have to work harder: complete graphs are no longer extremal, since it pays to have some edges of very high weight. Treating m as a large fixed parameter and letting α increase from 1 to $\frac{3}{2}$, the extremal graphs are close to the split graphs $K_t + \bar{K}_{m/t}$, where t rapidly decreases. Our result for $1 < \alpha < 2$, Theorem 6, only gives the correct leading term when α takes one of a discrete set of values. For $\alpha \ge 2$, it is not hard to show that $K_2 + \bar{K}_{m/2}$ is asymptotically best possible. Finally, in §4, we consider the case $\alpha < 0$. Here, repeated use of the Cauchy-Schwarz inequality shows that among graphs of size $\binom{k}{2}$, K_k has smallest α-weight (for $-1 \le \alpha < 0$ this was already noted in [1]).

2. Graphs of Extremal 1-weight

The aim of this section is to prove the following conjecture from [1].

Theorem 1. *Let k and r be positive integers with $0 < r \le k$. Then all graphs G of size $m = \binom{k}{2} + r$ and minimal degree at least one satisfy $w_1(G) \le w_1(G_m)$, where the graph G_m consists of a complete graph of order k together with an additional vertex joined to r vertices of the complete graph, and has 1-weight*

$$w_1(G_m) = \binom{r}{2}k^2 + \binom{k-r}{2}(k-1)^2 + rk(k-r)(k-1) + r^2k.$$

Before we are ready, we require three lemmas and the following generalisation of the notion of α-weight. For $\ell \in \mathbb{N}$ and $\alpha \in \mathbb{R}$, the (ℓ,α)-*weight* of an edge xy of a graph G is

$$w_{(\ell,\alpha)}(xy) = (d_G(x) + \ell)^\alpha (d_G(y) + \ell)^\alpha,$$

and the (ℓ,α)-*weight* $w_{(\ell,\alpha)}(G)$ of a graph G is the sum of the (ℓ,α)-weights of its edges. Note that the $(0,\alpha)$-weight (of an edge or of a graph) is just the α-weight. From now on, we write d_x for $d_G(x)$.

Lemma 2. *Let k, ℓ and r be positive integers with $0 < r \le k$. Let G be a graph of order n, without isolated vertices, having largest $(\ell,1)$-weight among all graphs of size $m = \binom{k}{2} + r$. Then $\Delta(G) = n - 1$.*

Proof. First observe that any two non-adjacent vertices in G have a common neighbour since otherwise by amalgamating the two vertices we could increase $w_{(\ell,1)}(G)$, while keeping $e(G) = m$. Let x be a vertex of maximal degree. Suppose, for a contradiction, that $d_x < n-1$ and let y be a vertex of maximal degree subject to the condition $xy \notin E(G)$. Let z be a common neighbour of x and y. Now let G' be G with the edge $yz \in E(G)$ replaced by the edge xy, and set $G_0 = G - \{x,y,z\}$. Also, write S_x for the sum of the $(\ell,1)$-weights (in G) of edges incident with x, except for edge xz, S_y for the sum of the $(\ell,1)$-weights (in G) of edges incident with y, except for edge yz, and S_z for the sum of the $(\ell,1)$-weights (in G) of edges incident with z, except for edges xz and yz. Then

$$w_{(\ell,1)}(G)=\sum_{e\in E(G_0)} w_{(\ell,1)}(e)+S_x+S_y+S_z+(d_x+\ell)(d_z+\ell)+(d_y+\ell)(d_z+\ell)$$

and

$$\begin{aligned} w_{(\ell,1)}(G') &= \sum_{e\in E(G_0)} w_{(\ell,1)}(e)+S_x\frac{d_x+\ell+1}{d_x+\ell}+S_y+S_z\frac{d_z+\ell-1}{d_z+\ell} \\ &+ (d_x+\ell+1)(d_z+\ell-1)+(d_y+\ell)(d_x+\ell+1). \end{aligned}$$

As $w_{(\ell,1)}(G)$ is maximal for graphs of size m,

$$0\geq w_{(\ell,1)}(G')-w_{(\ell,1)}(G)=\frac{S_x}{d_x+\ell}-\frac{S_z}{d_z+\ell}+(d_x+1-d_z)(d_y+\ell-1). \tag{1}$$

Notice that $d_x+1-d_z>0$ and $d_y+\ell-1\geq d_y-1\geq 0$. Therefore we have

$$\frac{S_z}{d_z+\ell}\geq\frac{S_x}{d_x+\ell}. \tag{2}$$

Next, let $W=\Gamma_G(x)-(\Gamma_G(z)\cup\{z\})$. Note that $W\neq\emptyset$, since $d_x\geq d_z$ and $|W|=|\Gamma_G(z)-(\Gamma_G(x)\cup\{x\})|+d_x-d_z\geq 1$, as $y\in\Gamma_G(z)-(\Gamma_G(x)\cup\{x\})$. Let $w\in W$, and write T_x for the sum of the $(\ell,1)$-weights (in G) of edges incident with x, except for the edges wx and xz, and T_z for the sum of the $(\ell,1)$-weights (in G) of the edges incident with z, except for the edge xz. (We suppress the simple dependence of T_x and T_z on w.) Let G'' be G with the edge $xw\in E(G)$ replaced by the edge wz. Arguing as in (1), we find that

$$0\geq w_{(\ell,1)}(G'')-w_{(\ell,1)}(G)=\frac{T_z}{d_z+\ell}-\frac{T_x}{d_x+\ell}+(d_z+1-d_x)(d_w+\ell-1). \tag{3}$$

But

$$\begin{aligned} T_z &= S_z+(d_y+\ell)(d_z+\ell), \\ T_x &= S_x-(d_x+\ell)(d_w+\ell), \end{aligned}$$

so (3) gives that

$$\begin{aligned} 0 &\geq \frac{S_z}{d_z+\ell}+(d_y+\ell)-\frac{S_x}{d_x+\ell}+(d_w+\ell)+(d_z+1-d_x)(d_w+\ell-1) \\ &\geq (d_x+1-d_z)(d_y+\ell-1)+(d_y+\ell)+(d_w+\ell)+(d_z+1-d_x)(d_w+\ell-1) \\ &= (d_x-d_z)(d_y-d_w)+2(d_y+d_w+2\ell-1) \\ &> (d_x-d_z)(d_y-d_w). \end{aligned}$$

Since $d_x\geq d_z$ we must have $d_x>d_z$ and $d_w>d_y$.

Therefore,

$$\begin{aligned}
\frac{S_x}{d_x+\ell} &= \sum_{v\in\Gamma(x)\cap\Gamma(z)} (d_v+\ell) + \sum_{w\in W}(d_w+\ell) \\
&> \sum_{v\in\Gamma(x)\cap\Gamma(z)} (d_v+\ell) + (d_y+\ell)|\Gamma(x)-(\Gamma(z)\cup\{z\})| \\
&> \sum_{v\in\Gamma(x)\cap\Gamma(z)} (d_v+\ell) + (d_y+\ell)|\Gamma(z)-(\Gamma(x)\cup\{x\})| \\
&\geq \frac{S_z}{d_z+\ell},
\end{aligned}$$

contradicting (2). □

In order to state the next lemma, we need another definition. The graph $G(d_1, d_2, \ldots, d_N)$ has vertex set defined as the disjoint union

$$\bigcup_{0\leq j\leq N} I_j,$$

where $I_0 = \{v_1, v_2, \ldots, v_N\}$, $|I_j| = d_j - d_{j+1}$ for $1 \leq j \leq N-1$ and $|I_N| = d_N - (N-1)$. For $1 \leq j \leq N$ we arrange that

$$\Gamma(v_j) = (I_0 - \{v_j\}) \cup \left(\bigcup_{j\leq k\leq N} I_k \right),$$

and

$$E\left(G\left[\bigcup_{1\leq j\leq N} I_j \right] \right) = \emptyset,$$

so that $d(v_j) = d_j$ for all j and

$$e(G(d_1, d_2, \ldots, d_N)) = \sum_{i=1}^{N} d_i - \binom{N}{2}.$$

We will, of-course, always have $d_1 \geq d_2 \geq \ldots \geq d_N \geq N-1$. Each of these graphs, of order n, say, is the unique realization of a sequence corresponding to a vertex of the polytope K^n of degree sequences in E^n, as defined in [4]. Let F denote the family of graphs of the form $G(d_1, d_2, \ldots, d_N)$ for $d_1 \geq d_2 \geq \ldots \geq d_N \geq N-1$.

Lemma 3. *Let k, ℓ and r be positive integers with $0 < r \leq k$. If G is a graph of minimal degree at least one, having largest $(\ell, 1)$-weight among all graphs of size $m = \binom{k}{2} + r$, then $G \in F$.*

Proof. Suppose G is as in the hypotheses of the lemma and write $|G| = n$. We define a sequence $G = G_0, G_1, G_2, \ldots$ of graphs as follows. From Lemma 2 we know that $\Delta(G) = n-1$. Suppose that $d_G(x_1) = n-1$. The graph $G - \{x_1\}$ consists of a graph

G_1 with no isolated vertices, together with a set J_1 of isolated vertices. If G_1 is the null graph, we are done. Otherwise we calculate

$$\begin{aligned} w_{(\ell,1)}(G) &= (n+\ell-1)\sum_{x_1 y\in E(G)}(d_y+\ell)+\sum_{yz\in E(G_1)}(d_y+\ell)(d_z+\ell) && (4)\\ &= (n+\ell-1)(2m-(n-1)+(n-1)\ell)+w_{(\ell+1,1)}(G_1) && (5)\\ &= (n+\ell-1)(2m+(\ell-1)(n-1))+w_{(\ell+1,1)}(G_1). && (6)\end{aligned}$$

We claim that $\Delta(G_1)=|G_1|-1$. For if not we can use the proof of Lemma 2 to replace G_1 by a graph G_1' on the same vertex set as G_1 satisfying

$$e(G_1')=e(G_1)$$

and

$$w_{(\ell+1,1)}(G_1')>w_{(\ell+1,1)}(G_1),$$

and thereby produce a graph $G'=(V(G),E(G)\cup E(G_1')-E(G_1))$ with

$$e(G')=e(G)$$

and

$$w_{(\ell,1)}(G')>w_{(\ell,1)}(G).$$

Suppose that $d_{G_1}(x_2)=|G_1|-1$. Then the graph $G_1-\{x_2\}$ consists of a graph G_2 with no isolated vertices, together with a set J_2 of isolated vertices. If G_2 is the null graph then $G=G(d_G(x_1),d_G(x_2))$ and we are done. Otherwise we continue and find a sequence of vertices $\{x_3,x_4,\ldots\}$ and graphs $\{G_3,G_4,\ldots\}$. Eventually the process terminates with a vertex $x_N\in V(G_{N-1})$ joined to a set J_N of isolated vertices. We then have $G=G(d_G(x_1),d_G(x_2),\ldots,d_G(x_N))\in F$. □

For example, the only graphs in F of size 6 are $G(6)$, $G(5,2)$, $G(4,3)$ and $G(3,3,3)$ with $(\ell,1)$-weights $36+42\ell+6\ell^2$, $39+36\ell+6\ell^2$, $44+34\ell+6\ell^2$ and $54+36\ell+6\ell^2$ respectively. For $0\le\ell\le 2$, $G(3,3,3)$ has largest $(\ell,1)$-weight, while when $\ell=3$ we have

$$w_{(3,1)}(G(3,3,3))=w_{(3,1)}(G(6))>w_{(3,1)}(G(5,2))>w_{(3,1)}(G(4,3)),$$

and when $l\ge 4$, $G(6)$ has largest weight.

The final ingredient in the proof of our main theorem is a technical inequality concerning decreasing sequences of integers.

Lemma 4. *Let $d_1,d_2,\ldots,d_N$ be positive integers satisfying*

$$\sum_{i=1}^{N}d_i=cN+l,l<N,d_1\ge d_2\ge\ldots\ge d_N\ge N-1. \tag{7}$$

Then

$$\sum_{i=1}^{N}(i-1)d_i^2\le\binom{N}{2}c^2+\binom{l}{2}(2c+1), \tag{8}$$

obtained by setting

$$d_1 = d_2 = \ldots = d_l = c+1, d_{l+1} = d_{l+2} = \ldots = d_N = c, \tag{9}$$

in other words making $(d_1, d_2, \ldots, d_N)$ *a* balanced sequence.

Proof. We use induction on N.

If $N = 2$ we have to maximize d_2^2 subject to $d_1 \geq d_2$ with $d_1 + d_2$ fixed, so we should make d_1 and d_2 as equal as possible. Thus the induction starts.

Consider now a fixed $N \geq 3$ and assume that balanced sequences maximize f for smaller values of N. Take an optimal sequence $(d_1, d_2, \ldots, d_N)$ satisfying (7), and write $d_N = b = a - x$. Then

$$\sum_{i=1}^{N}(i-1)d_i^2 = \sum_{i=1}^{N-1}(i-1)d_i^2 + (N-1)b^2,$$

and so $\sum_{i=1}^{N-1}(i-1)d_i^2$ is maximal subject to the constraints $\sum_{i=1}^{N-1} d_i = cN + l - b$ and $d_1 \geq d_2 \geq \ldots \geq d_{N-1}$. Therefore, by the induction hypothesis, $(d_1, d_2, \ldots, d_{N-1})$ is balanced, so that

$$d_1 = d_2 = \ldots = d_m = a+1, d_{m+1} = \ldots = d_{N-1} = a \tag{10}$$

with

$$Na + m - x = cN + l. \tag{11}$$

For notational simplicity, write

$$f(d_1, d_2, \ldots, d_N) = \sum_{i=1}^{N}(i-1)d_i^2.$$

In this notation, we must show that

$$f(a+1, a+1, \ldots, a+1, a, a, \ldots, a, a-x) \leq f(c+1, c+1, \ldots, c+1, c, c, \ldots, c).$$

Setting

$$\begin{aligned} F(N,a,m,x,c,l) &= \binom{N}{2}c^2 + \binom{l}{2}(2c+1) - \binom{N}{2}a^2 \\ &- \binom{m}{2}(2a+1) + (N-1)(2a-x)x, \end{aligned}$$

we need that

$$F(N,a,m,x,c,l) \geq 0, \tag{12}$$

provided the following four conditions hold:

$$c = a - \frac{x+l-m}{N}, \tag{13}$$

$$0 \leq m \leq N-2, \tag{14}$$

$$1 \leq l \leq N-1, \tag{15}$$

$$1 \leq x \leq a - N + 1. \tag{16}$$

Here, (16) comes from the condition $b \geq N-1$, and we can suppose that $l > 0$ since

$$f(c+1, c, c, \ldots, c) = f(c, c, \ldots, c),$$

while our proof will show that

$$f(a+1, a+1, \ldots, a+1, a, a, \ldots, a, a-x+1) \leq f(c+1, c, c, \ldots, c),$$

which will give

$$f(a+1, a+1, \ldots, a+1, a, a, \ldots, a, a-x) < f(c, c, \ldots, c).$$

Further, since a and c are integers, (13), (14), and (15) imply $c \leq a$.

The calculations involved in the proof of (12) are fairly lengthy, so we only outline them below.

It is convenient to deal with the cases $c = a$ and $c = a-1$ separately. When $c = a$, (13) implies $m = x + l$ and (12) reduces to an inequality $F_0(N, a, x, l) \leq 0$, where F_0 increases with l. When l is as large as possible, that is when $l = N - 2 - x$, this inequality is easily checked.

If $c = a - 1$, (13) implies that $m = x + l - N$, and (12) becomes an inequality $F_1(N, a, x, l) \geq 0$. Differentiating F_1 with respect to l shows that F_1 is minimized when l and m are approximately equal and so we need only prove some simple inequalities in N, a and x.

In the following, then, we may assume $c \leq a - 2$. Together with (13), this gives

$$x \geq 2N + m - l, \tag{17}$$

and, coupled with (16), (17) implies that

$$a \leq 3N + m - l - 1. \tag{18}$$

Differentiating (12), we find that $\frac{\partial F}{\partial x}$ dereases with x, so we need only check (12) when x is either as large as possible or as small as possible. As by (16) and (17),

$$2N + m - l \leq x \leq a - N + 1,$$

we have to consider the cases $x = a - N + 1$ and $x = 2N + m - l$.

Case A. $x = a - N + 1$. We can rewrite (12) as an inequality $F_2(N, a, m, l) \geq 0$, and $\frac{\partial F_2}{\partial m}$ decreases with m, so we must consider $F_2(N, a, m, l) \geq 0$ when m is either maximal or minimal subject to the constraints (14) and (18).

Case A1. $x = a - N + 1$ and $m = a - 3N + l + 1$. In this subcase, (13) yields $c = a - 2$. Relation (12) becomes $F_3(N, a, l) \geq 0$ and differentiation with respect to l identifies the few cases to check.

Case A2. $x = a - N + 1$ and $m = N - 2$. We may suppose (since we are not in case A1) that $m = N - 2 \leq a - 3N + l$. Relation (12) is now equivalent to a new inequality $F_4(N, a, l) \geq 0$, and this time F_4 increases with a. Therefore we need only look at the case when a is as small as possible, and from (18) this is precisely the case

$$x = 3N - 2 - l, m = N - 2, a = 4N - 3 - l, c = 4N - 5 - l. \tag{19}$$

Once again this subcase is readily checked, completing the proof of case A2.

Case A3. $x = a - N + 1$ and $m = 0$. Inequality (12) becomes $F_5(N, a, l) \geq 0$, where F_5 also increases with a, so the only case to examine is that where a is minimal, which is the easily checked case

$$x = 2N - l, m = 0, a = 3N - l - 1, c = 3N - l - 3. \tag{20}$$

This concludes case A3 and therefore case A.

Case B. $x = 2N + m - l$. From (16) we obtain

$$a \geq 3N + m - l - 1. \tag{21}$$

Moreover, $c = a - 2$. We find that if F_6 is the function obtained by substituting $x = 2N + m - l$ in F then $\frac{\partial F_6}{\partial a} > 0$. Therefore we need only check the case when a is minimal, and from (21) this is the case $a = 3N + m - l - 1$. But then we also have $x = a - N + 1$, and we are back in case A. This concludes the proof of (12), and therefore of (8). $\square$

Proof of Theorem 1. Lemma 3 shows that we have only to maximize

$$w_1(G(d_1, d_2, \ldots, d_N))$$

given the constraints

$$d_1 \geq d_2 \geq \ldots \geq d_N \geq N - 1 \tag{22}$$

and

$$\sum_{i=1}^{N} d_i = m + \binom{N}{2}. \tag{23}$$

An elementary calculation gives

$$w_1(G(d_1, d_2, \ldots, d_N)) = \left(\sum_{i=1}^{N} d_i\right)^2 + \sum_{i=1}^{N}(i-1)d_i^2 - N(N-1)\sum_{i=1}^{N} d_i. \tag{24}$$

First we fix N, thus also fixing $\sum_{i=1}^{N} d_i$. Lemma 4 shows that with these constraints, (24) is maximized by making the d_i as equal as possible. The remainder of the proof consists of comparing such balanced sequences, each one corresponding to a different value of N. The admissible values of N all satisfy $\binom{N}{2} \leq m$, from (22) and (23), and we will show that taking N maximal maximizes (24). The balanced sequence for this value of N corresponds to the graph G_m in the statement of the theorem.

Suppose that N is not maximal subject to $\binom{N}{2} \leq m$, and let $(d_1, d_2, \ldots, d_N)$ be a balanced sequence satisfying (22) and (23). Then $d_N \geq N$, for otherwise

$$d_N = N - 1,$$

$$d_1 \leq N$$

and

$$m + \binom{N}{2} = \sum_{i=1}^{N} d_i < N^2 = \binom{N+1}{2} + \binom{N}{2},$$

so that

$$m < \binom{N+1}{2},$$

a contradiction. Thus $d_N \geq N$. Create a new sequence by adding $d_{N+1} = N$. Conditions (22) and (23) are still valid, and the right hand side of (24) is unchanged. Therefore we can increase the right hand side of (24) by balancing our new sequence, and continue until N is maximal. This completes the proof of the theorem.

Note that if we had needed to maximize the function

$$g(d_1, d_2, \ldots, d_N) = \sum_{i=1}^{N} i d_i^2$$

instead of f, where the d_i are subject to the constraints in Lemma 4, we would make N as small as possible instead of as large as possible.

3. Graphs of maximal α-weight for $\alpha > 0$

As mentioned in the introduction, we distinguish three cases, $0 \leq \alpha \leq 1$, $1 < \alpha < 2$ and $\alpha \geq 2$. The following result deals with the first of these. For $m \geq 1$, we define k and r by the expressions

$$m = \binom{k}{2} + r,$$
$$0 < r \leq k,$$

and write

$$w(m) = w_1(G_m) = \binom{r}{2} k^2 + \binom{k-r}{2} (k-1)^2 + rk(k-r)(k-1) + r^2 k,$$

so that $w(m)$ is the largest possible 1-weight of a graph of size m.

Theorem 5. *Let G be a graph of size m with no isolated vertices. Then*

$$w_\alpha(G) \leq m^{1-\alpha} w(m)^\alpha$$

for $0 \leq \alpha < 1$. For $\alpha \neq 0$, we have equality if and only if G is complete.

Proof. Fix G with $e(G) = m$ and $\delta(G) \geq 1$. The case $\alpha = 0$ is trivial. Suppose then that $0 < \alpha < 1$. Setting $p = \frac{1}{\alpha}$ and $q = \frac{1}{1-\alpha}$, Hölder's inequality together with Theorem 1 shows that

$$\begin{aligned} w_\alpha(G) &= \sum_{xy \in E} (d_x d_y)^\alpha 1^{1-\alpha} \leq \left(\sum_{xy \in E} (d_x d_y)^{\alpha p} \right)^{\frac{1}{p}} \left(\sum_{xy \in E} 1 \right)^{\frac{1}{q}} \\ &= m^{1-\alpha} w(G)^\alpha \leq m^{1-\alpha} w(m)^\alpha, \end{aligned}$$

with equality iff $G \cong G_m$ and all edges have equal weight, so that $m = \binom{k}{2}$ and $G \cong K_k$. $\square$

We turn to the case $1 < \alpha < 2$. For convenience, we define

$$w_\alpha(m) = \max\{w_\alpha(G) : e(G) = m\}.$$

Here, when maximizing $w_\alpha(G)$ over graphs G of fixed size m, it is advantageous to have some vertices of very large degree (exactly how large depends on α). We therefore consider the *split graphs* $S(r,s)$ which are such that

$$\begin{aligned} V(S(r,s)) &= \{v_1, v_2, \ldots, v_r, v_{r+1}, v_{r+2}, \ldots, v_{r+s}\}, \\ E(S(r,s)) &= E_1 \cup E_2, \end{aligned}$$

where

$$\begin{aligned} E_1 &= \{\{v_i, v_j\} : 1 \le i < j \le r\}, \\ E_2 &= \{\{v_i, v_j\} : 1 \le i \le r, r+1 \le j \le r+s\}, \end{aligned}$$

so that $S(r,s)$ is simply $K_{r,s}$ with the first class "filled in". Note further that the split graphs are a subfamily of F. It seems natural to guess that, assuming m has the appropriate divisibility properties, a graph of size m and maximum α-weight is close to $S(t, \frac{m-\binom{t}{2}}{t})$ for some t. We have

$$\begin{aligned} w_\alpha\left(S\left(t, \frac{m-\binom{t}{2}}{t}\right)\right) &= \binom{t}{2}\left(t-1+\frac{m-\binom{t}{2}}{t}\right)^{2\alpha} \\ &+ \left(m-\binom{t}{2}\right)t^\alpha\left(t-1+\frac{m-\binom{t}{2}}{t}\right)^{\alpha} \\ &= \binom{t}{2}\left(\frac{m}{t}\right)^{2\alpha}\left(1+\frac{\binom{t}{2}}{m}\right)^{2\alpha} \\ &+ \left(m-\binom{t}{2}\right)m^\alpha\left(1+\frac{\binom{t}{2}}{m}\right)^{\alpha}. \end{aligned}$$

The first term is about $\frac{1}{2}m^{2\alpha}$ while the second is at most $4m^{1+\alpha}$. A quick differentiation shows that we should take t around $1+\frac{1}{2\alpha-2}$. To summarize, when $t = 1 + \frac{1}{2\alpha-2}$ is an integer, and when t divides $m-\binom{t}{2}$, $S(t, \frac{m-\binom{t}{2}}{t})$, with weight asymptotically equal to

$$\frac{(2\alpha-2)^{2\alpha-2}}{2(2\alpha-1)^{2\alpha-1}}m^{2\alpha},$$

is a good candidate for an extremal graph. For comparison, if in addition $m = \binom{k}{2}$, the complete graph of size m has α-weight asymptotically equal to $2^\alpha m^{1+\alpha}$.

The proof of the next theorem relies on the observation that only the terms in which d_x and d_y are both large contribute significantly to $w_\alpha(G) = \sum_{xy\in E(G)} d_x^\alpha d_y^\alpha$: a similar observation is made in [2].

Theorem 6. *For $\alpha > 1$ we have*

$$w_\alpha(m) \le \frac{(2\alpha-2)^{2\alpha-2}}{2(2\alpha-1)^{2\alpha-1}} m^{2\alpha} + O(m^{2\alpha-(\frac{\alpha-1}{\alpha+1})}).$$

In particular,

$$w_\alpha(m) \sim \frac{(2\alpha-2)^{2\alpha-2}}{2(2\alpha-1)^{2\alpha-1}} m^{2\alpha}$$

when $\frac{1}{2\alpha-2}$ is an integer.

Proof. Let G be a graph of size m. Suppose that $V(G) = \{v_1, v_2, \ldots, v_n\}$, where $d(v_i) = d_i$, and that $d_1 \ge d_2 \ge \ldots \ge d_n > 0$. Write

$$\begin{aligned} S &= \{i \in [n] : d_i > m^\gamma\}, \\ T &= \{i \in [n] : d_i \le m^\gamma\}, \\ W &= \{v_i : i \in S\}, \end{aligned}$$

for some $\frac{1}{2} < \gamma < 1$, so that W is the set of vertices of large degree. Now

$$\begin{aligned} w_\alpha(G) &= \sum_{xy \in E(G)} d_x^\alpha d_y^\alpha \le \sum_{1 \le i < j \le n} d_i^\alpha d_j^\alpha \\ &= \sum_{1 \le i < j \le n, j \in S} d_i^\alpha d_j^\alpha + \sum_{1 \le i < j \le n, j \in T} d_i^\alpha d_j^\alpha \\ &\le \sum_{1 \le i < j \le n, j \in S} d_i^\alpha d_j^\alpha + (\sum_{i=1}^n d_i^\alpha)(\sum_{j \in T} d_j^\alpha) \\ &= \sum_{1 \le i < j \le n, j \in S} d_i^\alpha d_j^\alpha + (\sum_{i=1}^n d_i d_i^{\alpha-1})(\sum_{j \in T} d_j d_j^{\alpha-1}) \\ &\le \sum_{1 \le i < j \le n, j \in S} d_i^\alpha d_j^\alpha + 2m^\alpha 2m^{1+\gamma(\alpha-1)} \\ &= \sum_{1 \le i < j \le n, j \in S} d_i^\alpha d_j^\alpha + 4m^{2+(1+\gamma)(\alpha-1)}. \end{aligned}$$

There are less than $2m^{1-\gamma}$ vertices in W, and so they span less than $2m^{2-2\gamma}$ edges. Writing $\beta = 1 + 2m^{1-2\gamma}$, we have

$$\begin{aligned} \sum_{1 \le i < j \le n, j \in S} d_i^\alpha d_j^\alpha &\le \frac{1}{2}(\sum_{1 \le i < j \le n, j \in S} d_i^{2\alpha-1} d_j + d_i d_j^{2\alpha-1}) \\ &= \frac{1}{2}(\sum_{i,j \in S, i \ne j} d_i^{2\alpha-1} d_j) = \frac{1}{2}(\sum_{i \in S} d_i \sum_{j \in S} d_j^{2\alpha-1} - \sum_{j \in S} d_j^{2\alpha}) \\ &\le \frac{1}{2}(\beta m \sum_{j \in S} d_j^{2\alpha-1} - \sum_{j \in S} d_j^{2\alpha}) = \frac{1}{2} \sum_{j \in S} d_j d_j^{2\alpha-2}(\beta m - d_j) \end{aligned}$$

$$\begin{aligned}
&\le \frac{1}{2}\sum_{j\in S} d_j(\beta m)^{2\alpha-1}\frac{(2\alpha-2)^{2\alpha-2}}{(2\alpha-1)^{2\alpha-1}} \le \frac{(2\alpha-2)^{2\alpha-2}}{2(2\alpha-1)^{2\alpha-1}}(\beta m)^{2\alpha}\\
&= \frac{(2\alpha-2)^{2\alpha-2}}{2(2\alpha-1)^{2\alpha-1}}m^{2\alpha} + O(m^{1+2\alpha-2\gamma}).
\end{aligned}$$

Putting the pieces together, we obtain

$$w_\alpha(G) \le \frac{(2\alpha-2)^{2\alpha-2}}{2(2\alpha-1)^{2\alpha-1}}m^{2\alpha} + 4m^{2+(1+\gamma)(\alpha-1)} + O(m^{1+2\alpha-2\gamma}).$$

Finally, we choose γ so that

$$2+(1+\gamma)(\alpha-1) = 1+2\alpha-2\gamma,$$

giving $\gamma = \frac{\alpha}{1+\alpha}$ and the stated result. □

When $\alpha < \frac{3}{2}$, $\frac{1}{2\alpha-2}$ is never an integer, so that the bound in Theorem 6 is not realized by the split graph $S(2, \frac{m-1}{2})$. However, due to the simple nature of $S(2, \frac{m-1}{2})$, it is possible to show that, at least for $\alpha \ge 2$, we have

$$w_\alpha(m) \sim w_\alpha(S(2, \frac{m-1}{2})) \sim \left(\frac{m}{2}\right)^{2\alpha}.$$

First we need a simple lemma.

Lemma 7. *Let $\alpha \ge 2$ and let $x_1, \dots, x_n$ be positive real numbers whose sum is unity. Then*

$$\sum_{1\le i<j\le n} (x_i x_j)^\alpha \le 4^{-\alpha},$$

with equality iff only two x_i are non-zero, and they are both $\frac{1}{2}$.

Proof. We use induction on n. For $n=2$ the result is immediate. Suppose $n \ge 3$ and $x_n = \min x_i$. If $x_n = 0$, we are done by the induction hypothesis. Otherwise,

$$\begin{aligned}
\sum_{1\le i<j\le n} (x_i x_j)^\alpha &= \sum_{1\le i<j\le n-1} (x_i x_j)^\alpha + x_n^\alpha \sum_{i=1}^{n-1} x_i^\alpha\\
&\le 4^{-\alpha}(1-x_n)^{2\alpha} + x_n^\alpha(1-x_n)^\alpha\\
&= 4^{-\alpha}\left\{(1-x_n)^{2\alpha} + (4x_n(1-x_n))^\alpha\right\}\\
&\le 4^{-\alpha}\left\{(1-x_n)^4 + (4x_n(1-x_n))^2\right\}\\
&< 4^{-\alpha},
\end{aligned}$$

using the induction hypothesis, the fact that $1-x_n$ and $4x_n(1-x_n)$ are both at most unity, *and* (crucially) the inequality $x_n \le \frac{1}{3}$. □

Theorem 8. *For $\alpha \geq 2$ fixed and $m \to \infty$, we have*

$$w_\alpha(m) = \left(\frac{m}{2}\right)^{2\alpha} + O\left(m^{2\alpha - \left(\frac{\alpha-1}{\alpha+1}\right)}\right)$$

Proof. The split graph $S(2, \frac{m-1}{2})$ has α-weight given by

$$w_\alpha(S(2, \frac{m-1}{2})) = \left(\frac{m+1}{2}\right)^{2\alpha} + (m-1)(m+1)^\alpha,$$

so we need only show that

$$w_\alpha(m) \leq \left(\frac{m}{2}\right)^{2\alpha} + O\left(m^{2\alpha - \left(\frac{\alpha-1}{\alpha+1}\right)}\right).$$

To this end, if $e(G) = m$ and $\frac{1}{2} < \gamma < 1$, the proof of Theorem 6 gives

$$w_\alpha(G) \leq \sum_{1 \leq i < j \leq n, j \in S} d_i^\alpha d_j^\alpha + 4m^{2+(1+\gamma)(\alpha-1)},$$

and this together with Lemma 7 implies that

$$w_\alpha(G) \leq \left(\frac{\beta m}{2}\right)^{2\alpha} + 4m^{2+(1+\gamma)(\alpha-1)}.$$

Choosing $\gamma = \frac{\alpha}{1+\alpha}$ as before, the theorem follows. $\square$

It would be interesting to investigate the case where m is not too large and $\alpha = 1 + \epsilon$, for small positive ϵ. Further, it is possible that one can prove an exact result for $\alpha \geq 2$.

4. Graphs of minimal α-weight for $\alpha < 0$

All we use in this section is Theorem 5 (which relies on Theorem 1) and the Cauchy-Schwarz inequality.

Theorem 9. *Let G be a graph of size m with no isolated vertices. Then*

$$w_\alpha(G) \geq m^{1-\alpha} w(m)^\alpha$$

for $\alpha < 0$, with equality if and only if G is complete.

Proof. Write

$$(0, \infty) = \bigcup_{j \geq 0} A_j,$$

where

$$A_j = [1 - 2^{j+1}, 1 - 2^j).$$

We proceed by induction on j. For $\alpha \in A_0$, we may write

$$w_\alpha(G) w_{-\alpha}(G) = \sum_{xy \in E} (d_x d_y)^\alpha \sum_{xy \in E} (d_x d_y)^{-\alpha} \geq \left\{ \sum_{xy \in E} (d_x d_y)^{\frac{\alpha}{2}} (d_x d_y)^{-\frac{\alpha}{2}} \right\}^2 = m^2$$

by the Cauchy-Schwarz inequality, so that using Theorem 5

$$w_\alpha(G) \geq \frac{m^2}{w_{-\alpha}(G)} \geq m^{1-\alpha} w(m)^\alpha,$$

with equality if and only if G is complete. Assume next that $w_\alpha(G) \geq m^{1-\alpha}w(m)^\alpha$ for $\alpha \in A_j$, with equality iff G is complete. Take $\alpha \in A_{j+1}$. Then, again by the Cauchy-Schwarz inequality,

$$w_\alpha(G)w_1(G) = \sum_{xy\in E} (d_x d_y)^\alpha \sum_{xy\in E} d_x d_y \geq \left\{ \sum_{xy\in E} (d_x d_y)^{\frac{\alpha}{2}} (d_x d_y)^{\frac{1}{2}} \right\}^2 = w_{\frac{1+\alpha}{2}}(G)^2.$$

Now

$$\alpha \in A_{j+1} \Leftrightarrow \frac{1+\alpha}{2} \in A_j,$$

so that

$$w_\alpha(G)w_1(G) \geq w_{\frac{1+\alpha}{2}}(G)^2 \geq m^{1-\alpha} w(m)^{1+\alpha}$$

by induction, and so

$$w_\alpha(G) \geq m^{1-\alpha} w(m)^\alpha,$$

with equality iff G is complete, completing the induction step. □

As mentioned in §1, the case $-1 \leq \alpha < 0$ appears in [1].

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