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An Extremal Problem on Degree Sequences of Graphs

Nathan Linial[1]* and Eyal Rozenman[2]

Institute of Computer Science, Hebrew University, Jerusalem 91904, Israel
e-mail: [1]nati, [2]eyalroz@cs.huji.ac.il

Abstract. Let $G = (I_n, E)$ be the graph of the n-dimensional cube. Namely, $I_n = \{0,1\}^n$ and $[x,y] \in E$ whenever $||x-y||_1 = 1$. For $A \subseteq I_n$ and $x \in A$ define $h_A(x) = \#\{y \in I_n \setminus A | [x,y] \in E\}$, i.e., the number of vertices adjacent to x outside of A. Talagrand, following Margulis, proves that for every set $A \subseteq I_n$ of size 2^{n-1} we have $\frac{1}{2^n}\sum_{x\in A}\sqrt{h_A(x)} \geq K$ for a universal constant K independent of n. We prove a related lower bound for graphs: Let $G = (V,E)$ be a graph with $|E| \geq \binom{k}{2}$. Then $\sum_{x\in V(G)}\sqrt{d(x)} \geq k\sqrt{k-1}$, where $d(x)$ is the degree of x. Equality occurs for the clique on k vertices.

1. Introduction

Let $G = (I_n, E)$ be the graph of the n-dimensional cube. That is $I_n = \{0,1\}^n$ and $[x,y] \in E$ whenever $||x-y||_1 = 1$. Let $A \subseteq I_n$ and define

$$h_A(x) = \#\{y \in I_n \setminus A | [x,y] \in E\}$$

Namely, $h_A(x)$ counts the number of vertices outside A which are adjacent to x. Using h_A we can measure the size of the boundary of A. For example, $\sum_{x\in A} h_A(x)$ is the number of edges between A and $I_n \setminus A$, i.e., the edge boundary of A. Similarly, the vertex boundary of A, namely, those vertices in A which have a neighbour in $I_n \setminus A$, are exactly those vertices for which $h_A(x) > 0$. Talagrand, in [2], following previous results of Margulis [1] and others, has derived isoperimetric inequalities for the n-dimensional cube in terms of h_A. For example, it is shown that

$$\frac{1}{2^n}\sum_{x\in A}\sqrt{h_A(x)} \geq K \tag{1}$$

for every $A \subseteq I_n$ with cardinality $|A| = 2^{n-1}$. The constant K is independent of n, the cube's dimension. More generally, lower bounds on $\frac{1}{2^n}\sum_{x\in A}\sqrt{h_A(x)}$ are established in terms of $|A|$. One can view the square root function as a "middle

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way'' between the two former quantities of edge and vertex boundaries. Natural questions that arise here are what the exact optimum is, and which sets are optimal for this inequality. Let us consider some families of sets that achieve $\sum_{x\in A}\sqrt{h_A(x)} = O(1)$. Half cubes

$$(x_1, x_2, \ldots, x_n); \quad x_1 = 1$$

do, as well as balls,

$$(x_1, x_2, \ldots, x_n); \quad \sum_{i=1}^{n} x_i \le n/2$$

In general, for $J \subseteq \{1, 2, \ldots, n\}$ and $|J|$ odd:

$$B_J = \left\{ (x_1, x_2, \ldots, x_n); \quad \sum_{i\in J} x_i \le |J|/2 \right\}$$

is a family with the same property. In our quest for sets which optimize this inequality, we first consider consecutive levels: Let $L_m = \{x; \sum x_i = m\}$ be the m-th level of the cube. Let $L_m(A) = A \cap L_m$, $l_m(A) = |(A \cap L_m)|$. For $x \in L_m(A)$ define

$$h_A^+(x) = \#\{y \in L_{m+1}(A) | [x, y] \in E\}$$

For monotone decreasing sets $h^+ = h$. (Recall that A is monotone decreasing when it is closed under the operation of changing a coordinate from 1 to 0). The question here is, given l_m, l_{m+1}, what are $L_m(A), L_{m+1}(A)$ that minimize $\sum_{x\in L_m(A)}\sqrt{h_A^+(x)}$? We can essentially solve the problem for $m = 1$:

Theorem 1.1. *Let $A \subseteq I_n$ contain the first level L_1. Suppose that $l_2(A) = \binom{n}{2} - \binom{k}{2}$. Then the minimum of $\sum_{x\in L_1(A)}\sqrt{h^+(x)}$ is attained when $L_2(A)$ is the suffix in colex order.*

Theorem 2.1 can be conveniently stated in the language of graphs and their degree sequence:

Theorem 1.2. *Let G be a graph with $\binom{k}{2}$ edges. Then*

$$\sum_{x\in V(G)} \sqrt{d(x)} \ge k\sqrt{k-1}$$

Equality occurs when G is the clique on k vertices.

$d(x)$ is, here and elsewhere, the degree of the vertex x.

Comment 1.3. Consider the more general problem of minimizing $\sum_{x\in V(G)} f(d(x))$ over all graphs with a given number of edges. One might suspect that a statement analogous to Theorem 2.2 holds for every concave increasing function f that vanishes at zero. This is, however, incorrect. Consider the function

$f(x) = \sqrt{x+a} - \sqrt{a}$. For this f, the minimizing graph need not be the clique. The star, for instance, is better for certain values of a. We show this for $a = k$. For the star with $\binom{k}{2}$ edges

$$F_{st}(k) = \sum_{V(G)} f(d(x)) = \binom{k}{2}\left(\sqrt{1+a} - \sqrt{a}\right) + \left(\sqrt{\binom{k}{2} + a} - \sqrt{a}\right)$$

The same quantity for the clique is

$$F_{cl}(k) = k\left(\sqrt{k-1+a} - \sqrt{a}\right)$$

Substitute $a = k$ to obtain (for large k)

$$\begin{aligned} F_{cl}(k) &\geq \left(\sqrt{2} - 1 - o(1)\right)k^{3/2} \\ F_{st}(k) &\leq \frac{k^2}{2}\left(\sqrt{k+1} - \sqrt{k}\right) + o\left(k^{3/2}\right) \\ &\leq k^{3/2}\left(\frac{1}{4} + o(1)\right) \end{aligned}$$

The $o(1)$ terms tend to zero for large k. This completes the counterexample.

Consider a monotone decreasing set $A \subseteq I_n$ with $l_1(A) = n - a$, $l_2(A) = \binom{n}{2} - \binom{k}{2}$. What is the minimum of $\sum_{x \in L_1(A)} \sqrt{h^+(x)}$? Theorem 2.1 provides the answer when $l_1(A) = n$. The graph-theoretic problem that corresponds to the case $l_1(A) = n - a$ is to minimize $\sum_{x \in V(G)} \sqrt{d(x) + a}$ on a graph with exactly $n - a$ vertices. An equivalent statement of the problem is to minimize $\sum_{x \in V(G)} \left(\sqrt{d(x) + a} - \sqrt{a}\right)$ on a graph with a given number of edges and with no restriction on the number of vertices. The function $f(x) = \sqrt{x+a} - \sqrt{a}$ therefore replaces $\sqrt{x}$ when $l_1(A) = n - a$ rather than n in theorem 2.1. The counterexample shows that the minimum of $L_2(A)$ is not attained by a suffix in colex order, as in the theorem.

2. A Family of Extremal Graphs

We turn to prove Theorem 2.2. As a starter, we show an easy argument which limits the family of possible extremal graphs. In contrast to comment 2.3 the discussion in this section is valid for every f that is concave and increasing. Here is an easy but useful observation:

Claim 3.1. *Let f be an increasing, concave function. Let G be a graph for which $\sum_{v \in V(G)} f(d(v))$ is minimal among all graphs with a given number of edges. If v, w are adjacent vertices of G, then v is adjacent to every vertex u s.t. $deg(u) \geq deg(w)$.*

Proof. Otherwise replace $[v, w]$ with $[v, u]$ to obtain a better G. □

From the claim we immediately derive a structural description of a minimizing G:

1. If x is a vertex of minimal degree and $[x, y] \in E(G)$, then y is adjacent to all the vertices in G.

2. In general, divide the graph to sets of vertices by increasing degree: Let $d_1 < d_2, \ldots < d_l$ be the sequence of distinct degrees appearing in the graph. Let S_i be the set of vertices of degree d_i. The vertices in S_l are adjacent to all the vertices in the graph, those in S_{l-1} to all vertices except those in S_1, the vertices in S_{l-2} to $\cup_{i=3}^{l} S_i$ and so forth. Thus, a vertex of degree d_i is adjacent to all vertices of degree d_j if $i + j \geq n + 1$.

We now see that the sequence of distinct degrees in the graph uniquely determines the graph. Define $a_i = |S_i|$, the number of vertices with degree d_i. Then

$$d_i = \begin{cases} \sum_{i+j \geq l+1} a_j - 1 & i \geq (l+1)/2 \\ \sum_{i+j \geq l+1} a_j & i \leq l/2 \end{cases}$$

Inverting this definition:

$$a_i = d_{l-i+1} - d_{l-i} + \delta_{i, \lceil \frac{l}{2} \rceil}$$

For each increasing sequence of integers d_i the corresponding graph is well defined, so we can now forget the graphs and concentrate on the following question (next section).

3. No Extremum Points

Let $\underline{d} = d_1 \leq d_2, \ldots \leq d_n$ be a nondecreasing sequence of real numbers. Define

$$a_i = d_{n-i+1} - d_{n-i} + \delta_{i, \lceil \frac{n}{2} \rceil} \tag{2}$$

$$F(\underline{d}) = \sum_{i=1}^{n} a_i d_i \tag{3}$$

$$G(\underline{d}) = \sum_{i=1}^{n} a_i \sqrt{d_i} \tag{4}$$

We want to find the minimum of $G(\underline{d})$ under the condition $F(\underline{d}) = const$. The connection with the question about graphs is as follows: If the d_i are positive integers, we can realize a graph with the given sequence of distinct degrees, as was shown in the end of section 3. The a_i are the number of vertices of degree d_i, $F(\underline{d})$ is the number of edges, and $G(\underline{d})$ is the functional $\sum_{v \in V(G)} f(d(v))$. A lower bound on G for real sequences yields a lower bound on integer sequences.

We proceed to show that the functional G has no local minimum for dimension (i.e. sequence length) greater than one. This is done using Lagrange multipliers. In the next section we shall deduce that the global minimum of G occurs in dimension 1.

Calculating partial derivatives for n even, $k = n/2$ produces (recall $a_k = d_{n-k+1} - d_{n-k} + \delta_{\lceil \frac{n}{2} \rceil}$),

$$\begin{aligned}
\frac{\partial F}{\partial d_k} &= \frac{\partial}{\partial d_k}(a_k d_k + a_{k+1} d_{k+1}) \\
&= d_{k+1} - d_k + 1 + d_{k+1} - d_k \\
&= 2(d_{k+1} - d_k) + 1 \\
\frac{\partial G}{\partial d_k} &= \frac{\partial}{\partial d_k}\left(a_k \sqrt{d_k} + a_{k+1}\sqrt{d_{k+1}}\right) \\
&= \frac{(d_{k+1} - d_k + 1)}{2\sqrt{d_k}} + \sqrt{d_{k+1}} - \sqrt{d_k}
\end{aligned}$$

For n odd let $k + 1 = \frac{n+1}{2}$ and take $\frac{\partial}{\partial d_{k+1}}$ to obtain:

$$\begin{aligned}
\frac{\partial F}{\partial d_{k+1}} &= \frac{\partial}{\partial d_{k+1}}(a_{k+1} d_{k+1} + a_k d_k) \\
&= d_{k+1} - d_k + 1 + d_{k+1} - d_k \\
&= 2(d_{k+1} - d_k) + 1 \\
\frac{\partial G}{\partial d_{k+1}} &= \frac{\partial}{\partial d_{k+1}}\left(a_{k+1}\sqrt{d_{k+1}} + a_k \sqrt{d_k}\right) \\
&= \frac{(d_{k+1} - d_k + 1)}{2\sqrt{d_{k+1}}} + \sqrt{d_{k+1}} - \sqrt{d_k}
\end{aligned}$$

Note that the F derivatives are the same, while in the G derivative the d_k in the denominator changes to d_{k+1}.

Similarly, for all $n > 1$,

$$\begin{aligned}
\frac{\partial F}{\partial d_n} &= 2(d_1 - d_0) \\
\frac{\partial G}{\partial d_n} &= \frac{(d_1 - d_0)}{2\sqrt{d_n}} + \sqrt{d_1} - \sqrt{d_0}
\end{aligned}$$

We claim that there is no local extremum for G when F is fixed if $\underline{d}$ is increasing. This is shown by calculating Lagrange multipliers. First with n even and $2k = n$. We must satisfy

$$\frac{\partial G}{\partial d_k} = \lambda \frac{\partial F}{\partial d_k}, \quad \frac{\partial G}{\partial d_n} = \lambda \frac{\partial F}{\partial d_n}$$

which produces the equations

$$\frac{(d_{k+1} - d_k + 1)}{2\sqrt{d_k}} + \sqrt{d_{k+1}} - \sqrt{d_k} = \lambda(2(d_{k+1} - d_k) + 1)$$
$$\frac{(d_1 - d_0)}{2\sqrt{d_n}} + \sqrt{d_1} - \sqrt{d_0} = \lambda 2(d_1 - d_0)$$

Set $u_k = \sqrt{d_k}$. The condition can be re-written as

$$(u_k + u_{k+1})(2\lambda - 1/2u_k) + \frac{\lambda - 1/2u_k}{u_{k+1} - u_k} = 1$$
$$(u_0 + u_1)(2\lambda - 1/2u_n) = 1$$

multiply each equation by 2 and replace 4λ with μ to get

$$(u_k + u_{k+1})(\mu - 1/u_k) + \frac{\mu/2 - 1/u_k}{u_{k+1} - u_k} = 2$$
$$(u_0 + u_1)(\mu - 1/u_n) = 2$$

The second equation gives (with monotonicity of the u_i) $u_k, u_{k+1} > 2/\mu$. Put this in the first equation to get: (note that the second summand of the first equation is positive – $\mu/2 - 1/u_k > 0$ by the second equation).

$$4/\mu(\mu - 1/u_k) < 2$$
$$4 - 4/(\mu u_k) < 2$$
$$\mu u_k < 2$$

which contradicts the second equation.

Now do all the calculations for odd n. The Lagrange condition becomes

$$\frac{(d_{k+1} - d_k + 1)}{2\sqrt{d_{k+1}}} + \sqrt{d_{k+1}} - \sqrt{d_k} = \lambda(2(d_{k+1} - d_k) + 1)$$
$$\frac{(d_1 - d_0)}{2\sqrt{d_n}} + \sqrt{d_1} - \sqrt{d_0} = \lambda 2(d_1 - d_0)$$

which produces, after the same calculation as above (the only difference is the d_k in the denominator, which changes to d_{k+1}):

$$(u_k + u_{k+1})(\mu - 1/u_{k+1}) + \frac{\mu/2 - 1/u_{k+1}}{u_{k+1} - u_k} = 2$$
$$(u_0 + u_1)(\mu - 1/u_n) = 2$$

Again $u_k, u_{k+1} > 2/\mu$ by the second equation, so

$$4/\mu(\mu - 1/u_{k+1}) < 2$$

which yields the same contradiction.

4. Vector Shortening

Claim 5.1. *Let* $\underline{d} = d_1 \le d_2, \ldots \le d_n$ *be a monotone vector and* $d_k = d_{k+1}$. *Then there exists a shorter vector* $\tilde{\underline{d}}$ *which satisfies* $H(\underline{d}) = H(\tilde{\underline{d}})$ *for all* H *of the form* $H(\underline{d}) = \sum a_i f(d_i)$ *where* a_i *is as in section 3.*

In particular this is true for F, G of the last section. The way to construct $\tilde{\underline{d}}$ is: if $2k = n$ or $2k+1 = n$ (i.e. $k = \lceil \frac{n}{2} \rceil$) omit d_k to create a new vector of length $n-1$. Otherwise omit d_k, d_{n-k} to create a vector of length $n-2$. The proof is by example on the three cases:

Case 1. $k \ne \lceil \frac{n}{2} \rceil$

Here is an example with $n = 10, k = 3$, i.e. $d_3 = d_4$. Let

$$\underline{d} = d_0, d_1, d_2, d_3, \ldots d_{10}$$

where $d_0 = 0$. Define

$$\tilde{\underline{d}} = d_0, d_1, d_2, d_4, d_5, d_6, d_8, d_9, d_{10}$$

We omitted d_3, d_7. We want to show that every element $a_i f(d_i)$ appears in $H(\tilde{\underline{d}})$. Let us examine the terms of $H(\tilde{\underline{d}})$. For $i < 3$ it is easy to note that $\tilde{a}_i$ is the same as a_i. $f(d_4)$ is multiplied by $d_8 - d_6 = a_3 + a_4$. $f(d_5)$ is multiplied by $=$ $d_6 - d_5 = a_5$. $f(d_6)$ is multiplied by $d_5 - d_3 + 1 = d_5 - d_4 + 1 = a_5$. (The $+1$ is because $4 = \lceil \frac{8}{2} \rceil$ and the new sequence has 8 terms). $f(d_7)$ is multiplied by $d_3 - d_2 = a_7$ and the same works up to d_{10}. It is easy to see that every element $a_i f(d_i)$ appears in $H(\tilde{\underline{d}})$. Note that the "missing" element $a_7 f(d_7)$ is zero since $a_7 = d_4 - d_3 = 0$, and the term $a_3 f(d_3)$ appears as a summand of the new term for $f(d_4)$, which is equal $f(d_3)$. Let us summarize in a table: define $b_i = d_{n-i+1} - d_{n-i}$, so $a_i = b_i + \delta_{\lceil \frac{n}{2} \rceil}$. The following array is the original $\underline{d}$ and the coefficient to multiply by:

d_1	d_2	d_3	d_4	d_5	d_6	d_7	d_8	d_9	d_{10}
b_1	b_2	b_3	b_4	b_5	b_6	b_7	b_8	b_9	b_{10}

And here is the same array for the new $\tilde{\underline{d}}$:

d_1	d_2	d_4	d_5	d_6	d_8	d_9	d_{10}
$d_{10} - d_9$	$d_9 - d_8$	$d_8 - d_6$	$d_6 - d_5$	$d_5 - d_4$	$d_4 - d_2$	$d_2 - d_1$	$d_1 - d_0$
b_1	b_2	$b_3 + b_4$	b_5	b_6	b_8	b_9	b_{10}

By observing the array, we can easily verify that $\sum b_i f(d_i) = \sum \tilde{b}_i f(\tilde{d}_i)$. Since the element number $\lceil \frac{n}{2} \rceil$ did not change its value, this is also true with a_i instead of b_i in the last equality. This works for every k, n when $k + 1 < n - k$, or

$k > n - k$, which is symmetrical. The idea is as above: We can omit d_{n-k} since $a_{n-k} = d_{k+1} - d_k = 0$, and to omit d_k is O.K. since in the new vector $f(d_{k+1})$ is multiplied by $d_{n-k+1} - d_{n-k-1} = a_k + a_{k+1}$, which compensates for $f(d_k)$ and $f(d_{k+1})$ simultaneously. The other terms are not affected by the shortening. Note that the special element $d_{\lceil \frac{n}{2} \rceil}$ is never affected by our erasures, and that it remains the special element (which is now $\lceil \frac{n-2}{2} \rceil = \lceil \frac{n}{2} \rceil - 1$), in the new, shortened vector.

Case 2. $2k = n$:

We do the example for $n = 10, k = 5$. Let

$$\underline{d} = d_0, d_1, d_2, d_3, \ldots d_{10}$$

where $d_0 = 0$ and $d_5 = d_6$. Define

$$\tilde{\underline{d}} = d_0, d_1, d_2, d_3, d_4, d_6, d_7, d_8, d_9, d_{10}$$

We omitted only d_5. Let us check the terms of $H(\tilde{\underline{d}})$: for $i < 5$ we get $\tilde{a}_i = a_i$. $f(d_6) = f(d_5)$ is multiplied by $d_6 - d_4 + 1 = d_5 - d_4 + 1 = a_5 + a_6$ (The $+1$ is because d_6 is the special element of the new sequence). $f(d_7)$ is multiplied by $d_4 - d_3 = a_7$ and this continues up to d_{10}. Again we see that all the terms coincide. The "missing" term $a_5 f(5)$ appears in the new term for d_6 – note that $a_5 = d_5 - d_4 + 1 = 1$. The following array is the original $\underline{d}$ and the coefficient to multiply:

d_1	d_2	d_3	d_4	d_5	d_6	d_7	d_8	d_9	d_{10}
b_1	b_2	b_3	b_4	b_5	b_6	b_7	b_8	b_9	b_{10}

And here is the same array for the new $\tilde{\underline{d}}$:

d_1	d_2	d_3	d_4	d_6	d_7	d_8	d_9	d_{10}
$d_{10} - d_9$	$d_9 - d_8$	$d_8 - d_7$	$d_7 - d_6$	$d_6 - d_4$	$d_4 - d_3$	$d_3 - d_2$	$d_2 - d_1$	$d_1 - d_0$
b_1	b_2	b_3	b_4	$b_5 + b_6$	b_7	b_8	b_9	b_{10}

Case 3. $2k + 1 = n$:

We do the special case for 11 elements,

$$\underline{d} = d_0, d_1, d_2, d_3, \ldots d_{10}, d_{11}$$

where $d_0 = 0$ and $d_5 = d_6$. Define

$$\tilde{\underline{d}} = d_0, d_1, d_2, d_3, d_4, d_6, d_7, d_8, d_9, d_{10}, d_{11}$$

d_1	d_2	d_3	d_4	d_6	d_7	d_8	d_9	d_{10}	d_{11}	
$d_{11}-d_{10}$	$d_{10}-d_9$	d_9-d_8	d_8-d_7	d_7-d_6	d_6-d_4	d_4-d_3	d_3-d_2	d_2-d_1	d_1-d_0	
b_1	b_2	b_3	b_4	b_5+b_6	b_7	b_8	b_9	b_{10}		

And we can check our equalities again. This completes the verification of the claim.

5. Global Minimum

Recall that we want to minimize $G(\underline{d})$ under $F(\underline{d}) = C$. Finding the global minimum is now easy: We claim that it occurs when the length of $\underline{d}$ is 1. First, there is only one solution for $F(\underline{d}) = C$ when the length is 1. Consider an increasing counterexample at a higher dimension, and assume this is the minimal dimension in which these exist. If it is not strictly increasing, apply vector shortening. Otherwise it is not a local minimum, so we can move to a worse example. Legal $\underline{d}$ values are bounded since $a_n d_n = d_1 d_n \leq F(\underline{d}) = C$ and our Lagrange multiplier considerations only changed $d_{\lceil \frac{n}{2} \rceil}, d_n$, so d_1 remains constant. Thus, we will reach a counterexample with two coordinates equal. Then we can apply vector shortening, which gives a shorter counterexample, a contradiction. Theorem 2.2 follows now by noting that a vector of length 1 corresponds to a clique in the identification we used. The condition that the number of edges is $\binom{k}{2}$ is used to get a vector of length 1 with integer value.

Open Questions. 1. We found the minimal graph for a graph with $\binom{k}{2}$ edges, and found that the clique is the minimal graph. What about $\binom{k}{2} + l$, where $l < k + 1$? We expect the minimal graph here to be a union of a clique on k vertices and a single vertex adjacent to l vertices of the clique. This result does not follow immediately from our methods, but we believe it could be derived with some extra effort.

2. Comment 2.3 shows the result cannot be extended to every concave increasing function. What is the family of functions for which the clique is the minimal graph? Are all functions x^c with $c < 1$ minimized on the clique ?

3. Perhaps there is a small family of graphs which contain the minimal graph for every increasing concave function f? For example, is every function minimized on the clique or the star?

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