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GRAPHS WITH EXTREMAL CONNECTIVITY INDEX

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Abstract. Let G be a graph and δ_v the degree of its vertex v. The connectivity index of G is $\chi = \sum(\delta_u \, \delta_v)^{-1/2}$, with the summation ranging over all pairs of adjacent vertices of G. We offer a simple proof that (a) among n-vertex graphs without isolated vertices, the star has minimal χ-value, and (b) among n-vertex graphs, the graphs in which all components are regular of non–zero degree have maximal (mutually equal) χ-values. Both statements (a) and (b) are deduced using the same proof technique, based on linear programming.

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1. Introduction

In this paper we are concerned with finite graphs without loops, multiple or directed edges. Let G be such a graph. Denote by uv the edge of G, connecting the vertices u and v. Denote by δ_v the degree of the vertex v. Then the *connectivity index*, also called *Randić index* or *Randić weight* or *branching index*, of the graph G is defined as

$$\chi = \chi(G) = \sum_{uv} \frac{1}{\sqrt{\delta_u \, \delta_v}} \tag{1}$$

with the summation going over all edges of G. (In the case when G possesses no edges, $\chi(G) = 0$). The graph invariant χ was first considered by Randić in 1975 [1].

Bollobás and Erdős [2] obtained the following result.

Theorem 1. *Among graphs with a fixed number of vertices, and without isolated vertices, the star has minimal connectivity index.*

Fajtlowicz [3, 4] characterized the graphs with maximal χ-values as follows:

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Theorem 2. *Among graphs with a fixed number of vertices, the graphs in which all components are regular of non–zero degree have maximal (mutually equal) connectivity indices.*

In what follows we deduce both Theorems 1 and 2 by means of essentially the same proof technique, based on linear programming, which is completely different from what has been used in the works of Bollobás–Erdős [2] and Fajtlowicz [4].

2. Preliminaries

Consider a graph G on n vertices, $n \geq 2$. The maximum possible vertex degree in such a graph is $n-1$. Denote by x_{ij} the number of edges of G connecting vertices of degree i and j. Clearly, $x_{ij} = x_{ji}$. Then Eq. (1) can be written as

$$\chi(G) = \sum_{1 \leq i \leq j \leq n-1} \frac{x_{ij}}{\sqrt{i\,j}} \ . \tag{2}$$

Directly from the definition of the connectivity index we conclude:

Lemma 1. *If the graph G consists of components $G_1, G_2, \ldots, G_p$, then $\chi(G) = \chi(G_1) + \chi(G_2) + \cdots + \chi(G_p)$.*

The star on n vertices has $n-1$ edges and each of its edges connects a vertex of degree one with a vertex of degree $n-1$. Therefore, in this case, $x_{ij} = 0$ for all choices of i, j, $1 \leq i \leq j \leq n-1$, except for $i = 1$, $j = n-1$ when $x_{1,n-1} = n-1$.

Lemma 2. *If S_n is the star on n vertices, then $\chi(S_n) = \sqrt{n-1}$.*

A regular graph on n vertices, having degree r, possesses $n\,r/2$ edges. Each edge of such a graph contributes by $1/r$ to the right–hand–side summation in Eq. (1).

Lemma 3. *If G is a regular graph of degree r, $r > 0$, then $\chi(G) = n/2$.*

Combining Lemmas 1 and 3 we obtain

Lemma 4. *If G is a graph on n vertices, all components of which are regular graphs of non-zero degree (not necessarily mutually equal), then $\chi(G) = n/2$.*

3. Proof of Theorem 1

Let G be a graph on n vertices, $n \geq 2$, possessing no isolated vertices. Denote by n_i the number of its vertices, having degree i. Then, $n_0 = 0$ and

$$n_1 + n_2 + \cdots + n_{n-1} = n \ . \tag{3}$$

Counting the edges incident to vertices of degree i we arrive at the identity

$$\sum_{j=1}^{n-1} x_{ij} + x_{ii} = i\, n_i \tag{4}$$

which holds for $i = 1, 2, \ldots, n-1$.

There is only one 2-vertex graph without isolated vertices and therefore Theorem 1 holds, in a trivial manner, for $n = 2$. By direct checking we see that Theorem 1 holds also for $n = 3$. In what follows we thus may assume that $n \geq 4$.

For n having a fixed and given value, the relations (3) & $\{(4)\,,\, i = 1, 2, \ldots, n-1\}$ can be viewed as a system of n linear equations in the unknowns n_i an x_{ij}, $i, j = 1, 2, \ldots, n-1$. Clearly, all these equations are linearly independent.

For the present proof it is purposeful to solve the system (3) & $\{(4)\,,\, i = 1, 2, \ldots,$
$n-1\}$ in the unknowns $n_1, n_2, \ldots, n_{n-1}, x_{1,n-1}$. This is immediate: For $i = 2, \ldots, n-2$ each n_i is directly expressed from Eq. (4):

$$n_i = \frac{1}{i} \left(\sum_{j=1}^{n-1} x_{ij} + x_{ii} \right) \ . \tag{5}$$

What remains is to solve a system of three linear equations in the unknowns n_1, n_{n-1} and $x_{1,n-1}$, viz.,

$$n_1 - x_{1,n-1} = \sum_{j=1}^{n-2} x_{1j} + x_{11}$$

$$(n-1)\, n_{n-1} - x_{1,n-1} = \sum_{j=2}^{n-1} x_{j,n-1} + x_{n-1,n-1}$$

$$n_1 + n_{n-1} = n - \sum_{i=2}^{n-2} \frac{1}{i} \left(\sum_{j=1}^{n-1} x_{ji} + x_{ii} \right) \ .$$

Direct calculation yields:

$$x_{1,n-1} = n - 1 - \sum{}^{\star}\ \frac{n-1}{n} \left(\frac{1}{i} + \frac{1}{j} \right) x_{ij} \tag{6}$$

as well as analogous expressions for n_1 and n_{n-1}. In formula (6), $\sum^{\star}$ indicates summation over all i and j satisfying $1 \leq i \leq j \leq n-1$, except $i = 1$, $j = n-1$.

By substituting Eq. (6) back into Eq. (2) we readily arrive at:

$$\chi(G) = \sqrt{n-1} + \sum{}^{\star}\ \left[\frac{1}{\sqrt{i\,j}} - \frac{\sqrt{n-1}}{n} \left(\frac{1}{i} + \frac{1}{j} \right) \right] x_{ij}$$

which can also be written as

$$\chi(G) = \sqrt{n-1} + \sum_{1 \le i \le j \le n-1} \left[\frac{1}{\sqrt{i\,j}} - \frac{\sqrt{n-1}}{n} \left(\frac{1}{i} + \frac{1}{j} \right) \right] x_{ij} \tag{7}$$

because the term

$$\frac{1}{\sqrt{i\,j}} - \frac{\sqrt{n-1}}{n} \left(\frac{1}{i} + \frac{1}{j} \right) \tag{8}$$

is equal to zero for $i = 1$, $j = n-1$.

It is an elementary task to show that for all $1 \le i \le j \le n-1$, except for $i = 1$, $j = n-1$, the expression (8) is positive–valued. On the other hand, the quantities x_{ij} are necessarily non-negative. Consequently, the right–hand side of Eq. (7) will attain its minimal possible value if $x_{ij} = 0$ for all $1 \le i \le j \le n-1$, except for $i = 1$, $j = n-1$. This minimal value is $\sqrt{n-1}$, which is just the connectivity index of the n-vertex star (cf. Lemma 2). Among n-vertex graphs without isolated vertices, the conditions $x_{ij} = 0$ for all $1 \le i \le j \le n-1$, except for $i = 1$, $j = n-1$, are obeyed by the n-vertex star and only by it.

This completes the proof of Theorem 1.

We mention in passing that among all n-vertex graphs, the graph without edges has minimal value ($\chi = 0$) of the connectivity index. The second–minimal value ($\chi = 1$) of this index has the graph with just one edge. Etc.

4. Proof of Theorem 2

Theorem 2 can be deduced by means of a fully analogous argument. Again, by direct checking we confirm that Theorem 2 holds for $n = 2$ and $n = 3$ and assume that $n \ge 4$. Initially we consider n-vertex graphs without isolated vertices.

This time we solve the system (3) & $\{(4)\,,\, i = 1, 2, \ldots, n-1\}$ in the unknowns $n_1, n_2, \ldots, n_{n-1}$, $x_{n-1,n-1}$. The task is even simpler than what we had in the preceding section: First, expressions of the form (5) hold for $i = 1, 2, \ldots, n-2$. Second, n_{n-1} is calculated by combining Eqs. (3) and (4):

$$n_{n-1} = n - \sum_{i=1}^{n-2} \frac{1}{i} \left(\sum_{j=1}^{n-1} x_{ij} + x_{ii} \right) .$$

Finally, $x_{n-1,n-1}$ is obtained from Eq. (4) for $i = n-1$:

$$\sum_{j=1}^{n-2} x_{n-1,j} + 2\, x_{n-1,n-1} = (n-1)\, n_{n-1}$$

i. e.,

$$(9)\quad x_{n-1,n-1} = \frac{1}{2}(n-1)\left[n - \sum_{i=1}^{n-2}\frac{1}{i}\left(\sum_{j=1}^{n-1} x_{ij} + x_{ii}\right)\right] - \frac{1}{2}\left[\sum_{j=1}^{n-2} x_{n-1,j}\right] .$$

Substituting Eq. (9) into Eq. (2), and performing pertinent transformations we obtain

$$(10)\qquad \chi(G) = \frac{n}{2} + \sum_{1\le i<j\le n-1}\left[\frac{1}{\sqrt{i\,j}} - \frac{1}{2}\left(\frac{1}{i}+\frac{1}{j}\right)\right] x_{ij} .$$

It is easy to see that

$$\frac{1}{\sqrt{i\,j}} - \frac{1}{2}\left(\frac{1}{i}+\frac{1}{j}\right)$$

is negative–valued for $i \neq j$. Consequently, the right–hand side of Eq. (10) will be maximal if, and only if, $x_{ij} = 0$ for all i, j , such that $1 \le i < j \le n-1$. The respective, maximal, value of the connectivity index is $n/2$ (cf. Lemma 4).

The above result can be formulated also as follows: The connectivity index of a graph G without isolated vertices is maximal if, and only if, G does not possess edges connecting vertices of different degrees.

On the other hand, the parameters $x_{11}, x_{22}, \ldots, x_{n-1,n-1}$ do not occur on the right–hand side of Eq. (10), which means that these may assume arbitrary values. In other words, the connectivity index of an n-vertex graph without isolated vertices is maximal if, and only if, all its edges connect vertices of equal degrees. This, in turn, implies that each component of the respective graph is regular of non–zero degree.

We thus proved that the connectivity index of any n-vertex graph without isolated vertices is less than or equal to $n/2$, and characterized the graphs for which this index is equal to $n/2$.

Let the n-vertex graph G' possess p isolated vertices, $p > 0$. Let G'' be the $(n-p)$-vertex graph obtained from G' by deleting its isolated vertices. Then G'' is a graph without isolated vertices and its connectivity index does not exceed $(n-p)/2$, which is less than $n/2$. By Lemma 1 the graphs G' and G'' have equal connectivity indices. Consequently, the connectivity index of any n-vertex graph does not exceed $n/2$.

This completes the proof of Theorem 2.

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