LE MATEMATICHE
Vol. LIX (2004) – Fasc. I–II, pp. 349–365

CONNECTED GRAPHS OF FIXED ORDER AND SIZE WITH MAXIMAL INDEX: STRUCTURAL CONSIDERATIONS

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The largest eigenvalue, or index, of simple graphs is extensively studied in literature. Usually, the authors consider the graphs from some fixed class and identify within it those graphs with maximal (or minimal) index. So far maximal graphs with fixed order, or with fixed size, are identified, but not maximal connected graphs with fixed order and size. In this paper we add some new observations related to the structure of the latter graphs.

1. Introduction.

We consider only *simple graphs*, i.e. finite, undirected graphs without loops or multiple edges. The *spectrum* of a graph G is the spectrum of its (0, 1)-adjacency matrix. As is well known (see, for example, [5]) the spectrum of G is a collection of its real invariants. The largest eigenvalue, to be denoted by $\lambda(G)$, is also called the *index* (or *spectral radius*) of G. If G is connected then $\lambda(G)$ is of multiplicity one. The corresponding eigenvector (as it follows from the theory of non-negative irreducible matrices, see also [5]) can be assumed to be positive; it is also called the *Perron eigenvector of G*.

Following [6] we will take that $\mathcal{G}(\nu, \varepsilon)$ denotes the set of all graphs of order ν and size ε, while $\mathcal{H}(\nu, \varepsilon)$ is its subset consisting of connected graphs.

2000 *Mathematical Subject Classification*: 05C50
Key words and phrases: graph spectrum, largest eigenvalue, spectral radius, graph index, nested split graphs

(In addition, see Section 2, $\mathcal{S}(\nu, \varepsilon)$ will stand for those which are nested split graphs). In the set of graphs with fixed order, or fixed size, *maximal graphs* (i.e. graphs with maximum index) are identified. For the order ν, this is K_ν (see, for example, [5]). For the size ε the corresponding graph is formed from a single clique of maximal allowed size and a single vertex adjacent to at least one (possibly all) vertices of the clique: more precisely, if $\varepsilon = \binom{q-1}{2} + r$, where $1 \leq r \leq q - 1$, then the clique order is $q - 1$ and the single vertex is adjacent to r vertices from the clique. This graph will be denoted by $P(\varepsilon)$ (note, it is connected). The corresponding problem was open for many years. The structure of maximal graphs had been for the first time described by R. A. Brualdi and A. J. Hoffman, but the complete solution to the problem was provided later, by P. Rowlinson (see [9]). Thus, if we ask for a graph in $\mathcal{G}(\nu, \varepsilon)$ with maximal index, then the corresponding graph consists of one copy of $P(\varepsilon)$ and $n - q$ of isolated vertices.

The problem of finding maximal graphs in $\mathcal{H}(\nu, \varepsilon)$ has not been solved yet (in general).

To mention some known results from literature, we next define two types of graphs of order ν and size $\nu + \kappa$, to be denoted by $B(\nu, \kappa)$ and $S(\nu, \kappa)$ (here, we assume that $\kappa \geq 0$; for $\kappa = -1$, i.e. for trees, the maximal graphs are stars - see, for example, [5]). Let d be the largest integer such that $\binom{d-1}{2} \leq \kappa + 1$. Then we can write (uniquely) that $\binom{d-1}{2} + r = \kappa + 1$, where $0 \leq r \leq d - 2$. If $r = 0$ (then $3 \leq d \leq \nu$), $B(\nu, \kappa)$ is obtained from a complete graph K_d by adding $\nu - d$ pendant edges at one of its vertices - this graph will be also denoted by $F(\nu, d)$; otherwise, if $r > 0$ (then $3 \leq d \leq \nu - 1$), $B(\nu, \kappa)$ is obtained from $F(\nu, d)$ by joining one vertex of degree 1 to r vertices of degree $d - 1$. Note, if $d \leq 2$ then $F(\nu, 1) = F(\nu, 2) = K_{1,\nu-1}$ and then $\kappa < 0$; for $d > 2$, it is noteworthy that the subgraph obtained by deleting the vertex of maximal degree from $B(\nu, \kappa)$ coincides (up to isolated vertices) with $P(\kappa+1)$. $S(\nu, \kappa)$ is defined only for $\kappa \leq \nu - 3$. It is the graph obtained from the star $K_{1,\nu-1}$ by joining one vertex of degree 1 to $\kappa + 1$ other vertices of degree 1. Note that $B(\nu, \kappa)$ and $S(\nu, \kappa)$ coincide if and only if $\kappa = 0$ or 1.

Consider now the graphs from $\mathcal{H}(\nu, \varepsilon)$. Then the maximal graphs in several cases, depending on ε, are identified. For example, if $\binom{\nu-1}{2} < \varepsilon \leq \binom{\nu}{2}$ then $P(\varepsilon)$ is maximal (follows from the result of P. Rowlinson since all graphs in question are now connected). In what follows we will put, as in [6], that $\varepsilon = \nu + \kappa$. Due to R. A. Brualdi and E. S. Solheid (see [4]), the problem is completely solved for some small values of κ, i.e. for $\kappa \leq 2$. For $\kappa \leq 1$, $B(\nu, \kappa)$ ($= S(\nu, \kappa)$) is maximal; for $\kappa = 2$, only $B(\nu, \kappa)$ is maximal. In the same paper, it was shown that for $3 \leq \kappa \leq 5$ the maximal graph is not of the prescribed form. Namely, for small values of ν, $B(\nu, \kappa)$ is maximal, while, for large values of ν, $S(\nu, \kappa)$ is maximal. These results were extended by D. Cvetković and P. Rowlinson in [6]. Their result is asymptotic. Namely, for any fixed $\kappa \geq 6$, and for all sufficiently large values of ν, only $S(\nu, \kappa)$ is maximal. Finally, it was proved by F. K. Bell (see [1]) that for $\kappa = \binom{d-1}{2} - 1$ (and ν arbitrary), that $F(\nu, d)$ is maximal for $\nu \leq g$; $S(\nu, \kappa)$ is maximal for $\nu > g$ (see Section 4 for the meaning of g). Based on these results, many questions were posed by F. K. Bell in the mentioned paper. Some further results of F.K. Bell are mentioned in Section 4.

In Section 2 we give some preparatory results (including new ones), and introduce the type of graphs to be considered (also called, by P. Hansen, nested split graphs, or NSGs for short). In Section 3 we investigate various modifications of NSGs which keep them within the same class. In Section 4 we add some general comments, while Section 5 is an appendix containing the tree-like representations of the graphs $P(\varepsilon)$, $B(\nu, \kappa)$ and $S(\nu, \kappa)$.

2. Preliminaries.

We first consider some results belonging to graph perturbations (see, for example, [8], Chapter 6). Of course, we are mainly interested to see how the index of a graph is changed under the relocation of its edges.

Let e be an edge of a graph G. Assume first that $e = rs$, and that r is not adjacent to t. A *relocation of type* $\mathcal{R}_1$ (in fact, a rotation around r) consists of a deletion of the edge e followed by an addition of the edge $e' = rt$. Next, assume that $e = st$, and that two vertices, say u and v ($\{u, v\} \cap \{s, t\} = \emptyset$), are not adjacent. A *relocation of type* $\mathcal{R}_2$ consists of a deletion of the edge e followed by an addition of the edge $e' = uv$.

The basic argument to be used in the next proof, is the following description of the largest eigenvalue of any hermitian matrix. In particular, let here A be the adjacency matrix of a graph G. Then, as well known (see, for example, [8]), we have

$$\lambda(G) = \sup_{||x||=1} \mathbf{x}^T A \mathbf{x}. \tag{1}$$

The following lemma now easily follows.

Lemma 2.1. *Let G' be a graph obtained from a connected graph G (of order ν) by one of the relocations as above. Let $\mathbf{x} = (x_1, x_2, \ldots, x_\nu)^T$ be the Perron eigenvector of G. Then we have:*

(i) if $x_t \geq x_s$ then $\lambda(G') > \lambda(G)$ (for $\mathcal{R}_1$);
(ii) if $x_u x_v \geq x_s x_t$ then $\lambda(G') > \lambda(G)$ (for $\mathcal{R}_2$).

Proof. Consider only (i) (the proof of (ii) is almost the same and will be omitted here because this result is not needed later on). Without loss of generality, assume that $||x|| = 1$. Then we have:

$$\lambda(G') - \lambda(G) = \sup_{||\mathbf{y}||=1} \mathbf{y}^T A'\mathbf{y} - \mathbf{x}^T A\mathbf{x} \geq \mathbf{x}^T A'\mathbf{x} - \mathbf{x}^T A\mathbf{x} = \mathbf{x}^T(A' - A)\mathbf{x} = \Delta.$$

Further, we easily get $\Delta = 2x_r(x_t - x_s)$. So, $\lambda(G') \geq \lambda(G)$. The equality holds if and only if $\Delta = 0$ and $\mathbf{x}$ is an eigenvector of G'. But then we easily get that the eigenvalue equation does not hold (in G') for the vertices s and t, and the proof follows. $\square$

In what follows we will give a new characterization of graphs whose index is maximal within the graphs of fixed size (but not necessarily order).

Theorem 2.2. *Let G be a graph of a fixed size, and assume that its index is maximal. Then G does not contain, as induced subgraph, any of the graphs: $2K_2$, P_4 and C_4.*

Proof. Let H be an induced subgraph of G, equal to one of the graphs supposed to be forbidden. Let v be a vertex of H whose weight (with respect to $\mathbf{x}$) is minimal. Let u be a vertex of H adjacent to v, while w a vertex of H non-adjacent to u. So we have that u is adjacent to v, but non-adjacent to w, and in addition that $\mathbf{x}(v) \leq \mathbf{x}(w)$. It is a matter of routine to check that such triplet of vertices always exists in H (provided H is one of the graphs in question). But then (see Lemma 2.1(i)) we can rotate the edge uv around u to the non-edge uw to get a graph (say G'), with a greater index, a contradiction. $\square$

The above result deserves some comments.

Firstly, the graphs having no $2K_2$, nor P_4 as induced subgraphs were already studied in literature (see, for example, [2], [13]). In the spectral graph theory, they already appear in the context of the second largest eigenvalue. Graphs for which the second largest eigenvalue is too small (actually, less than the golden section, i.e. $\frac{\sqrt{5}-1}{2}$, or some smaller numbers) were investigated to some extent. In [10], these graphs are represented by the so called expression trees (see below). In [11] all graphs having together with their complements the second largest eigenvalue less than golden section were found. These graphs belong to the class of graphs for which C_4, in addition to $2K_2$ and P_4, is forbidden.

Secondly, graphs with maximal index from Theorem 2.2 are not necessarily connected. They can have one non-trivial component and certain number of isolated vertices (note, just $2K_2$ is forbidden). The question we can now pose is what happens if we require that a graph G (from Theorem 2.2) is connected. Then we need some additional considerations.

Theorem 2.2'. *Let G be a connected graph of a fixed order and size, and maximal index. Then G does not contain, as an induced subgraph, any of the graphs: $2K_2$, P_4 and C_4.*

Proof. We will follow the previous proof. If G', as defined there, is connected we are done. Assume now that G' is disconnected. If so, uv must be a bridge in G, and then $G - uv$ consists of two components, say G_1 and G_2, such that, say u and w are in G_1, and v is in G_2. Since G has a maximal index, $\mathbf{x}(u) > \mathbf{x}(s)$ for any $s \in V(G_1)$ other than u. (Notice, otherwise we can rotate the edge vu around v to the non-edge vs to get a graph with a greater index). Consider now a vertex t, adjacent to w, belonging to a (say, the shortest) path between u and w. Then we can rotate the edge wt around w to the non-edge wu to get a connected graph with a greater index, a contradiction. □

We now introduce some notation and necessary results from [10] in order to keep the paper more self-contained.

A *rooted tree* T is the tree with one vertex, say r (also called the *root*), distinguished. In describing some relations between the vertices of a rooted tree, we shall use (besides the usual terminology) the terminology of family trees. Thus all vertices of T are the *descendants* of the root r, while r is their *ancestor*. We can also imagine that the edges of a tree are oriented from the root to its descendants. If f is joined with s by an (oriented) edge, then s is regarded as a *son* of f (while f is the father of s). The vertices without sons are called *leaves*; other vertices, except the root, are called *internal vertices*. Two vertices of a tree are called *incomparable* if they are not connected by an oriented path. The *height* of a tree T, also denoted by $h(= h(T))$, is the maximal distance between the root and the leaves.

Weighted rooted trees (with weights assigned to vertices) were used in [10] in representing graphs from the class, called $\mathcal{C}$, which is defined as follows:

(i) $\emptyset \in \mathcal{C}$ ($\emptyset$ being an empty graph);
(ii) if $G \in \mathcal{C}$, then $G \cup K_1 \in \mathcal{C}$;
(iii) if $G_1, G_2 \in \mathcal{C}$, then $G_1 \nabla G_2 \in \mathcal{C}$

Of course, these rules can be repeated only finitely many times.

Here ∇ denotes the join of two graphs, while $\cup$ refers to union of two disjoint graphs. Notice that $G_1 \nabla G_2 = \overline{\overline{G_1} \cup \overline{G_2}}$, and also that these two (graph) operations are associative.

Remark. An alternative way to describe graphs from the class $\mathcal{C}$ is in terms of minimal forbidden induced subgraphs. Actually, $\mathcal{C}$ is a class of graphs having no induced subgraphs equal to $2K_2$ or P_4.

To any graph G from $\mathcal{C}$ we may associate a weighted rooted tree T_G (also called an *expression tree* of G) in the following way:

> if $H = (H_1 \nabla H_2 \nabla \cdots \nabla H_m) \cup nK_1$ is any subexpression of a graph G (i.e. a graph obtained by using the above rules), then a subtree T_H with a root v corresponds to H; $n(= w(v))$ is a weight of v, whereas for each i $(i = 1, 2, \dots, m)$ there is a vertex v_i (a son of v) representing a root of H_i.

Conversely, given a tree T_G, we get G by assigning to each vertex of T_G, say v, a co-clique of order $w(v)$; vertices from two co-cliques are adjacent if and only if these co-cliques originated from the incomparable vertices of T_G.

Remark. It is also worth mentioning (see [10], Lemma 3.4) that this representation may be turned into a canonical one. Then all vertices except possibly the root have non-zero weights, and each father has at least two sons. If so, then any canonical representation determines the graph up to isomorphism. The corresponding tree is called the *canonical expression tree*.

To fix some new ideas, consider a graph G from $\mathcal{C}$ defined as follows:

$$G = ((((2K_1 \nabla (K_1 \nabla K_1)) \cup K_1)) \nabla (K_1 \nabla K_1 \nabla K_1)) \cup 2K_1$$

Clearly, G can be represented (in a more compressed form) as follows:

$$G = ((((2K_1 \nabla K_2) \cup K_1)) \nabla K_3) \cup 2K_1.$$

In Fig. 1(a) G is represented by its canonical expression tree; in Fig. 1(b) this tree is turned to a compressed form (namely, some vertices of the tree are joined together). More generally, we can now say that white vertices (as earlier) correspond in G to co-cliques, while black vertices (after the compression) correspond in G to cliques - in both cases, their weights determine the orders of co-cliques, or cliques. The main idea used here is to represent "brothers" which are leaves of weight one by a common vertex. We will also say that this compressed tree is a *coloured expression tree*, or CET for short. It is assumed to be a canonical one, if it cannot be simplified (in the same sense as uncoloured ones).

We will now use the fact (see Theorems 2.2 and 2.2') that C_4 is forbidden in any graph G with maximal index. This fact is reflected in the T_G as follows: if two vertices of such a tree are incomparable, then at least one must be a leaf, and at least one must be of weight one (otherwise, in both situations, C_4 appears). Thus, we can easily conclude that each father has at most one son whose weight

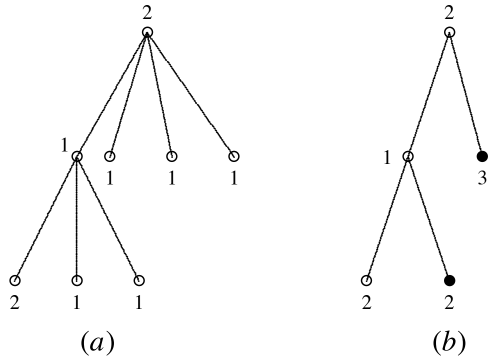


Fig. 1: Representations of the graph G.

is greater than one, and that all other sons are the leaves of weight one. So if we start from the root, and use this argument, then the compressed form of our tree gets the following structure: all white vertices can be put into chain-like patten, and each of them has a pendant edge whose other end is a black vertex (see Fig. 2(b)), which will be also a model for drawing the (canonical) CETs in the situations when three graphs from Theorem 2.2 (or 2.2') are forbidden.

It can be also easily verified that any graph which can be represented by a CET of the later form, does not contain as an induced subgraph, besides $2K_2$ and P_4, C_4 as well. So we can say that any graph with maximal index (with a fixed order and size, connected or disconnected) can be represented (uniquely) by its canonical CET.

We can now summarize the above considerations as follows: Graphs in $\mathcal{G}(\nu, \varepsilon)$ (disconnected or connected) with maximal index can be characterized by minimal forbidden subgraphs as in Theorems 2.2 and 2.2'. They can be represented by the canonical CETs as above. Therefrom, their structure is completely determined. If isolated vertices are ignored, they are generally split graphs, and due to some further structural properties (implied from their tree-like representation) they will be called *nested split graphs*.

Remark. The above characterization is equivalent to the characterization (in terms of the adjacency matrix) given by R. A. Brualdi and A. J. Hoffman (see [3]). Namely, the graphs in question admit the labelling (of vertices) in which their adjacency matrix takes the *stepwise form*. We recall here that a (0, 1) symmetric matrix $A = (a_{ij})$ (with zeroes at the main diagonal) is in the stepwise form if it satisfies the condition:

$(*)$ if $i < j$ and $a_{ij} = 1$ then $a_{st} = 1$ whenever $s < t \leq j$ and $s \leq i$.

We now introduce some parameters of the NSGs. Firstly, any NSG, say G, is completely determined by the following $2h$ parameters

$$(m_1, \ldots, m_h; n_1, \ldots, n_h),$$

in fact, the vertex weights in the canonical CET; see also Fig. 2(b).

Note, if some of these parameters are equal to zero, we can then turn that tree into the canonical one to get the "canonical" parameters. Here, in fact, m_i is the order of i-th co-clique (whose vertex set will be denoted by U_i), while n_j is the order of j-th clique (whose vertex set will be denoted by V_j) (see also Fig. 2(a)).

We next put

$$M_s = \sum_{i=1}^{s} m_i,\, N_t = \sum_{j=1}^{t} n_j \quad (1 \le s, t \le h)$$

So, the corresponding graph G is of order $\nu = M_h + N_h$, and size $\varepsilon = \sum_{k=1}^{h} m_k N_k + \binom{N_h}{2}$.

In Fig. 2 an NSG and its expression tree are depicted. The white circles correspond to co-cliques, while the black ones to cliques (their vertex sets are indicated); here, the line between any two circles means that any two vertices belonging to corresponding circles are mutually adjacent.

In Section 5 (see Figs. 5–7) one can find the representations of the graphs $P(\epsilon)$, $B(\nu, \kappa)$ and $S(\nu, \kappa)$ defined in Section 1.

Remark. We will now mention a result of P. Rowlinson (see [9]) which gives an additional condition for graphs with a fixed number of edges to be maximal. This condition, provided (*) is satisfied, reads:

(**) If
(i) $g < p < q < k$, and
(ii) $a_{gk} = 1$, $a_{gj} = 0$ whenever $j > k$, $a_{ik} = 0$ whenever $i > g$, and
(iii) $a_{pq} = 0$, $a_{pj} = 1$ whenever $p < j < q$, $a_{iq} = 1$ whenever $i < p$,
then $p + q \le g + k + 1$.

It is based on relocation $\mathcal{R}_2$ (actually, the edge $e = gk$ is relocated to the position of the non-edge $f = pq$). In proving (**) an elegant rearrangement of eigenvector components is used in getting the inequality required in Theorem 2.1(ii) (see [9] for more details). Here we will give an equivalent form of (**), based on the parameters introduced for the NSGs.

If $1 \le s < t \le h - 1$ then $M_t - M_{s-1} \ge N_t - N_s + 1$; in addition, if $t = h$ and $m_h \ge 2$ then $M_t - M_{s-1} \ge N_t - N_s + 2$.

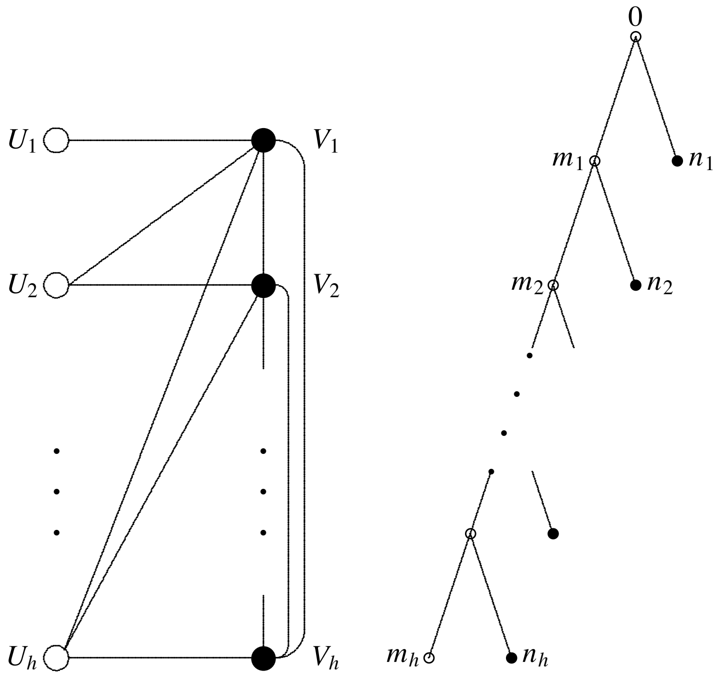


Fig. 2: An NSG and its representation.

3. Modifications of NSGs.

We will now focus our attention on some modifications of NSGs which keep them within the same class. Notice first that any induced subgraph of an NSG, is (again) an NSG. For spanning subgraphs, this is not true (in general). Actually, a deletion (or an addition) of an edge can give a graph which is not an NSG. In the next two theorems we will give criteria under which, for a given nested split graph G and an edge e, the graphs $G \pm e$ are (or are not) NSGs.

For this aim, we assume in what follows that $e = pq$, and that s and t are another two vertices (if any) such that H, the subgraph (of G) induced by these four vertices, is equal (in $G \pm e$) to one of the graphs: $2K_2$, P_4 and C_4.

Theorem 3.1. *Let G be an NSG, and let $e = pq$ be its edge. Then $G - e$ is an NSG if and only if (a) $p \in U_i$, $q \in V_i$ for some $i (1 \leq i \leq h)$, or (b) $p, q \in V_h$ provided $|U_h| = 1$.*

Proof. Firstly, we have that either $p \in U_i$, $q \in V_j$ (with $i \geq j$), or $p \in V_i$, $q \in V_j$. We now assume that $p \in U_i$, $q \in V_j$, where $i > j$. Take then that $s \in V_i$,

$t \in U_j$. If so, $H - e = P_4$, and $G - e$ is not an NSG. Assume next that $p \in V_i$, $q \in V_j$. If $i \neq j$, take that $s \in U_i$, $t \in U_j$. But then $H - e = P_4$, and $G - e$ is not an NSG. If $i = j < h$ (or $i = j = h$ and $|U_h| > 1$), take that $s \in U_i$, $t \in U_h$ (resp. $s, t \in U_h$). Then $H - e = C_4$, and $G - e$ is not an NSG.

Consider now the converse. Then we have to prove that P_4 and C_4 cannot appear in $G - e$ (this is obvious for $2K_2$; otherwise, G contains P_4). Assume now to the contrary, i.e. that $H - e = P_4$ or C_4.

Suppose first that (a) holds. Let s be a vertex adjacent (in H) to p and q (such a vertex must exist, if $H - e$ is as taken above). Then $s \in V_k$ for some $k \leq i$. Since t is non-adjacent (in H) to s, $t \in U_l$ for some $l < k$. But then t is an isolated vertex of H, a contradiction. Suppose next that (b) holds. Then we can take the single vertex from U_h and, say p, from V_h and exchange their positions within these sets. If this is done, then this case is reduced to the former one. Thus, none of the forbidden subgraphs appears in $G - e$. This completes the proof. □

Remark. From the above proof, we see that (b) is a special case of (a) that appears if $U_h = \{p\}$; call it (b'). Further, it is noteworthy that M_h and N_h do not change if (a) but not (b') holds; if (b) or (b') holds then M_h is increased by one, while N_h is decreased by one.

Remark. In Fig. 3 we show how some details in the CETs are changed in a more general case, namely if more than one edge is deleted. Extending the case (a) of Theorem 3.1, we delete kl edges which join k vertices from U_i to l vertices in V_i (for some $1 \leq i \leq h$). Note, if h' is the height of a new tree, then it is equal to $h + 1$ if $m_i - k$ and $n_i - l$ are non-zero, or to h if either $m_i - k$ or $n_i - l$ is equal to zero, or to $h - 1$ if both $m_i - k$ and $n_i - l$ are zero (in the latter two situations the obtained trees are not canonical; see Fig. 3(a) for more details). The case (b) can be extended as well. If $|U_h| = 1$, we can delete (in G) a complete graph K_k from the clique induced by the vertex set V_h. Note, if h' is the height of a new tree, then it is equal to h if $n_h - k + 1$ is non-zero, or to $h - 1$ if $n_h - k + 1$ is zero (in the latter case the obtained tree is not canonical; see Fig. 3(b) for more details). The procedure to make such trees canonical will be explained in one of the remarks that follow. Finally, it is also possible to combine (a) and (b) (with $m_h = 1$) and to delete K_{n_h+1} from the last level to get a CET of some NSG. More generally, we can also delete all edges from the h-th level (or, to repeat this in turns).

Theorem 3.2. *Let G be an NSG, and let $e = pq$ be its non-edge. Then $G + e$ is an NSG if and only if (a) $p \in U_i$, $q \in V_{i+1}$ for some $i (1 \leq i \leq h - 1)$, or (b) $p \in U_{h-1}$, $q \in U_h$ provided $|U_h| = 1$, or (c) $p, q \in U_h$.*

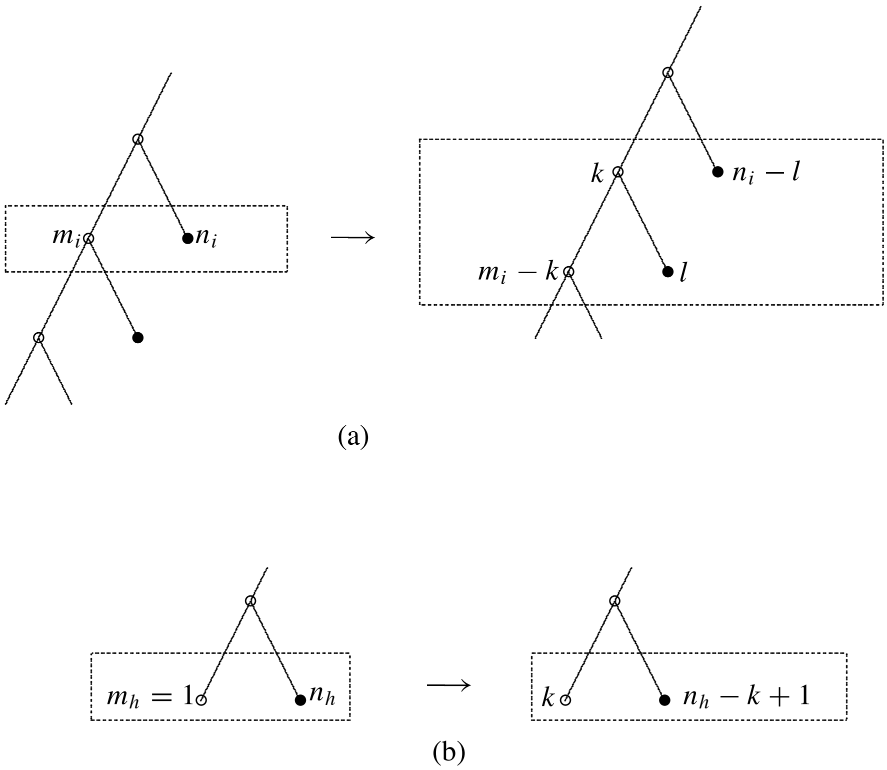


Fig. 3: A change in a CET (if edges are deleted).

Proof. Firstly, we have that either $p \in U_i$, $q \in V_j$ (with $j \geq i + 1$), or $p \in U_i$, $q \in U_j$. We now assume that $p \in U_i$, $q \in V_j$, where $j > i + 1$. Take then that $s \in U_{i+1}$, $t \in V_{i+1}$. If so, $H + e = P_4$, and $G + e$ is not an NSG. Assume next that $p \in U_i$, $q \in U_j$. If $i, j \leq h - 1$, take that $s \in U_h$, $t \in V_h$. But then $H + e = 2K_2$, and $G + e$ is not an NSG. If, say $i \leq h - 1$, $j = h$ and $|U_h| > 1$, take that $s \in U_h$, $t \in V_h$. But then $H + e = P_4$, and $G + e$ is not an NSG. If $i \leq h - 2$, $j = h$ and $|U_h| = 1$, take that $s \in U_{h-1}$, $t \in V_{h-1}$. But then $H + e = P_4$, and $G + e$ is not an NSG.

Consider now the converse. Then we have to prove that $2K_2$ and P_4 cannot appear in $G + e$ (this is obvious for C_4; otherwise, G contains P_4). Assume now to the contrary, i.e. that $H + e = 2K_2$ or P_4.

Suppose first that (a) holds. Let s be a vertex non-adjacent (in H) to p and q (such a vertex must exit, if $H + e$ is as taken above). Then $s \in U_k$ for some $k \leq i$. Since t is adjacent (in H) to s, $t \in V_l$ for some $l \leq k$. But then t is adjacent to all vertices of H, a contradiction. Suppose next that (b) holds. But then we can take q (from U_h) and any vertex from V_h, and exchange their positions within these sets. If this is done, then this case is reduced to the former one. Finally, suppose that (c) holds. Let again, as above, s be a vertex non-adjacent (in H) to p and q. Then $s \in U_k$ for some k. Since t is adjacent (in H) to s, $t \in V_l$ for some $l \leq k$. But then t is adjacent to all vertices of H, a contradiction. Thus, none of the forbidden subgraphs appears in $G + e$. This completes the proof. $\square$

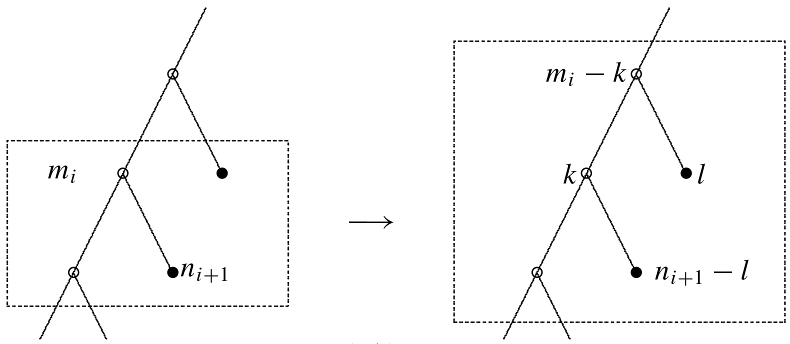
Remark. From the proof, we see that (b), as in Theorem 3.1, is a special case of (a) that appears if $U_h = \{p\}$; call it again (b'). Further, it is noteworthy that M_h and N_h do not change if (a) but not (b') holds; if (b) or (b') holds then M_h is increased by one, while N_h is decreased by one. Finally, if (c) holds, then M_h is decreased by one, while N_h is increased by one.

Remark. In Fig. 4 we show how some details in the CETs are changed in a more general case, namely if more than one edge is added. Extending the case (a) of Theorem 3.2, we add kl edges which join k vertices from U_i to l vertices in V_{i+1} (for some $1 \leq i \leq h-1$) Note, if h' is the height of a new tree, then it is equal to $h+1$ if $m_i - k$ and $n_{i+1} - l$ are non-zero, or to h if either $m_i - k$ or $n_{i+1} - l$ is equal to zero, or to $h-1$ if both $m_i - k$ and $n_{i+1} - l$ are zero (in the latter two situations the obtained trees are not canonical; see Fig. 4(a,b) for more details). Note, the case (b) can be extended as well, but it can be considered as a special case of (a) (with $q \in V_h$ and $l = 1$). We will now consider (c). It can be extended by adding edges between vertices of U_h so that they induce an arbitrary NSG. If, in particular, they induce K_k, we then get the easiest situation. If so, and if h' is the height of a new tree, then it is equal to $h+1$ if $m_h - k$ is non-zero, or to h if $m_i - k$ is equal to zero (in the latter situation the obtained tree is not canonical; see Fig. 4(c) for more details). The procedure to make such trees canonical is explained in the next remark.

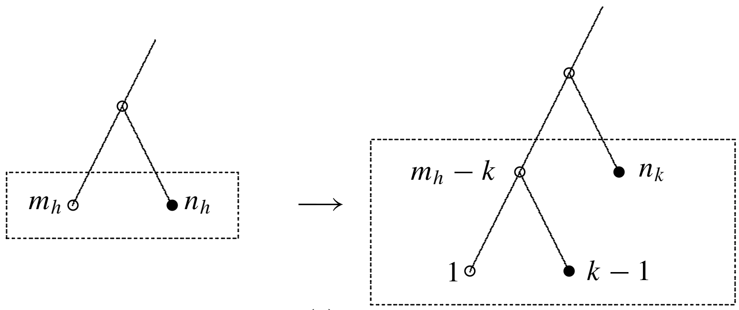
Remark. It is worth mentioning how some CETs are changed if some vertices (other than a root), after deletion or addition of edges, get the zero weights. We will then consider the following cases:

(a) u is a white internal vertex: Now the subtree with u as a root is moved up by one level. Then u is identified with its father, while the brother of u and the (black) son of u are identified.

(b) v is a black vertex not on the last level: Now consider u the white brother of v. Then the same applies as in (a).



(a,b)



(c)

Fig. 4: A change in a CET (if edges are added).

(c) u is a white leaf: Consider now v, the brother of u. If $w(v) = 1$ then v is identified with a father of u (or v); if $w(v) > 1$, then we put $w(u) = 1$, while $w(v)$ is decreased by one (in respect to the previous value).

(d) v is a black leaf on the last level: Consider now u, the brother of v. Now v deleted, while u is identified with its father.

Note also, that the weight of the vertex obtained by the identification of two vertices is the sum of their weights.

Let G be an NSG. We finally consider the situation when some edges are deleted (from G), while some other ones added (to G). Let E^* be the edges being deleted, while F^* the edges being added. Then G becomes $G^* = G - E^* + F^*$. If $|E^*| = |F^*|$, as we will assume, then, in fact, G^* is obtained from G by a relocation of some edges. In further we will assume that the edge sets E^* and F^* are disjoint (have no common vertices). According to the above remarks we will assume that they induce in G or in G^* either a complete graph, or a complete bipartite graph. Under these conditions the structures of T_G and T_{G^*} are related in accordance of Fig. 3 and 4. In fact, T_G is changed to T_{G-E^*} (see Fig. 3), and then T_{G-E^*} is changed to $T_{G-E^*+F^*}(= T_{G^*})$ (see Fig. 4). We also note here that in this case the heights of T_G and T_{G^*} can differ at most by two.

Remark. A natural question now arises: Are there any other (more general) means for transforming an NSG to any other NSG? For example, for NSGs of height two and fixed bi-partition (i.e. (M_2, N_2)) the number of edges is of the form $\binom{N_2}{2} + M_2N_2 - m_1n_2$. So, it is easy to see that each factorization of $c(= m_1n_2)$ can give rise to a new NSG. The (open) question is whether such relocations can be deduced from the ones mentioned above.

4. Concluding Remarks.

Here we will give some general remarks. The problem of identifying graphs from $\mathcal{H}(\nu, \varepsilon)$ with maximal index is still open (according to some sources, it is open for more than 40 years). It can be viewed as a problem of combinatorial optimization, where we are searching (in a discrete set) an object being extremal in some sense. For this reason an interaction with computers will be very important. The obtained results can be viewed as tools for examining the search space in a more efficient way. Namely, instead of examining the complete space $\mathcal{H}(\nu, \varepsilon)$, we will restrict us to its subset of NSGs, and moreover, we have a mechanism to jump from any NSG to its “neighbours”. So far, we have not got a result which states that the complete space of NSGs can be traversed by doing step by step certain types of local modifications. Note, such a situation appears with graphs with fixed degree sequences; then, each one can be obtained from any other by a sequence of local switchings - see, for example, [12], p. 45. By the way, it can be interesting to mention that each NSG is uniquely determined by its degree sequence, as can be easily deduced either from the form of its adjacency matrix (stepwise form) or from the minimal forbidden subgraphs (which do not allow any local switching).

We will now mention some experimental results. By a computer search (conducted by A. Obuljen) it was noticed that for small values of ν and fixed κ maximal graphs are of the type $B(\nu, \kappa)$, while for large values of ν there exists a function (defining the transition value, say g) so that maximal graphs for $\nu \leq g$ are of type $B(\nu, \kappa)$, while for $\nu \geq g$ of type $S(\nu, \kappa)$. In a particular case, for $\kappa = \binom{d-1}{2} - 1$ and $d \in \{5, \ldots, \nu - 1\}$, this fact was proved by F.K. Bell (see,

[1]); the corresponding function reads:

$$g(d) = \frac{1}{2}d(d+5) + 7 + \frac{32}{d-4} + \frac{16}{(d-4)^2}.$$

In addition, it was also noticed for ν big enough that the indices of the above two types of graphs are (surprisingly) very close to each other.

Finally, we mention two conjectures:

(i) $h \leq 3$ for any maximal graph;
(ii) if $\varepsilon \leq \binom{\nu-1}{2} + 1$ then $n_1 = 1$.

Remark. So far we have shown that that $2K_2$, P_4 and C_4 are minimal forbidden (induced) subgraphs for graphs with maximal index belonging to $\mathcal{H}(\nu, \varepsilon)$. A sensible question is to ask: are there any other such graphs? For example, if conjecture (i) from above is true then the graph with parameters $(1, 1, 1, 1; 1, 1, 1, 1)$, or

$$(((((K_2 \cup K_1)\nabla K_1) \cup K_1)\nabla K_1) \cup K_1)\nabla K_1$$

is one such graph.

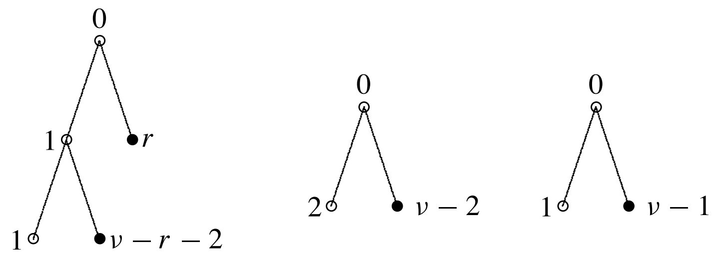
The research on this topic is in progress. In our next paper, we will consider the bounds on the index of the NSGs.

5. Appendix.

Here we show, as announced in Section 2, the (canonical) CETs for the graphs $P(\varepsilon)$, $B(\nu, \kappa)$ and $S(\nu, \kappa)$ introduced in Section 1 (see Figs. 5–7).

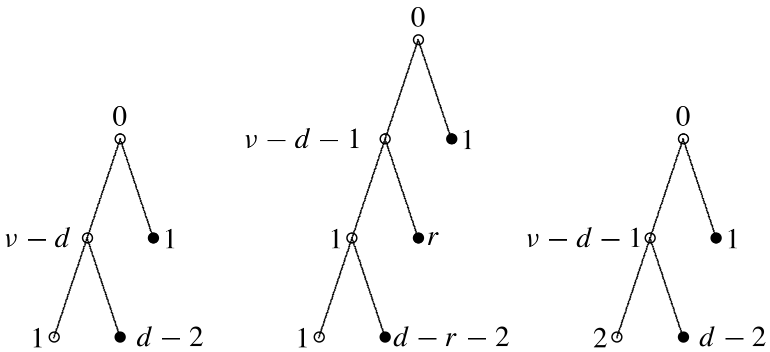
Note, all these representations are canonical ones.

Acknowledgement. The authors are indebted to M. Gionfriddo for enabling us to communicate these results at the conference Combinatorics 2004 (Acireale, September 13-18, 2004). We are grateful to F.K. Bell for his useful remarks which have improved the presentation of our results, and also to A. Obuljen, the student of Faculty of Computer Sciences (in Belgrade), for his computational results which have helped very much in these investigations. Research of the first author was supported in part by INDAM(Italy) and the Grant 1389 of the Serbian Ministry of Science. Research of the second author was supported by MIUR (cofin 2003 "Strutture geometriche, combinatoria e loro applicazioni").



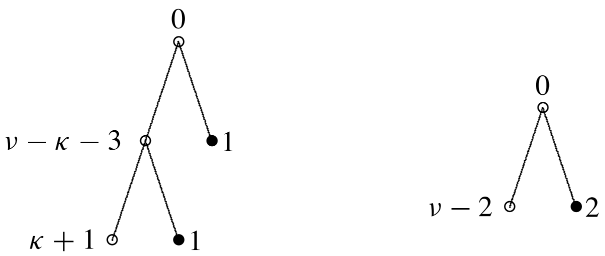
(a) $1 \leq r < \nu - 2$ (b) $r = \nu - 2$ (c) $r = \nu - 1$

Fig. 5: Representation of $P(\varepsilon)$ ($\varepsilon = \binom{\nu-1}{2} + r;\ 1 \leq r \leq \nu - 1$).



(a) $r = 0$ (b) $0 < r < d - 2$ (c) $r = d - 2$

Fig. 6: Representation of $B(\nu, \kappa)$ ($\kappa + 1 = \binom{d-1}{2} + r;\ 0 \leq r \leq d - 2$).



(a) $\kappa < \nu - 3$ (b) $\kappa = \nu - 3$

Fig. 7: Representation of $S(\nu, \kappa)$ ($\kappa \leq \nu - 3$).

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