Chapter 2
Extremal Graphs with Respect to Harary Index

In recent years, characterizing the extremal (maximal or minimal) graphs in a given set of graphs with respect to some distance-based topological index has become an important direction in chemical graph theory.

Let us briefly recall the chemical background of this problem as follows. A class of molecular graphs representing carbon compounds is a class of connected graphs with maximum degree at most 4. It models the skeletons of hydrocarbons [1], an important class of molecules in organic chemistry. The bounds of a molecular descriptor are important information of a molecular graph in the sense that they establish the approximate range of the descriptor in terms of molecular structural parameters. Therefore, it is important to establish the (lower or upper) bounds for topological indices and to characterize the corresponding extremal graphs at which the lower or upper bounds are attained.

Alternatively, topological index of a graph can be viewed as a graph invariant under the isomorphism of graphs, that is, for some topological index TI, $\mathrm{TI}(G) = \mathrm{TI}(H)$ if $G \cong H$. Therefore, the results in this chapter can also be seen as a topic in extremal graph theory. For some other interesting results in extremal graph theory, see [2].

In this chapter, we determine the upper or lower bounds on the Harary indices of graphs in various sets of structures, including general graphs, trees and generalized trees, and characterize the corresponding extremal graphs at which these bounds are attained. For some recent related results to this topic, see a recent survey [3].

2.1 General Graphs

In this section, we present some extremal results on general graphs with respect to Harary index.

Denote by $G^{\circledast} = (V, E)$ a graph with diameter d ($3 \le d \le 4$ and $|V(G^{\circledast})| \ge d+2$) such that, for any two distinct vertices $u \in V(G^{\circledast}) \setminus V(P_{d+1})$ and $v \in V(G^{\circledast})$, $d_{G^{\circledast}}(u, v) = 1$ *or* 2 where P_{d+1} is a path with $d + 1$ vertices in $G^{\circledast}$. Two graphs depicted in Fig. 2.1 are all of $G^{\circledast}$ type.

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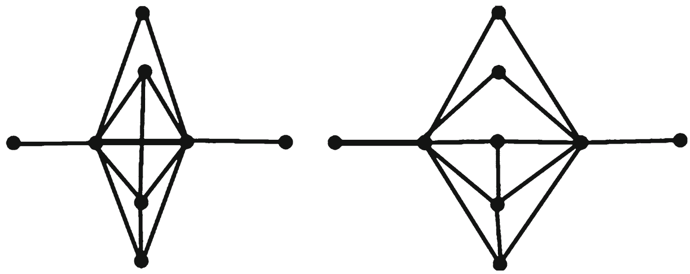

Fig. 2.1 Examples of graphs of $G^{\circledast}$-type

Theorem 2.1.1 ([4]) *Let G be a connected graph of order n and with m edges and diameter $D(G) = d$. Set $A = H(P_{d+1})$. Then*

$$A + \frac{n(n-1) + 2(m-d)(d-1)}{2d} - \frac{d+1}{2} \leq H(G) \leq A + \frac{n(n-1) + 2m}{4} - \frac{d(d+3)}{4}$$

with left equality holding if and only if G is a graph with diameter $d \leq 2$ or $G \cong P_n$, and right equality holding if and only if G is a graph with diameter $d \leq 2$ or $G \cong P_n$, or G is isomorphic to some $G^{\circledast}$.

A connected graph G is called a *cactus* if each block of G is either an edge or a cycle. Denote by C at (n, r) the set of connected cacti possessing n vertices and r cycles. Let $C^0(n, r)$ be the cactus graph obtained from a star S_n by adding r independent edges between the leaves of S_n.

Theorem 2.1.2 ([5, 6]) *Let G be any graph in C at (n, r). Then we have*

$$H(G) \leq \frac{1}{4}(n-2r-1)(n-2r-2) - r^2 + (n-1)(r+1)$$

with equality holding if and only if $G \cong C^0(n, r)$.

Theorem 2.1.3 ([7]) *Among all cacti of order 2n and with a perfect matching, the graph $C^0(2n, n-1)$ is the unique graph having the maximal Harary index.*

Let $C^*_{n,k}$ be a cactus obtained by identifying the vertex of degree $n-4$ of $C^0(n-3, \frac{n-k-4}{2})$ with one vertex of C_4. For example, the graph $C^*_{11,3}$ is shown in Fig. 2.2.

Theorem 2.1.4 ([7]) *Among all cacti of order n and with k cut edges, the graph $C^0(n, \frac{n-k-1}{2})$ is the unique graph with maximal Harary index when $n-k$ is odd; and $C^*_{n,k}$ uniquely has the maximal Harary index if $n-k$ is even.*

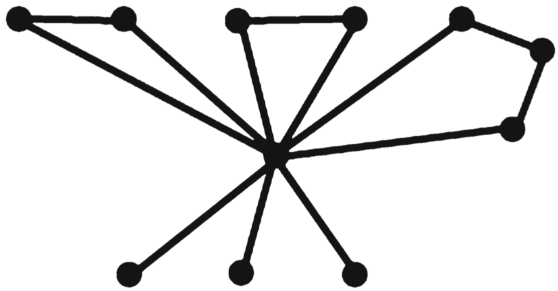

Fig. 2.2 The cactus $C^*_{11,3}$

Theorem 2.1.5 ([7]) *Among all cacti of order n and with k pendant vertices, the graph* $C^0(n, \frac{n-k-1}{2})$ *is the unique graph with maximal Harary index when* $n-k$ *is odd; and* $C^*_{n,k}$ *uniquely has the maximal Harary index if* $n-k$ *is even.*

Denote by $C^\dagger(2n, r)$ a graph of order $2n$ obtained by attaching $n-r-1$ paths of length 2 at the vertex of maximum degree in $C^0(2r+2, r)$.

Theorem 2.1.6 ([6]) *Let* $G \in \mathcal{C}at(2n, r)$ *with a perfect matching. Then we have*

$$H(G) \leq \frac{1}{24}(n-r-1)(23n+17r-2)+2n+r^2-1$$

with equality holding if and only if $G \cong C^\dagger(2n, r)$.

Let $1 \leq k < n$ and KC_n^k be the graph obtained by attaching k pendant vertices to one vertex of the complete graph K_{n-k}.

Theorem 2.1.7 ([8]) *Among all connected graphs with n vertices and k cut edges, the graph* KC_n^k *uniquely has the maximal Harary index.*

Note that the *kite graph* $Ki_{n,k}$ is obtained by identifying one vertex of K_k with one pendant vertex of P_{n-k+1} and the *Turán graph* $T_n(k)$ is a complete k-partite graph of order n in which any two partition sets differ in size by at most one.

Theorem 2.1.8 ([9]) *Among all connected graphs with n vertices and clique number k, the Turán graph* $T_n(k)$ *uniquely has the maximal Harary index, the kite graph* $Ki_{n,k}$ *uniquely has the minimal Harary index.*

Moreover, in [10], the authors also determined some extremal bipartite graphs with respect to Harary index, which are all complete bipartite graphs. Hence, these results can be viewed as the special cases of Theorem 2.1.8.

Theorem 2.1.9 ([9]) *Among all connected graphs with n vertices and chromatic number k, the Turán graph* $T_n(k)$ *uniquely has the maximal Harary index, the kite graph* $Ki_{n,k}$ *uniquely has the minimal Harary index.*

In graph theory, the well-known *Moore graph* is a r-regular graph with diameter k whose order attains the upper bound

$$1 + r \sum_{i=0}^{k-1} (r-1)^i.$$

Hoffman and Singleton [11] proved that every r-regular Moore graph G with diameter 2 must have $r \in \{2, 3, 7, 57\}$. They pointed out that $G \cong C_5$ if $r = 2$, G is just Petersen graph for $r = 3$; G is the well-known Hoffman-Singleton graph for $r = 7$ and while $r = 57$ we do not know whether such graph G exists or not.

Theorem 2.1.10 ([12]) *Let G be a connected triangle- and quadrangle-free graph with $n \geq 2$ vertices and m edges. Then*

$$H(G) \leq \frac{n(n-1)}{4} + \frac{m}{2}$$

with equality holding if and only if G is a star or a Moore graph of diameter 2.

In the next theorem, we will characterize the extremal graphs maximizing the Harary index among all connected graphs with a given matching number. Obviously, either $G = C_3$ or $G = S_n$ holds for any connected graph G with $n \geq 2$ vertices and matching number $\beta = 1$. For the connected graph G with $n \geq 4$ vertices and matching number $\beta \geq 2$, we have

Theorem 2.1.11 ([13]) *Let G be a connected graph with $n \geq 4$ vertices and matching number β, where $2 \leq \beta \leq \left\lfloor \frac{n}{2} \right\rfloor$.*

(1) *If $\beta = \left\lfloor \frac{n}{2} \right\rfloor$, then $H(G) \leq H(K_n)$ with equality holding if and only if $G \cong K_n$;*
(2) *If $\frac{2n}{5} < \beta \leq \left\lfloor \frac{n}{2} \right\rfloor - 1$, then $H(G) \leq H(K_1 \bigvee (K_{2\beta-1} \cup \overline{K_{n-2\beta}}))$ with equality holding if and only if $G \cong K_1 \bigvee (K_{2\beta-1} \cup \overline{K_{n-2\beta}})$;*
(3) *If $2 \leq \beta < \frac{2n}{5}$, then $H(G) \leq H(K_\beta \bigvee \overline{K_{n-\beta}})$ with equality holding if and only if $G \cong K_\beta \bigvee \overline{K_{n-\beta}}$;*
(4) *If $\beta = \frac{2n}{5}$, then $H(G) \leq H(K_\beta \vee \overline{K_{n-\beta}}) = H(K_1 \vee (K_{2\beta-1} \cup \overline{K_{n-2\beta}}))$ with equality holding if and only if $G \cong K_\beta \bigvee \overline{K_{n-\beta}}$ or $G \cong K_1 \bigvee (K_{2\beta-1} \cup \overline{K_{n-2\beta}})$.*

By the definition of Harary index, one can easily observe that any edge addition will increase the Harary index. Thus, we have

Proposition 2.1.12 ([9]) *Let G be a connected graph with $e \notin E(G)$. Then we have $H(G) < H(G+e)$.*

By Proposition 2.1.12, it easily follows that

Theorem 2.1.13 ([12]) *Let G be a connected graph of order n. Then $H(G) \leq H(K_n)$ with equality holding if and only if $G \cong K_n$.*

A graph G is called *quasi-tree graph* if there exists a vertex $x \in V(G)$ such that $G - x$ is a tree. Clearly, any tree is a quasi-tree graph since the deletion of any pendant vertex will deduce another new tree. So, we call any tree a trivial quasi-tree graph, and other quasi-tree graphs are called nontrivial quasi-tree graphs. Very recently in [14] we introduced a new definition of k-generalized quasi-tree graph. A graph G is called *k-generalized quasi-tree graph* if there exists a subset $V_k \subseteq V(G)$ with $|V_k| = k$ such that $G - V_k$ is a tree but, for any subset $V_{k-1} \subseteq V(G)$ with cardinality $k-1$, $G - V_{k-1}$ is not a tree. For $k \geq 2$, we denote by $\mathcal{QT}^{(k)}(n)$ the set of k-generalized quasi-tree graphs of order n. Here, we think nontrivial quasi-tree graphs and generalized quasi-tree graphs as general graphs because of their more complicated structure [14] than unicyclic or bicyclic graphs.

Let $C_k((n-k)^1)$ be a graph obtained by attaching a path of length $n-k$ to any one vertex of C_k. We denote by $C_{3,3}^{n-5}$ (see Fig. 2.3) a graph obtained by connecting two vertex-disjoint triangles by a path of length $n-5$. Extremal graphs with respect to Harary index are characterized, respectively, in the following three theorems among all nontrivial quasi-tree graphs of order $n \geq 4$ and k-generalized graphs of order $n \geq 6$ (including the minimal case for $k = 2$ and the maximal case for all values of k).

Theorem 2.1.14 ([14]) *Let G be a nontrivial quasi-tree graph of order $n \geq 4$. Then we have*

$$3 + n\sum_{k=2}^{n-2}\frac{1}{k} \leq H(G) \leq \frac{(n-2)(n+5)}{4} + 1$$

with left equality holding if and only if $G \cong C_3((n-3)^1)$, and right equality holding if and only if $G \cong K_2 \bigvee \overline{K_{n-2}}$.

Theorem 2.1.15 ([14]) *Let G be a 2-generalized quasi-tree graph of order $n \geq 6$. Then we have*

$$H(G) \geq 5 + n\sum_{k=2}^{n-3}\frac{1}{k} + \frac{1}{n-3}$$

with equality holding if and only if $G \cong C_{3,3}^{n-5}$.

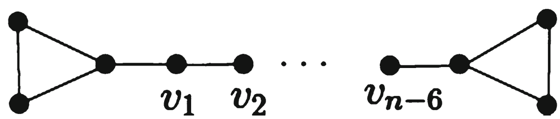

Fig. 2.3 The graph $C_{3,3}^{n-5}$

Theorem 2.1.16 ([14]) *For any graph $G \in \mathcal{QT}^{(k)}(n)$ with $n \geq 6$, we have*

$$H(G) \leq \frac{n(n-1)}{4} + \frac{(k+1)(n-k-1)}{2} + \frac{(k+1)k}{4}$$

with equality holding if and only if $G \cong K_{k+1} \bigvee \overline{K_{n-k-1}}$.

For a connected graph G, the kth power G^k (see Ref. [15]) is a new graph with vertex set $V(G^k) = V(G)$ such that two vertices are adjacent in G^k if and only if they are at distance at most k in G. The bounds on Harary index have been presented in the following theorem among all kth power of trees. Moreover the corresponding extremal graphs were also characterized implicitly with respect to Harary index.

Theorem 2.1.17 ([15]) *For any tree T of order n, we have*

$$H(P_n^k) \leq H(T^k) \leq H(S_n^k)$$

with left equality holding if and only if $T^k \cong P_n^k$ and right equality holding if and only if $T^k \cong S_n^k$.

From Proposition 2.1.12, the corollary below can be easily obtained.

Corollary 2.1.18 ([15]) *Let G be a connected graph of order n. Then we have $H(P_n^k) \leq H(G^k)$.*

In the several theorems below, we present some extremal results with respect to Harary index on disconnected graphs. First, we define

$$f(n,k) = \begin{cases} k + n\displaystyle\sum_{l=2}^{r-1} \frac{1}{l} + \frac{s(r+1)}{r} & \text{if } k \leq \dfrac{n}{2}; \\ n-k & \text{if } k > \dfrac{n}{2}, \end{cases}$$

where r, s are integers with $n = rk + s$ and $0 \leq s < k$.

Theorem 2.1.19 ([16]) *Let G be a graph of order n and with k components where $1 \leq k \leq n$. Then we have*

$$f(n,k) \leq H(G) \leq \frac{(n-k+1)(n-k)}{2}$$

with left equality holding if and only if $G \cong (k-s)P_r \cup sP_{r+1}$ and right equality holding if and only if $G \cong (k-1)K_1 \cup K_{n-k+1}$.

Theorem 2.1.20 ([16]) *Let G be a graph of order n and with m edges and k components $G_1, G_2, \ldots, G_k$ where $|V(G_i)| = n_i$ for $i = 1, 2, \ldots, k$. Then we have*

$$\sum_{i=1}^{k} H(P_{n_i}) + \frac{m-n+k}{2} \leq H(G) \leq \frac{\sum_{i=1}^{k} n_i^2}{4} - \frac{n}{4} + \frac{m}{2}$$

with left equality holding if and only if $G_i \cong P_{n_i}$ *or* K_3 *for* $i = 1, 2, \ldots, k$ *and right equality holding if and only if* G_i *has diameter at most* 2 *for* $i = 1, 2, \ldots, k$.

Theorem 2.1.21 ([16]) *Let* G *be a graph of order* n *and with* m *edges and* k *components where* $1 \leq k \leq n$. *Then we have*

$$f(n,k) + \frac{m-n+k}{2} \leq H(G) \leq \frac{(n-k+1)(n-k)}{4} + \frac{m}{2}$$

with left equality holding if and only if $G \cong (k-s)P_r \cup sP_{r+1}$ *and right equality holding if and only if* $G \cong (k-1)K_1 \cup K_{n-k+1}$, *where* r, s *are integers with* $n = rk+s$ *and* $0 \leq s < k$.

2.2 Trees

When we study some property of graphs, a tree is generally viewed as the simplest graph to consider first as a starting point. In this section, we report some extremal results on trees with respect to Harary index.

Theorem 2.2.1 ([17, 18]) *Let* T *be a tree of order* n. *Then we have*

$$H(P_n) \leq H(T) \leq H(S_n)$$

with left equality holding if and only if $T \cong P_n$, *and right equality holding if and only if* $T \cong S_n$.

By Proposition 2.1.12, among all connected graphs, the extremal graph with the minimal Harary index must be a tree. Thus, by Theorem 2.2.1, we have

Corollary 2.2.2 ([12]) *Let* G *be a connected graph of order* n. *Then we have* $H(G) \geq H(P_n)$ *with equality holding if and only if* $G \cong P_n$.

Although by now, in chemical graph theory, the measure of branching cannot be formally defined [19], there are several properties that any proposed measure has to satisfy [20, 21]. Basically, a topological index (TI) acceptable as a measure of branching must satisfy the inequalities

$$\mathrm{TI}(S_n) < \mathrm{TI}(T) < \mathrm{TI}(P_n) \;\; or \;\; \mathrm{TI}(P_n) < \mathrm{TI}(T) < \mathrm{TI}(S_n)$$

for any tree T of order $n \geq 5$ different from S_n and P_n. From Theorem 2.2.1, we find that Harary index (H) satisfies the basic requirement to be a branching index.

Taking Theorem 2.2.1 into consideration, we naturally ask: *Which trees have the extremal Harary indices among the trees of order* n *different from* S_n *and* P_n? The next two theorems will give an answer to this question, in which the ordering of trees will be extended with respect to Harary index.

Before stating these two theorems, we first introduce some necessary notations and definitions. A vertex v of a tree T is called a *branching point* if $d_T(v) \geq 3$. Let $T_n(n_1, n_2, \ldots, n_m)$ be a starlike tree of order n obtained by inserting $n_1 - 1, \ldots, n_m - 1$ vertices into m edges of the star S_{m+1}, respectively, where $n_1 + \cdots + n_m = n - 1$. Note that any tree with exactly one branching point is a starlike tree. Assume that T is a tree of order n with exactly two branching points v_1 and v_2 with $d_T(v_1) = r$ and $d_T(v_2) = t$. The orders of $r - 1$ components, which are paths, of $T - v_1$ are $p_1, \ldots, p_{r-1}$, the order of the component which is not a path of $T - v_1$ is $p_r = n - p_1 - \cdots - p_{r-1} - 1$. The orders of $t - 1$ components, which are paths, of $T - v_2$ are $q_1, \ldots, q_{t-1}$, the order of the component which is not a path of $T - v_2$ is $q_t = n - q_1 - \cdots - q_{t-1} - 1$. We denote this tree by $T = T_n(p_1, \ldots, p_{r-1}; q_1, \ldots, q_{t-1})$, where $r \leq t$, $p_1 \geq \cdots \geq p_{r-1}$ and $q_1 \geq \cdots \geq q_{t-1}$.

For convenience, when considering the trees $T_n(n_1, n_2, \ldots, n_k, \ldots, n_m)$ or $T_n(p_1, \ldots, p_k, \ldots, p_{r-1}; q_1, \ldots, q_k, \ldots, q_{t-1})$, we use the symbols $n_k^{l_k}$ or $p_k^{l_k}$ (resp. $q_k^{l_k}$) to indicate that the number of n_k or p_k (resp. q_k) is $l_k > 1$ in the following. For example, $T_{16}(2, 2, 3, 3, 5)$ will be written as $T_{16}(2^2, 3^2, 5^1)$. Let $T_2, T_3, \ldots, T_8$ be the trees of order $n \geq 14$ as shown in Fig. 2.4.

Theorem 2.2.3 ([18]) *Suppose that T is a tree of order $n \geq 16$. Then we have*

$$\begin{aligned} H(P_n) &< H(T_n(n-3, 1^2)) < H(T_n(n-4, 2, 1)) < H(T_n(1^2; 1^2)) \\ &< H(T_n(n-5, 3, 1)) < H(T_n(1^2; 2, 1)) < H(T_n(n-4, 1^3)) < H(T). \end{aligned}$$

Theorem 2.2.4 ([18]) *Suppose that T is a tree of order $n \geq 16$. Then we have*

$$\begin{aligned} H(T) &< H(T_8) < H(T_7) < H(T_6) < H(T_5) \\ &< H(T_4) < H(T_3) < H(T_2) < H(S_n). \end{aligned}$$

In the theorem below, we assume that $n - 1 = kq + r$ with $0 \leq r < k$, that is, $q = \left\lfloor \frac{n}{k} \right\rfloor$. Obviously, we have $n - 1 = k\left\lfloor \frac{n}{k} \right\rfloor + r = (k - r)\left\lfloor \frac{n}{k} \right\rfloor + r\left\lceil \frac{n}{k} \right\rceil$.

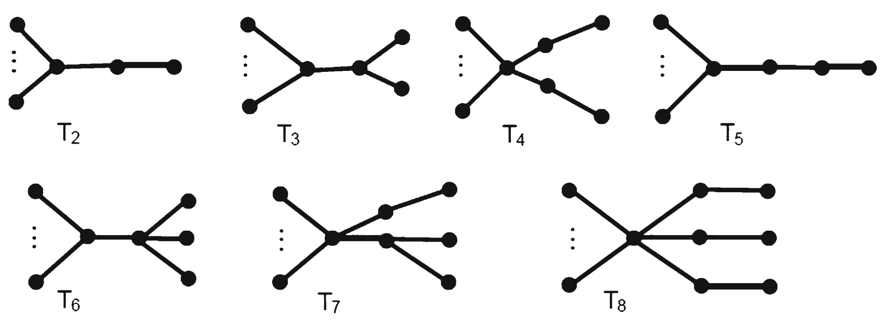

Fig. 2.4 The trees $T_2, T_3, \ldots, T_8$ encountered in Theorem 2.2.4

Theorem 2.2.5 ([22]) *Let T be a tree with n vertices and k pendant vertices, where $2 \le k \le n-2$. Then*

$$H(T) \le H\left(T_n\left(\left\lceil \frac{n}{k} \right\rceil^r, \left\lfloor \frac{n}{k} \right\rfloor^{k-r}\right)\right)$$

with equality holding if and only if $T \cong T_n(\left\lceil \frac{n}{k} \right\rceil^r, \left\lfloor \frac{n}{k} \right\rfloor^{k-r})$.

Recall that $T_n(2^{\beta-1}, 1^{n-2\beta+1})$ is a tree defined as above. Clearly, the matching number of $T_n(2^{\beta-1}, 1^{n-2\beta+1})$ is β, and there is exactly one tree with n vertices and matching number $\beta = 1$, which is just the star S_n. Recently, the maximal Harary index in the class of trees with n vertices and matching number $\beta \ge 2$ were determined in the following theorem.

Theorem 2.2.6 ([22, 23]) *Let T be a tree with n vertices and matching number $2 \le \beta \le \left\lfloor \frac{n}{2} \right\rfloor$. Then*

$$H(T) \le H(T_n(2^{\beta-1}, 1^{n-2\beta+1}))$$

where the equality holds if and only if $T \cong T_n(2^{\beta-1}, 1^{n-2\beta+1})$.

It is well-known that $\alpha + \beta = n$ for a bipartite graph G of order n and with matching number β and independence number α (see, e.g., [24]). Therefore, the following corollary can be easily obtained from Theorem 2.2.6.

Corollary 2.2.7 ([22, 23]) *Let T be a tree with n vertices and independence number α. Then*

$$H(T) \le H(T_n(2^{n-\alpha-1}, 1^{2\alpha-n+1}))$$

with equality holding if and only if $T \cong T_n(2^{n-\alpha-1}, 1^{2\alpha-n+1})$.

For $2 \le \Delta \le n-1$, the *Volkmann tree* $V_{n,\Delta}$ is defined as follows [25, 26]:

If $n = \Delta + 1$, then $V_{n,\Delta}$ is just a star of order n;

For $n > \Delta + 1$, define n_i as $n_i = 1 + \sum_{j=1}^{i} \Delta(\Delta-1)^j$ for $i = 1, 2, \ldots$, and choose k such that $n_{k-1} < n \le n_k$.

Then calculate the parameters m and h by $m = \dfrac{n - n_{k-1}}{\Delta - 1}$ and $h = n - n_{k-1} - (\Delta - 1)m$.

The vertices of $V_{n,\Delta}$ are arranged into $k+1$ levels. In level 0, there is only one vertex labeled as $v_{0,1}$. In level i for $i = 1, 2, \ldots, k-1$, there are $\Delta(\Delta-1)^i$ vertices labeled as $v_{i,1}, v_{i,2}, \ldots, v_{i,\Delta(\Delta-1)^i}$. These are connected (in that order) to the vertices in level i, so that $\Delta - 1$ vertices from level i are adjacent to each vertex from level $i-1$. At level k there are $n - n_{k-1}$ vertices, labeled as $v_{k,1}, v_{k,2}, \ldots, v_{k,n-n_{k-1}}$. They are connected (in that order) to the vertices in level $k-1$, so that $\Delta - 1$ vertices from level k are adjacent to vertices $v_{k-1,1}, v_{k-1,2}, \ldots, v_{k-1,m}$. The remaining h vertices at level k (if any) are connected to the vertex $v_{k-1,m+1}$ in level $k-1$. To illustrate the structure of $V_{n,\Delta}$, we give an example in Fig. 2.5 for $n = 22$ and $\Delta = 4$.

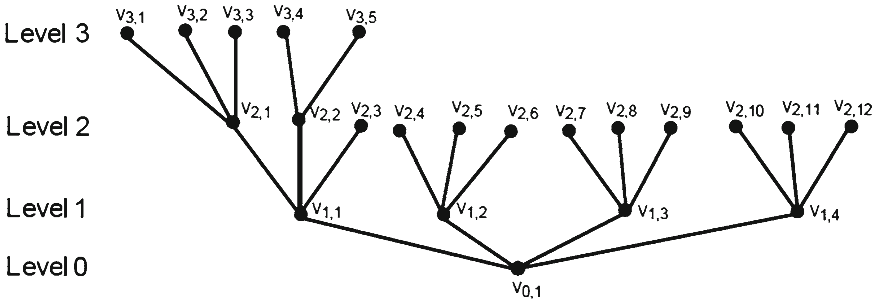

Fig. 2.5 The Volkmann tree $V_{22,4}$ with its vertices labeled

Theorem 2.2.8 ([15, 22, 27, 28]) *Let T be a tree with n vertices and maximum degree $\Delta \geq 3$. Then we have*

$$H(T_n(n-\Delta, 1^{\Delta-1})) \leq H(T) \leq H(V_{n,\Delta})$$

with left equality holding if and only if $T \cong T_n(n-\Delta, 1^{\Delta-1})$ and right equality holding if and only if $T \cong V_{n,\Delta}$.

In view of Proposition 2.1.12 and Theorem 2.2.8, the following result can be easily obtained.

Corollary 2.2.9 ([27]) *Let G be a connected graph of order n and with maximum degree Δ. Then we have*

$$H(G) \geq H(T_n(n-\Delta, 1^{\Delta-1}))$$

with equality holding if and only if $T \cong T_n(n-\Delta, 1^{\Delta-1})$.

In the next theorem, the extremal tree maximizing the Harary index is characterized completely among all trees of order n and with diameter d.

Theorem 2.2.10 ([22, 27]) *Let T be a tree with n vertices and diameter d, where $3 \leq d \leq n-2$. Then*

$$H(T) \leq H\left(T_n\left(\left\lceil \frac{d}{2} \right\rceil, \left\lfloor \frac{d}{2} \right\rfloor, 1^{n-d-1}\right)\right)$$

with equality holding if and only if $T \cong T_n(\left\lceil \frac{d}{2} \right\rceil, \left\lfloor \frac{d}{2} \right\rfloor, 1^{n-d-1})$.

2.3 Generalized Trees

A unicyclic graph is a connected graph of order n and with n edges, which can be obtained by adding a new edge into a tree. Similarly, a bicyclic graph is a connected graph of order n and with $n + 1$ edges, which can be obtained by adding two new edges into a tree, i.e., by adding a new edge into a unicyclic graph. Therefore these two classes of graphs can be viewed as generalized trees. In this section we will determine some extremal results with respect to Harary index on these two classes of generalized trees.

Before presenting our main results, we first introduce some necessary notations. Denote by $C_k(n_1^{l_1}, n_2^{l_2}, \ldots, n_m^{l_m})$ the unicyclic graph obtained by attaching l_1 paths of length n_1, l_2 paths of length n_2, $\ldots$, l_m paths of length n_m, respectively, to one vertices of C_k, where $n_1 > n_2 > \cdots > n_m$. Note that the graph $C_k(l^1)$ defined in Sect. 2.1 is a special graph of $C_k(n_1^{l_1}, n_2^{l_2}, \ldots, n_m^{l_m})$. For example, the graph $C_5(4^1, 3^2, 2^2)$ is shown in Fig. 2.6. There are exactly two unicyclic graphs C_4 and $C_3(1^1)$ of order 4 with $H(C_4) = H(C_3(1^1))$. So we assume that $n \geq 5$ in the following theorem.

Theorem 2.3.1 ([29]) *Let G be a unicyclic graph of order $n \geq 5$. Then we have*

$$H(C_3((n-3)^1)) \leq H(G) \leq H(C_3(1^{n-3}))$$

where the left equality holds if and only if $G \cong C_3((n-3)^1)$, and the right equality holds if and only if $G \cong C_3(1^{n-3})$ for $n \geq 6$ and $G \cong C_3(1^{n-3})$ or $G \cong C_5$ for $n = 5$.

There is exactly one unicyclic graph C_3 with n vertices and matching number 1. For $n = 5$ and $\beta = 2$, we can easily check [29] that only two graphs C_n and $C_3(1^2)$ have the maximal Harary index among all unicyclic graphs of order n and with matching number 2. We find that [30] the unique graph $C_3(1^{n-3})$ has the maximal Harary index among these unicyclic graphs of order n and with matching number 2. Next, we present the extremal unicyclic graphs with maximal Harary index among all the unicyclic graphs with n vertices and matching number $\beta \geq 3$.

Theorem 2.3.2 ([31]) *Let G be a unicyclic graph with $n \geq 9$ vertices and matching number $\beta \geq 3$. Then*

$$H(G) \leq H(C_3(2^{\beta-2}, 1^{n-2\beta+1}))$$

with equality holding if and only if $G \cong C_3(2^{\beta-2}, 1^{n-2\beta+1})$.

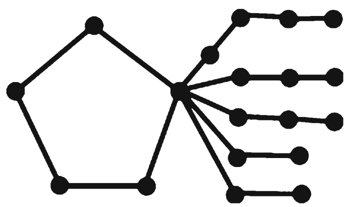

Fig. 2.6 The graph $C_5(4^1, 3^2, 2^2)$

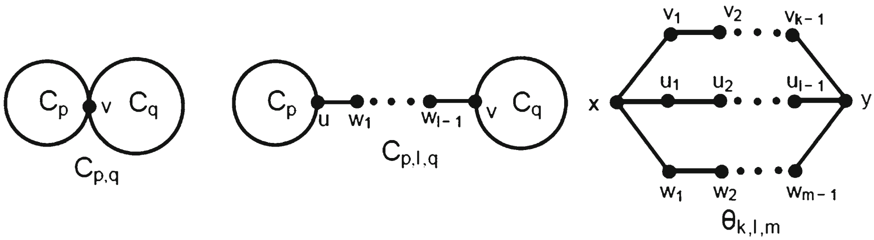

Fig. 2.7 The base graphs of type (I), (II), and (III)

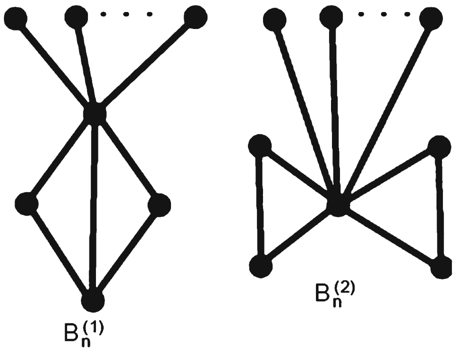

Fig. 2.8 The bicyclic graphs $B_n^{(1)}$ and $B_n^{(2)}$

In the next step, we turn to the determination of extremal Harary indices of bicyclic graphs. For any bicyclic graph G, the structure of cycles in G can be divided into the following three cases (see [32]):

(I) The two cycles C_p and C_q in G have only one common vertex v;
(II) The two cycles C_p and C_q in G are linked by a path of length $l > 0$;
(III) The two cycles C_{l+k} and C_{l+m} in G have a common path of length $l > 0$.

As shown in Fig. 2.7, the bicyclic graphs $C_{p,q}$, $C_{p,l,q}$ and $\theta_{k,l,m}$ (where $1 \le l \le \min\{k, m\}$) corresponding to the above three cases are called the base subgraphs of bicyclic graph G of type (I), (II) and (III), respectively. For $n \ge 5$, let $B_n^{(1)}$ and $B_n^{(2)}$ be the bicyclic graphs as shown in Fig. 2.8.

For $n \ge 5$, let $B_n^{(0)}$ be a graph obtained by attaching a path of length $n - 4$ to one vertex of degree 2 pertaining to $\theta_{2,1,2}$ (see Fig. 2.9). In [33], the extremal graph with maximal Harary index has been determined among all bicyclic graphs of order n and with exactly two cycles. In the following two theorems, we characterize completely the extremal bicyclic graphs with respect to Harary index in the class of bicyclic graphs of order $n \ge 5$.

Theorem 2.3.3 ([29]) *Let G be a bicyclic graph of order $n \ge 5$ and $i \in \{1, 2\}$. Then we have*

$$H(G) \le H(B_n^{(i)})$$

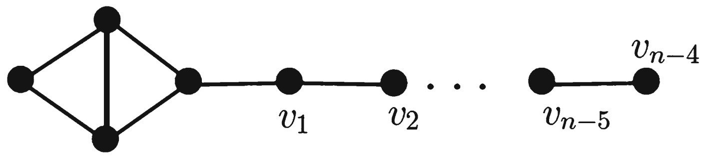

Fig. 2.9 The graph $B_n^{(0)}$

with equality holding if and only if $G \cong B_n^{(i)}$ *for* $n \geq 7$ *and* $G \cong B_n^{(i)}$ *or* $G \cong \theta_{2,2,3}$ *for* $n = 6$ *and* $G \cong B_n^{(i)}$ *or* $G \cong \theta_{2,1,3}$ *or* $G \cong K_{2,3}$ *for* $n = 5$.

Theorem 2.3.4 ([29]) *Let* G *be a bicyclic graph of order* $n \geq 5$. *Then we have*

$$H(B_n^{(0)}) \leq H(G)$$

where the equality holds if and only if $G \cong B_n^{(0)}$.

Although the extremal graphs with respect to Harary index have been completely determined among all unicyclic or bicyclic graphs of order n, there are still some interesting and challenging problems on this topic, such as determining the extremal graphs with respect to Harary index among all graph in some classes of unicyclic or bicyclic graphs, dealing with some extremal results among all connected graphs of order n and $m \geq n + 2$ edges. These problems seem to be attractive to many mathematical researchers.

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