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ORIGINAL PAPER

On the connectivity index of trees

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Abstract The connectivity index $\chi_1(G)$ of a graph G is the sum of the weights $d(u)d(v)$ of all edges uv of G, where $d(u)$ denotes the degree of the vertex u. Let $T(n, r)$ be the set of trees on n vertices with diameter r. In this paper, we determine all trees in $T(n, r)$ with the largest and the second largest connectivity index. Also, the trees in $T(n, r)$ with the largest and the second largest connectivity index are characterized.

Keywords Connectivity index · Tree · Diameter

1 Introduction

Mathematical descriptors of molecular structure, such as various topological indices, have been widely used in structure-property-activity studies [6,7,14]. Among the numerous topological indices considered in chemical graph theory, only a few have been found noteworthy in practical application [12]. One of these is the connectivity index or Randić index. The connectivity index of an organic molecule whose molecular graph is G is defined [3,13] as

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$$\chi_\alpha(G) = \sum_{u,v} (d(u)d(v))^\alpha,$$

where $d(u)$ denotes the degree of the vertex u of the molecular graph G, the summation goes over all pairs of adjacent vertices of G and α is a pertinently chosen exponent. Randić introduced the respective structure-descriptor in [13] for $\alpha = -\frac{1}{2}$ in his study of alkanes. However, other choice of α were also considered, in particular $\alpha = 1$ [1,4,5] was treated as an adjustable parameter to optimize the correlation between χ_1 and some selected class of organic compounds.

We only consider trees here. For a vertex x of a tree T, we denote the neighborhood and the degree of x by $N_T(x)$ and $d_T(x)$, respectively. For two vertices v_i and v_j $(i \neq j)$, the distance between v_i and v_j is the number of edges in a shortest path joining v_i and v_j. The diameter of T is the maximum distance between any two vertices of T. We will use $T - xy$ to denote the graph that arises from T by deleting the edge $xy \in E(T)$. Similarly, $T + xy$ is a graph that arises from T by adding an edge $xy \notin E(T)$, where $x,\ y \in V(T)$.

Let T be a tree. We denote by $T(n,r)$ the set of all trees with order n and diameter r. Let $T \in T(n,r)$. We call a path P^r of T *a main chain* if the length of P^r is r and denote $P^r = u_0u_1\ldots u_r$. Obviously, $d(u_0) = d(u_r) = 1$. Denote by S_n and P_n the star and the path with n vertices, respectively.

Let $T \in T(n,r)$ $(r \geq 2)$ and $P^r = u_0u_1\ldots u_r$ the main chain of T. Let $U_0(k_1,\ldots,k_{r-1})$ be a tree of order n obtained from P^r by attaching k_i pendant vertices to each $u_i \in V(P^r) \setminus \{u_0, u_r\}$, respectively. Denote

$$T^*(n,r) = \left\{ U_0(k_1,\ldots,k_{r-1}) : \sum_{i=1}^{r-1} k_i = n - r - 1 \right\}.$$

We use $T_i^*(n, r, n-r-1)$ to denote the tree in $T^*(n,r)$ with $k_i = n-r-1 \geq 1$ and $k_j = 0$ for $j \neq i$, where $1 \leq i, j \leq r-1$, and let $T_1^* = \{T_i^*(n,r,n-r-1) | 1 \leq i \leq r-1\}$. Let $T_{i,j}^*(n,r,k_i,k_j)$ be the tree in $T^*(n,r)$ with $k_i, k_j \geq 1$ and $k_l = 0$ for $l \neq i, j$, where $1 \leq i, j, l \leq r-1$, and $T_2^* = \{T_{i,j}^*(n,r,k_i,k_j) | 1 \leq i, j \leq r-1,\ i \neq j\}$.

Let T be a tree of order n. In [15], Yu gave a sharp upper bound of T for $\alpha = -\frac{1}{2}$ and in [2], Clark and Moon gave bounds of T for $\alpha = -1$. In [11] and [8], the sharp upper and lower bounds of $\chi_\alpha(G)$ of graph G were considered for arbitrary real number α involving the degrees of the vertices and the order of G, respectively. In [9], trees with small and large Randić index are considered. In [16], Zhao and Li gave the smallest lower bound of $\chi_{-1/2}$ of T with order n and diameter r.

The research on $\alpha = 1$ was discussed by Liu, et al. [10] in 2004, who gave the upper and lower bound of connectivity index of trees with order n and pending vertex m.

In the paper, we will give sharp upper bound for $\chi_1(T)$. Also, the second largest of $\chi_1(T)$ are determined.

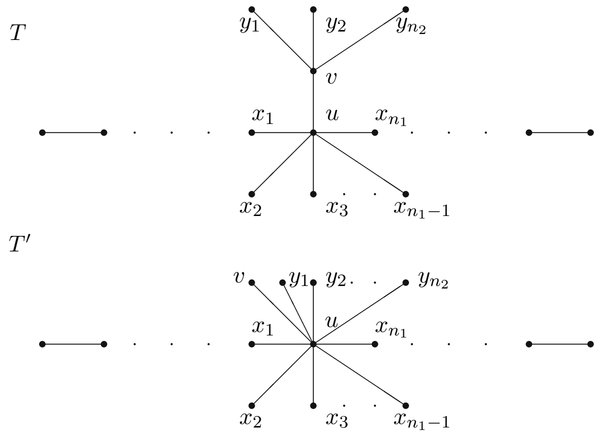

Fig. 1 T and T'

Note that if $r = 2$ or $r = n - 1$, then the only trees in $T(n, r)$ are S_n and P_n, respectively. Since $\chi_1(S_n) = (n-1)^2$ and $\chi_1(P_n) = 4(n-2)$, we always assume that $3 \le r \le n-2$ in Sects. 2 and 3.

2 Lemmas

We first give some lemmas that will be used in the proof of our main results.

Lemma 1 *Let $T \in T(n, r)$, $P^r = u_0u_1 \ldots u_r$ be the main chain of T and $u \in V(P^r)$ with $d_T(u) = n_1 + 1$, $n_1 \ge 2$. Suppose there exists $v \notin V(P^r)$ such that $uv \in E(T)$ and $d_T(v) = n_2 + 1$, $n_2 \ge 1$. Denote $N_T(u) = \{v, x_1, x_2, \ldots, x_{n_1}\}$ and $N_T(v) = \{u, y_1, y_2, \ldots, y_{n_2}\}$. Let $T' = T - \sum_{i=1}^{n_2} y_iv + \sum_{i=1}^{n_2} y_iu$, (see Fig. 1). Then $\chi_1(T') > \chi_1(T)$.*

Proof Let $Q_1 = \{xu | x \in N_T(u)\} \cup \{yv | y \in N_T(v)\}$, $Q_2 = \{xu | x \in N_{T'}(u)\}$, $\Omega_1 = \sum_{xy \in E(T) - Q_1} d_T(x)d_T(y)$ and $\Omega_2 = \sum_{xy \in E(T') - Q_2} d_{T'}(x)d_{T'}(y)$. Obviously $\Omega_1 = \Omega_2$, and

$$\begin{aligned}
\chi_1(T) &= \Omega_1 + d_T(u)d_T(v) + \sum_{i=1}^{n_2} d_T(y_i)d_T(v) + \sum_{i=1}^{n_1} d_T(x_i)d_T(u) \\
&= \Omega_1 + (n_1+1)(n_2+1) + (n_2+1)\sum_{i=1}^{n_2} d_T(y_i) + (n_1+1)\sum_{i=1}^{n_1} d_T(x_i), \\
\chi_1(T') &= \Omega_2 + d_{T'}(u)d_{T'}(v) + \sum_{i=1}^{n_2} d_{T'}(y_i)d_{T'}(u) + \sum_{i=1}^{n_1} d_{T'}(x_i)d_{T'}(u) \\
&= \Omega_2 + (n_1+n_2+1) + (n_1+n_2+1)\left(\sum_{i=1}^{n_2} d_{T'}(y_i) + \sum_{i=1}^{n_1} d_{T'}(x_i)\right).
\end{aligned}$$

Note that $d_T(y_i) = d_{T'}(y_i)$ $(1 \leq i \leq n_2)$ and $d_T(x_j) = d_{T'}(x_j)$ $(1 \leq j \leq n_1)$. Then

$$\chi_1(T') - \chi_1(T) = -n_1 n_2 + n_2 \sum_{i=1}^{n_1} d_T(x_i) + n_1 \sum_{i=1}^{n_2} d_T(y_i).$$

Since $d_T(y_i),\ d_T(x_j) \geq 1$, for $1 \leq i \leq n_2$ and $1 \leq j \leq n_1$, we have $\sum_{i=1}^{n_1} d_T(x_i) \geq n_1$ and $\sum_{i=1}^{n_2} d_T(y_i) \geq n_2$. Thus $\chi_1(T') - \chi_1(T) = -n_1 n_2 + n_1 n_2 + n_2 n_1 = n_1 n_2 > 0$. Hence $\chi_1(T') - \chi_1(T) > 0$. □

Lemma 2 *Let $T \in T(n, r)$. Then there exists $T^* \in T^*(n, r)$, such that $\chi_1(T^*) \geq \chi_1(T)$.*

Proof Let $P^r = u_0 u_1 \ldots u_r$ be the main chain of T.

For all $u_i \in V(P^r) \setminus \{u_0, u_r\}$, denote $m(T_{u_i}) = |\{v | d_T(v) \geq 2, v \in N_T(u_i) \setminus \{u_{i-1}, u_{i+1}\}\}|$. Let $m(T) = \sum_{i=1}^{r-1} m(T_{u_i})$. Obviously, if $m(T) = 0$, then $T \in T^*(n, r)$.

If $m(T) = 1$, then from Lemma 1, there exists $T' \in T(n, r)$ such that $\chi_1(T') > \chi_1(T)$ and $m(T') = 0$. This implies the lemma holds.

If $m(T) = k \geq 2$, then from Lemma 1, we have trees $T^k, T^{k-1}, \ldots, T^1$ such that

$$\chi_1(T^k) > \chi_1(T^{k-1}) > \cdots > \chi_1(T^1) > \chi_1(T)$$

and $m(T^k) = 0$, i.e., $T^k \in T^*(n, r)$. Thus the lemma holds. □

Lemma 3 *For $r \geq 3$ and $T \in T^*(n, r) \setminus T_1^*$, there exists $T' \in T_1^*$ such that $\chi_1(T') > \chi_1(T)$.*

Proof Let $T \in T^*(n, r) \setminus T_1^*$, $P^r = u_0 u_1 \ldots u_r$ be the main chain of T and $t = |\{k_i : k_i \neq 0\}|$. Then $t \geq 2$.

Let $k_i, k_j \neq 0,\ i < j$. Denote $\Theta(u_l) = \sum_{x \in N_T(u_l)} d_T(x) + d_T(u_l)$, $l = i, j$. Assume, without loss of generality, that $\Theta(u_j) \geq \Theta(u_i)$. Let $N_T(u_i) = \{v_1, v_2, \ldots, v_{k_i}, u_{i-1}, u_{i+1}\}$ and $N_T(u_j) = \{w_1, w_2, \ldots, w_{k_j}, u_{j-1}, u_{j+1}\}$. Suppose $d_T(u_k) = n_k$ for $0 \leq k \leq r$. Then $\Theta(u_l) = n_{l-1} + n_l + n_{l+1} + k_l$, $l = i, j$.

Let $Q = \{x u_i | x \in N_T(u_i)\} \cup \{y u_j | y \in N_T(u_j)\}$ and $\Omega = \sum_{xy \in E(T) - Q} d_T(x) d_T(y)$. Set $T^1 = T - \sum_{k=1}^{k_i} v_k u_i + \sum_{k=1}^{k_i} v_k u_j$. We first consider the following two cases.

Case 1 $j \geq i + 2$ (see Fig. 2).

In this case, we have

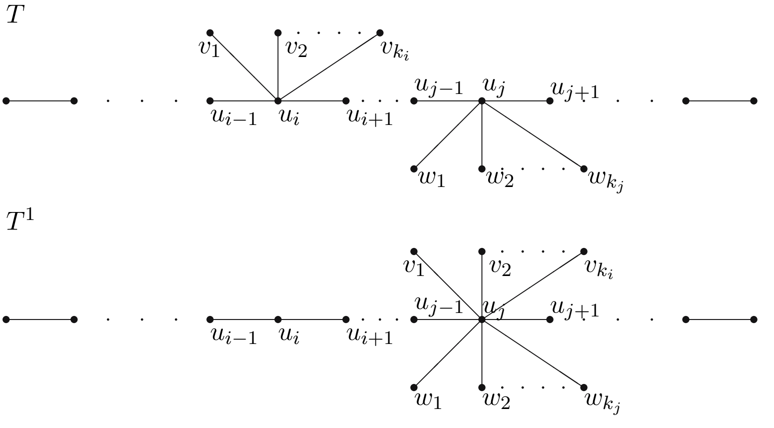

Fig. 2 T and T^1

$$\begin{aligned}\chi_1(T) &= \Omega + \sum_{k=1}^{k_i} d_T(v_k)d_T(u_i) + \sum_{k=1}^{k_j} d_T(w_k)d_T(u_j) + d_T(u_i)d_T(u_{i-1}) \\ &\quad + d_T(u_i)d_T(u_{i+1}) + d_T(u_{j-1})d_T(u_j) + d_T(u_{j+1})d_T(u_j) \\ &= \Omega + (k_i + n_{i-1} + n_{i+1})n_i + (k_j + n_{j-1} + n_{j+1})n_j,\end{aligned}$$

and

$$\begin{aligned}\chi_1(T^1) &= \Omega + \sum_{k=1}^{k_i} d_{T^1}(v_k)d_{T^1}(u_j) + \sum_{k=1}^{k_j} d_{T^1}(w_k)d_{T^1}(u_j) + d_{T^1}(u_i)d_{T^1}(u_{i-1}) \\ &\quad + d_{T^1}(u_i)d_{T^1}(u_{i+1}) + d_{T^1}(u_{j-1})d_{T^1}(u_j) + d_{T^1}(u_{j+1})d_{T^1}(u_j) \\ &= \Omega + (n_{i-1} + n_{i+1})(n_i - k_i) + (n_j + k_i)(k_j + k_i + n_{j-1} + n_{j+1}).\end{aligned}$$

So

$$\begin{aligned}\chi_1(T^1) - \chi_1(T) &= k_i(n_j + k_j + n_{j-1} + n_{j+1}) + {k_i}^2 - k_i(n_i + n_{i-1} + n_{i+1}) \\ &= k_i(n_{j-1} + n_j + n_{j+1} + k_j) - k_i(n_i + n_{i-1} + n_{i+1} + k_i) + 2{k_i}^2 \\ &= k_i(\Theta(u_j) - \Theta(u_i)) + 2{k_i}^2 > 0.\end{aligned}$$

Case 2 $j = i + 1$ (see Fig. 3)

In this case, we get

$$\begin{aligned}\chi_1(T) &= \Omega + \sum_{k=1}^{k_i} d_T(v_k)d_T(u_i) + \sum_{k=1}^{k_j} d_T(w_k)d_T(u_j) \\ &\quad + d_T(u_i)d_T(u_{i-1}) + d_T(u_i)d_T(u_j) + d_T(u_{j+1})d_T(u_j) \\ &= \Omega + k_i n_i + k_j n_j + n_{i-1}n_i + n_i n_j + n_j n_{j+1},\end{aligned}$$

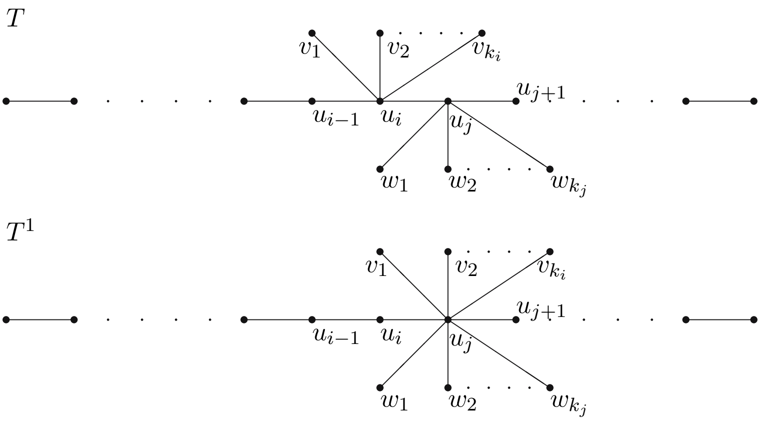

Fig. 3 T and T^1

and

$$\begin{aligned}\chi_1(T^1) &= \Omega + \sum_{k=1}^{k_i} d_{T^1}(v_k)d_{T^1}(u_j) + \sum_{k=1}^{k_j} d_{T^1}(w_k)d_{T^1}(u_j)\\ &\quad + d_{T^1}(u_i)d_{T^1}(u_{i-1}) + d_{T^1}(u_i)d_{T^1}(u_j) + d_{T^1}(u_{j+1})d_{T^1}(u_j)\\ &= \Omega + (k_i + k_j)(n_j + k_i) + n_{i-1}(n_i - k_i)\\ &\quad + (n_i - k_i)(n_j + k_i) + (n_j + k_i)n_{j+1}.\end{aligned}$$

So

$$\begin{aligned}\chi_1(T^1) - \chi_1(T) &= k_i(k_j + n_{j+1} - n_{i-1})\\ &= k_i((k_j + n_i + n_j + n_{j+1}) - (k_i + n_{i-1} + n_i + n_j) + k_i)\\ &= k_i(\Theta(u_j) - \Theta(u_i) + k_i) > 0.\end{aligned}$$

Note that $T^1 \in T_1^*$ if $t = 2$ and $\chi_1(T^1) > \chi_1(T)$ from Cases 1 and 2. If $t > 2$, then we will use T^1 to repeat the above step until the cardinality of k_i being nonzero is only one. So we get

$$T^2, T^3, \ldots, T^{t-1} \text{ and } \chi_1(T^1) < \chi_1(T^2) < \cdots < \chi_1(T^{t-1}).$$

Note that $T^{t-1} \in T_1^*$, and hence the lemma holds. □

Lemma 4 *Let $r \geq 4$. Then $\chi_1(T^*_{i,i+1}(n, r, k_i, s)) > \chi_1(T^*_{i,j}(n, r, k_i, s))$ if $1 \leq i, j \leq r - 1$ and $j \geq i + 2$.*

Proof For short, denote $T = T^*_{i,j}(n, r, k_i, s)$. Assume $P^r = u_0u_1 \ldots u_r$ is the main chain of T. Denote $d_T(u_i) = n_i$. Then $n_0 = n_r = 1$, $n_j = 2 + s$, $n_i = k_i + 2 \geq 3$ and $n_t = 2$ if $t \neq 0, i, j, r$. We will complete the proof by considering the following two cases.

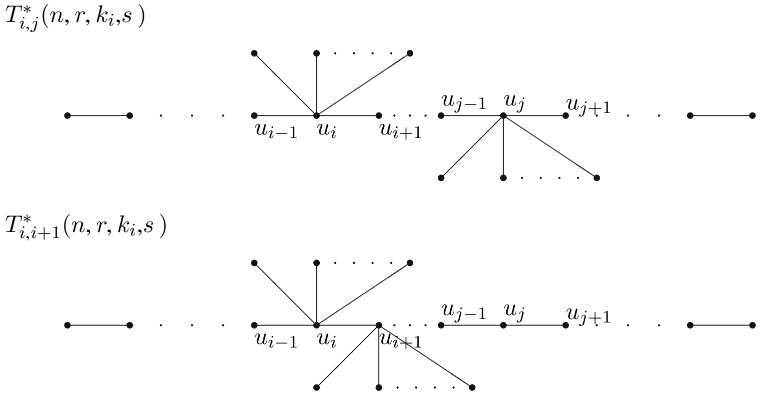

Fig. 4 $T^*_{i,j}(n, r, k_i, s)$ and $T^*_{i,i+1}(n, r, k_i, s)$

Case 1 $j \geq i + 3$ (see Fig. 4).

In this case, we have $n_{j+1} \leq 2$. Thus

$$\begin{aligned}
&\chi_1(T^*_{i,i+1}(n, r, k_i, s)) - \chi_1(T^*_{i,j}(n, r, k_i, s)) \\
&\quad = n_{i-1}n_i + k_i n_i + n_i(n_{i+1} + s) + s(n_{i+1} + s) + n_{i+2}(n_{i+1} + s) + n_{j-1}(n_j - s) \\
&\qquad + n_{j+1}(n_j - s) - (n_{i-1}n_i + k_i n_i + n_{i+1}n_i + n_{i+1}n_{i+2} + n_{j-1}n_j + sn_j + n_{j+1}n_j) \\
&\quad = s(n_i + n_{i+1} + s + n_{i+2} - n_j - n_{j-1} - n_{j+1}) \\
&\quad \geq s(n_i - 2) > 0.
\end{aligned}$$

Case 2 $j = i + 2$.

In this case, we have $n_{i+3} \leq 2$. Thus

$$\begin{aligned}
&\chi_1(T^*_{i,i+1}(n, r, k_i, s)) - \chi_1(T^*_{i,j}(n, r, k_i, s)) \\
&\quad = n_{i-1}n_i + k_i n_i + n_i(n_{i+1} + s) + s(n_{i+1} + s) + (n_{i+2} - s)(n_{i+1} + s) \\
&\qquad + (n_{i+2} - s)n_{i+3} - (n_{i-1}n_i + k_i n_i + n_{i+1}n_i + n_{i+1}n_{i+2} + sn_{i+2} + n_{i+2}n_{i+3}) \\
&\quad = s(n_i - n_{i+3}) > 0.
\end{aligned}$$

Thus the lemma holds. □

Lemma 5 *Let* $r \geq 5$. *Then* $\chi_1(T^*_{i,i+1}(n, r, s, t)) > \chi_1(T^*_{1,2}(n, r, s, t)) = \chi_1(T^*_{r-2,r-1}(n, r, t, s))$ *if* $2 \leq i \leq r - 3$.

Proof It is no difficult to check that $\chi_1(T^*_{i,i+1}(n, r, s, t)) = \chi_1(T^*_{i,i+1}(n, r, t, s))$ for $2 \leq i \leq r - 3$ and $\chi_1(T^*_{i,i+1}(n, r, s, t)) = \chi_1(T^*_{j,j+1}(n, r, s, t))$ for $2 \leq i, j \leq r - 3$ and $i \neq j$. Hence, we just need to show $\chi_1(T^*_{2,3}(n, r, s, t)) > \chi_1(T^*_{1,2}(n, r, s, t)) = \chi_1(T^*_{r-2,r-1}(n, r, t, s))$. Since

$$\begin{aligned}
&\chi_1(T^*_{2,3}(n,r,s,t)) - \chi_1(T^*_{1,2}(n,r,s,t))\\
&\quad = 2 + 2(s+2) + s(s+2) + (s+2)(t+2) + t(t+2) + 2(t+2)\\
&\qquad -[(s+2) + s(s+2) + (s+2)(t+2) + t(t+2) + 2(t+2) + 4]\\
&\quad = (s+2) - 2 > 0,
\end{aligned}$$

the lemma holds immediately. □

Lemma 6 *Let $r \geq 3$ and $1 \leq i \leq r-2$. Then*

$$\chi_1(T^*_{i,i+1}(n,r,s,t)) \begin{cases} \leq \chi_1(T^*_{i,i+1}(n,r,s-1,t+1)) & \text{if } t \geq s;\\ < \chi_1(T^*_{i,i+1}(n,r,s+1,t-1)) & \text{if } s > t.\end{cases}$$

Proof Let $P^r = u_0u_1\ldots u_r$ be the main chain of $T^*_{i,i+1}(n,r,s,t)$ and $d(u_i) = n_i$ for $0 \leq i \leq r$. Then $1 \leq n_{i-1} \leq 2$ and $1 \leq n_{i+2} \leq 2$. If $t \geq s$, then we have

$$\begin{aligned}
&\chi_1(T^*_{i,i+1}(n,r,s-1,t+1)) - \chi_1(T^*_{i,i+1}(n,r,s,t))\\
&\quad = n_{i-1}(s+1) + (s-1)(s+1) + (s+1)(t+3) + (t+1)(t+3) + n_{i+2}(t+3)\\
&\qquad -[n_{i-1}(s+2) + s(s+2) + (s+2)(t+2) + t(t+2) + n_{i+2}(t+2)]\\
&\quad = 1 + n_{i+2} - n_{i-1} + (t-s) \geq 0.
\end{aligned}$$

If $s > t$, then

$$\begin{aligned}
&\chi_1(T^*_{i,i+1}(n,r,s+1,t-1)) - \chi_1(T^*_{i,i+1}(n,r,s,t))\\
&\quad = n_{i-1}(s+3) + (s+1)(s+3) + (s+3)(t+1) + (t-1)(t+1) + n_{i+2}(t+1)\\
&\qquad -[n_{i-1}(s+2) + s(s+2) + (s+2)(t+2) + t(t+2) + n_{i+2}(t+2)]\\
&\quad = 1 + n_{i-1} - n_{i+2} + (s-t) > 0.
\end{aligned}$$

Thus the lemma holds. □

3 Results

Theorem A *Let $T \in T(n,r)$. Then*

$$\chi_1(T) \leq \begin{cases} n^2 - 3n + 4 & \text{if } r = 3; & (1)\\ (n-r+1)(n-r+3) + 4(r-3) & \text{if } r \geq 4. & (2)\end{cases}$$

Equalities hold in (1) *and* (2) *if and only if* $T \cong T^*_i(n,3,n-4)$, $i = 1,2$ *and* $T \in T^*_1 \setminus \{T^*_1(n,r,n-r-1), T^*_{r-1}(n,r,n-r-1)\}$, *respectively.*

Proof For any $T \in T(n,3)$, we have $T \in T^*(n,3)$. Since $\chi_1(T^*_1(n,3,n-4)) = \chi_1(T^*_2(n,3,n-4)) = n^2 - 3n + 4$, (1) holds by Lemma 3 and the equality holds if and only if $T \cong T^*_i(n,3,n-4)$, $i = 1,2$.

Now we consider the case $r \geq 4$. From Lemmas 2 and 3, for any $T \in T(n, r)$, there exists $T' \in T_1^*$ such that $\chi_1(T') \geq \chi_1(T)$. By an elementary calculation, we have $\chi_1(T_i^*(n, r, n-r-1)) = \chi_1(T_j^*(n, r, n-r-1))$ if $2 \leq i, j \leq r-2$ and $\chi_1(T_1^*(n, r, n-r-1)) = \chi_1(T_{r-1}^*(n, r, n-r-1))$. On the other hand, we have

$$\chi_1(T_i^*(n, r, n-r-1)) = (n-r+1)(n-r+3) + 4(r-3), \quad i \neq 1, r-1$$

and

$$\chi_1(T_1^*(n, r, n-r-1)) = (n-r+1)(n-r+2) + 4(r-3) + 2.$$

Hence $\chi_1(T_i^*(n, r, n-r-1)) - \chi_1(T_1^*(n, r, n-r-1)) = n-r+1-2 = n-r-1 > 0$ by $r \leq n-2$. Thus (2) holds and the equality holds if and only if $T \in T_1^* \setminus \{T_1^*(n, r, n-r-1), T_{r-1}^*(n, r, n-r-1)\}$. □

Theorem B *Let $r \geq 5$ and $T \in T(n, r) \setminus T_1^*$. Then*

$$\chi_1(T) \leq (n-r)(n-r+3) + 4(r-4) + 9$$

and the equation holds if and only if $T \cong T_{i,i+1}^*(n, r, 1, n-r-2)$, $2 \leq i \leq r-3$.

Proof By the proof of Lemma 3, for any $T \in T(n, r) \setminus T_1^*$, there exists $T' \in T_2^*$ such that $\chi_1(T') \geq \chi_1(T)$. By Lemmas 4 and 5, we have $\chi_1(T') \leq \chi_1(T_{i,i+1}^*(n, r, s, t))$, where $2 \leq i \leq r-3$. By lemma 6 and note that for $2 \leq i \leq r-3$,

$$\begin{aligned}\chi_1(T_{i,i+1}^*(n, r, 1, n-r-2)) &= \chi_1(T_{i,i+1}^*(n, r, n-r-2, 1)) \\ &= (n-r)(n-r+3) + 4(r-4) + 9,\end{aligned}$$

Theorem B holds immediately. □

Theorem C *Let $r \geq 5$ and $T \in (T(n, r) \cup \{T_1^*(n, r, n-r-1), T_{r-1}^*(n, r, n-r-1)\}) \setminus T_1^*$. Then $\chi_1(T) \leq (n-r)(n-r+3) + 4(r-4) + 9$ and the equation holds if and only if $T \cong T_{i,i+1}^*(n, r, 1, n-r-2)$, $2 \leq i \leq r-3$.*

Proof By Theorem B, for any $T \in T(n, r) \setminus T_1^*$, there exists i with $2 \leq i \leq r-3$ such that

$$\chi_1(T) \leq \chi_1(T_{i,i+1}^*(n, r, 1, n-r-2)) = (n-r)(n-r+3) + 4(r-4) + 9.$$

Note that

$$\begin{aligned}\chi_1(T_1^*(n, r, n-r-1)) = \chi_1(T_{r-1}^*(n, r, n-r-1)) &= (n-r+1)(n-r+2) \\ &\quad +4(r-3) + 2\end{aligned}$$

and

$$\chi_1(T^*_{i,i+1}(n, r, 1, n-r-2)) - \chi_1(T^*_1(n, r, n-r-1)) = 1 > 0,$$

Theorem C holds obviously. □

Theorem D *Let $T \in T(n,r) \setminus T^*_1$. Then*

$$\chi_1(T) \leq \begin{cases} n^2 - 4n + 9 & \text{if } r = 3; \quad (3) \\ n^2 - 5n + 12 & \text{if } r = 4. \quad (4) \end{cases}$$

Equalities hold in (3) and (4) if and only if $T \cong T^*_{1,2}(n, 3, 1, n-5)$ and $T \cong T^*_{1,2}(n, 4, 1, n-6)$, respectively.

Proof For $T \in T(n, 3) \setminus T^*_1$, by Lemma 6, we have $\chi_1(T) \leq \chi_1(T^*_{1,2}(n, 3, 1, n-5))$ or $\chi_1(T) \leq \chi_1(T^*_{1,2}(n, 3, n-5, 1))$. Since

$$\chi_1(T^*_{1,2}(n, 3, 1, n-5)) = \chi_1(T^*_{1,2}(n, 3, n-5, 1)) = n^2 - 4n + 9,$$

(3) holds and equality holds if and only if $T \cong T^*_{1,2}(n, 3, 1, n-5)$.

By the proof of Lemma 3, for $T \in T(n, 4) \setminus T^*_1$, there exists $T' \in T^*_2$ such that $\chi_1(T') \geq \chi_1(T)$. By Lemmas 4 and 6, we have $\chi_1(T') \leq \chi_1(T^*_{1,2}(n, 4, 1, n-6))$ or $\chi_1(T) \leq \chi_1(T^*_{1,2}(n, 4, n-6, 1))$. Note that

$$\chi_1(T^*_{1,2}(n, 4, 1, n-6)) = n^2 - 5n + 12,$$

and

$$\chi_1(T^*_{1,2}(n, 4, n-6, 1)) = n^2 - 6n + 19.$$

Then

$$\chi_1(T^*_{1,2}(n, 4, 1, n-6)) - \chi_1(T^*_{1,2}(n, 4, n-6, 1)) = n - 7 \geq 0.$$

Thus (4) holds and equality holds if and only if $T \cong T^*_{1,2}(n, 4, 1, n-6)$. □

Theorem E *Let $T \in (T(n, 4) \cup \{T^*_1(n, 4, n-5), T^*_3(n, 4, n-5)\}) \setminus T^*_1$.* Then

$$\chi_1(T) \leq n^2 - 5n + 12$$

and equality holds if and only if $T \cong T^*_{1,2}(n, 4, 1, n-6)$ or $T \cong T^*_1(n, 4, n-5)$ or $T \cong T^*_3(n, 4, n-5)$.

Proof Let $T \in T(n, 4)\backslash T_1^*$. By Theorem D, we have $\chi_1(T) \leq \chi_1(T_{1,2}^*(n, 4, 1, n-6))$. Note that

$$\chi_1(T_1^*(n, 4, n-5)) = \chi_1(T_3^*(n, 4, n-5)) = \chi_1(T_{1,2}^*(n, 4, 1, n-6)) \\ = n^2 - 5n + 12.$$

Theorem E holds immediately. □

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