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Maximal hitting times for random walks on bicyclic graphs with a given number of pendant vertices

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Abstract. Let $H_G(x, y)$ be the expected hitting time from vertex x to vertex y for the first time on a simple connected graph G and $\varphi(G) = \max_{x,y \in V(G)} H_G(x, y)$. Let $\mathcal{G}_n^t$ be the set of simple connected graphs with n vertices and t pendant vertices. In this paper, we proved the upper bound of the $\varphi(G)$ for $G \in \mathcal{G}_n^t$ and determined the extremal graph in all n-vertex bicyclic graphs with given t pendant vertices.

1. Introduction

Let $G = (V(G), E(G))$ be a graph with vertex set $V(G)$ and edge set $E(G)$. For any vertex $x \in V(G)$, $N(x)$ is used to be the set of adjacent vertices of vertex x, i.e., $N(x)$ is the neighbor set of x. Let $N[x]$ be the induced subgraph of G induced by x and all vertices adjacent to x. The degree of vertex x in G is denoted by $d_G(x)$ and if $d_G(x) = 1$, then we call vertex x a pendant vertex. The distance between vertices x and y in G is denoted by $d_G(x, y)$, abbreviated as $d(x, y)$ if G is clear. For vertices x and y in G, the hitting time $H_G(x, y)$ is the expected number of steps it takes from vertex x to vertex y for the first time. If the graph G is clear from the context, we use $H(x, y)$ instead of $H_G(x, y)$. If $A \subseteq V(G)$, then $H_G(x, A)$ is the expected hitting time from vertex x to reach a vertex in set A for the first time. If $x \in A$, then $H_G(x, A) = 0$. For a given graph G, the hitting time of G is defined as

$$\varphi(G) = \max_{x,y \in V(G)} H_G(x, y).$$

Let $\mathcal{G}_n^t$ be the set of simple connected graphs with n vertices and t pendant vertices. Let $\phi(n) := \max\{\varphi(G) : G \in \mathcal{G}_n^t\}$. If there is a graph G in $\mathcal{G}_n^t$ such that $\phi(n) = \varphi(G)$, then G is called an n-maximal graph for $\mathcal{G}_n^t$.

Let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ be two simple connected graphs such that $V_1 \cap V_2 = \{x, y\}$ and $E_1 \cap E_2 = \emptyset$. If G is composed of G_1 and G_2, then there is $V(G) = V_1 \cup V_2$ and $E(G) = E_1 \cup E_2$. In this case, G can be described as a graph obtained by pasting G_1 and G_2 through vertices x and y, in other words, G_1 and G_2 are two subgraphs obtained by decomposing G through vertices x and y. The effective resistance

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$R(x, y)$ between x and y can be defined as the potential difference between x and y when a unit current from x to y is maintained. While G is treated as an electrical network and each edge of G is replaced with a unit resistor, $R_G(x, y)$ is the effective resistance between x and y in G by Ohm's law.

An n-vertex bicyclic graph is a graph that contains two cycles with $n + 1$ edges. For any bicyclic graph, the two cycles in the graph can be divided into two cases, one case is that two cycles have no edges in common and the other case is that two cycles have at least one edge in common. Let $\mathcal{B}^t(n)$ be the set of all bicyclic graphs with n vertices and t pendant vertices. In particular, $\mathcal{B}_1^t(n)$ is defined as the subset of $\mathcal{B}^t(n)$ in consisting of all bicyclic graphs in which the two cycles share no common edges, and the set $\mathcal{B}_2^t(n)$ is defined as the subset of $\mathcal{B}^t(n)$ comprising all bicyclic graphs in which the two cycles share at least one common edge.

If $G \in \mathcal{B}_1^t(n)$, then G has two cycles, say C_p and C_q, which intersect with no edges. Without loss of generality, we assume that $C_p = uu_1 \cdots u_{p-1}u$, $C_q = vv_1 \cdots v_{q-1}v$, and $P_m = uw_1 \cdots w_{m-1}v$ is a unique path of length m from vertex u to vertex v, and the trees T_u, T_v, T_{u_i}, T_{v_j}, and T_{w_k} are pasted onto u, v, u_i, v_j, and w_k, respectively. Moreover, we denote G by $G = B(C_p, P, C_q)$ (see the left graph in Figure 1). If $m = 0$, then the length of P is zero, so C_p and C_q have a common vertex, that is, $u = v$; if $m = 1$, then $P = uv$. In addition, let $B_{n,t}^{p,q}$ be a bicyclic graph of order n with t pendant vertices in which two cycles C_p and C_q have only one intersection vertex. A star tree S_t is attached at any vertex of C_p (excluding the intersection vertex), which contains $t - 1$ pendant vertices, a path of length $(n - p - q - t + 2)$ is pasted on vertex v_i on C_q. Specifically, if $p = q = 3$, then we denote this bicyclic graph by $B_1^t(n)$ (see Figure 2).

If $G \in \mathcal{B}_2^t(n)$, then G has two cycles C_p and C_q which share at least one common edge, it means that G contains paths with three non-intersecting edges at the same start vertex and end vertex. Without loss of generality, we denote $P_a = xu_1u_2 \cdots u_{a-1}y$, $P_b = xw_1w_2 \cdots w_{b-1}y$, and $P_c = xv_1v_2 \cdots v_{c-1}y$ to be three paths. Then the lengths of these three paths are a, b, and c, respectively. Therefore, graph G mainly consists of eight parts, namely P_a, P_b, P_c and $T_{u_i}(1 \le i \le a-1)$, $T_{v_j}(1 \le j \le b-1)$, $T_{w_k}(1 \le k \le c-1)$, T_x, T_y with root vertices u_i, v_j, w_k, x, and y, respectively. (see the right graph in Figure 1). Let $B_{n,t}^{a,b,c}$ be a bicyclic graph that consists of three non-intersecting paths P_a,P_b, P_c, and a star tree with $t-1$ pendant vertices is pasted on some vertex of P_a, and a path of length $(n-a-b-c-t-1)$ is pasted on any vertex of P_c, excluding vertices x and y. Specifically, if $a = c = 1$ and $b = 0$, i.e., then the bicyclic graph contains three disjoint paths $P_a = xu_1y$, $P_b = xy$, $P_c = xv_1y$, and a path of length $(n-t-3)$ is pasted at vertex v_1 and a star tree S_t is pasted at vertex u_1, then let $B_2^t(n)$ be such a bicyclic graph (see Figure 3).

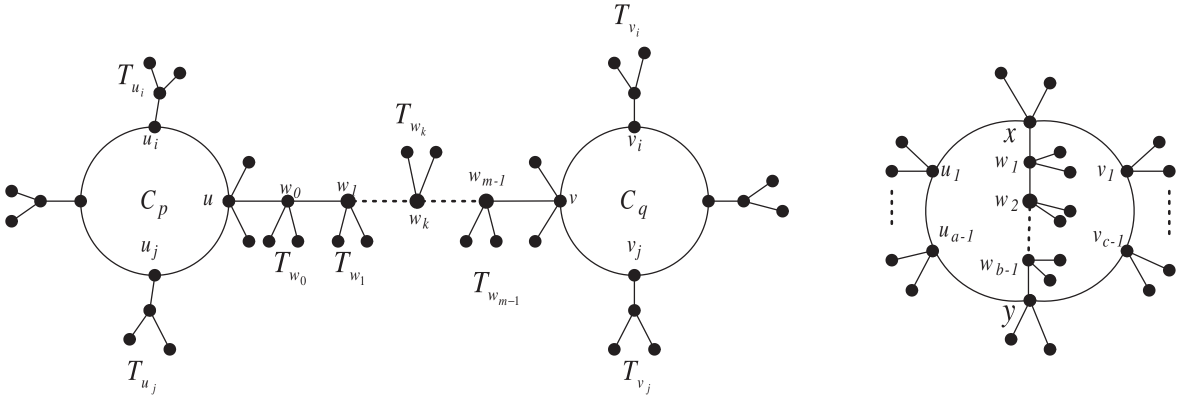


Figure 1: $\mathcal{B}_1^t(n)$ and $\mathcal{B}_2^t(n)$.

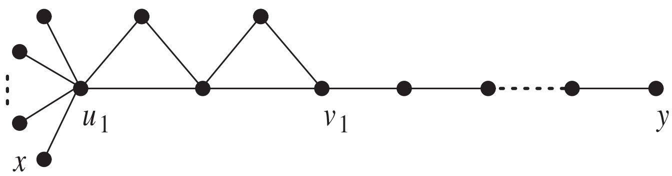


Figure 2: $B_1^t(n)$.

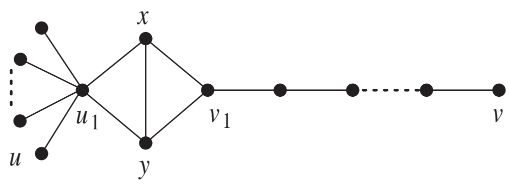


Figure 3: $B_2^t(n)$.

Random walks on graphs have been investigated in many aspects and fields. The theory of random walk is generally related to graphs and their related branches, such as effective resistance distance, topological index, and the hitting time of some special graph classes. Hitting time, access time, cover time, and other key parameters are used for studying random walks on graphs. Bollobás [1] introduced the basic knowledge of random walks on graphs and the relevant calculation formulas and methods for the hitting time on graphs. Río and Palacios [15] derived a formula to decompose the walking hitting time on the graph into simpler times. Tetali [16] indicated the relationship between the number of traversals between effective resistance nodes x and y and the expected number of random walks along any specific edge of the two nodes x and y. Similarly, Klein and Randić [10] also indicated the close relationship between random walks and effective resistance distance. Cheng and Zhang [5] used the power network method to prove the formula for the hitting time of simple random walks on trees and unicyclic graphs with cutpoints. Huang, Li, and Xie [9] explained the close relationship between the hitting time, Kirchhoff index, resistance centrality, and related invariants of simple random walks on the graph, and clarified the upper and lower bounds on the cover cost of a single loop graph. Zhang and Li [19] studied some extreme value problems of the ZZ-index on trees, and under certain given parameters, clarified in detail the upper and lower bounds on the hitting time of the tree under the condition of given diameter, given number of matches, given number of pendant vertices and vertex partition. González-Arévalo and Palacios [7] derived a formula from the symmetry in the graph weak product inherited from the coordinate graph to calculate the expected hitting time of random walks on the graph. Palacios [13] utilized the symmetry and properties of the power network to provide a general boundary for a simple random walk of hitting times and cover times on some special undirected connected graphs.

In addition, Brightwell and Winkler [2] proved that the lollipop graph G with n vertices and vertices x and y make $H_G(x, y)$ the maximum hitting time among all n vertices in the graphs, and provided the maximum values of the extremal graph and $\varphi(G)$. Therefore, if the number of vertices in a graph remains constant, then its extremal graph is also fixed. This result prompts us to consider the following problem when the number of vertices and edges remains constant. Zhang and Li [19] obtained the upper bound on the hitting time of a tree under the condition that the number of pendant vertices remains unchanged. The extremal graph can be described as a path with a length of $(n - p - 1)$ and a star graph with $p - 1$ pendant vertices are pasted at the starting vertex of this path. In addition, Zhu and Zhang [22, 23] provided upper and lower bounds on the hitting time of unicyclic graphs and bicyclic graphs and gave the extremal graphs of unicyclic graphs and bicyclic graphs. Zhu and Yang [21] provided upper and lower bounds on the hitting time of tricyclic graphs and gave the extremal graphs.

In this paper, we continue to study the maximal hitting times for random walks on bicyclic graphs with a given number of pendant vertices and use induction to prove relevant conclusions and derive its extremal graph. We have learned the relationship between the hitting time of a graph and its subgraph. The results are used to establish the upper bound for the hitting times of n-vertex bicyclic graphs with a given number of pendant vertices. The main result is stated as follows:

Theorem 1.1. *Let G be a bicyclic graph of order n with t pendant vertices. Then*

$$\varphi(G) \leq n^2 - t^2 + 2n - 6t - 11.$$

In addition, the equality holds if and only if G is a graph obtained by a path with $n - t - 2$ vertices, a star graph S_t, and $K_4 - e$, where $K_4 - e$ is a graph obtained by deleting one edge from complete graph K_4.

The rest of this paper is arranged as follows. In Section 2, we present symbols and some key results which will be used to prove the main results. In Section 3, we investigate the extremal problem of hitting times for n-vertex bicyclic graphs with t pendant vertices, classified according to the structure of their cycles. Specifically, the graphs are categorized into two distinct types: one type consists of bicyclic graphs whose two cycles are edge-disjoint, while the other type comprises bicyclic graphs whose two cycles share at least one common edge. In Section 4, we use the results of Section 3 to prove Theorem 1.1.

2. Preliminary

Theorem 2.1. *[19] Let T be an n-vertices tree with t pendant vertices for $n \geq 3$. Then*

$$\varphi(T) \leq n^2 - t^2 + 2t - 2n + 1. \tag{1}$$

The equality holds if and only if T is composed of P_{n-t} and a star tree S_t pasted at the start vertex of this path.

Theorem 2.2. *[20] Let G be any n-vertices unicyclic graph with t pendent vertices. Then*

$$\varphi(G) \leq n^2 - t^2 - \frac{8}{3}t - \frac{7}{3}. \tag{2}$$

Theorem 2.3. *[10] Let G be a connected graph and $x, y \in V(G)$. If there exists a cut vertex z such that x and y are not in a same component of $G - z$, then*

$$H_G(x, y) = H_G(x, z) + H_G(z, y). \tag{3}$$

Moreover, if there exists a unique path $P = xv_1 \dots v_{k-1}y$ in G, then

$$H_G(x, y) = H_G(x, v_1) + H_G(v_1, v_2) + \dots + H_G(v_{k-1}, y). \tag{4}$$

Theorem 2.4. *[2] Let G be a simple connected graph on n vertices and $x, y \in V(G)$. If there exists a unique path $P = v_0v_1 \dots v_k$ with $v_0 = x$ and $v_k = y$, and m_i is the number of edges of subgraph G_i, where G_i is the component of $G - v_0v_1, v_1v_2, \dots, v_{k-1}v_k$ containing v_i for $i = 0, \dots, k$, then*

$$H_G(x, y) = k^2 + 2\sum_{i=0}^{k-1} m_i(k - i). \tag{5}$$

Theorem 2.5. *[15] Let G_1 and G_2 be decomposition of G through x and y with $V(G_1) \cap V(G_2) = \{x, y\}$ and $E(G_1) \cap E(G_2) = \emptyset$. Then*

$$H_G(x, y) = \frac{R_2(x, y)}{R_1(x, y) + R_2(x, y)} H_{G_1}(x, y) + \frac{R_1(x, y)}{R_1(x, y) + R_2(x, y)} H_{G_2}(x, y). \tag{6}$$

where $R_1(x, y)$ and $R_2(x, y)$ are the effective resistance between x and y computed in graph G_1 and G_2 respectively.

Theorem 2.6. *[1] Let G be a simple connected graph on n vertices, $y, z \in V(G)$ and $z \in N(x)$, x, y, z represent three different vertices, respectively. Then*

$$H_G(x,y) = 1 + \frac{1}{d(x)} \sum_{z \in N(x)} H_G(z,y). \tag{7}$$

Lemma 2.7. *[22] Let G be a simple connected graph. If there exist two vertices $x, y \in V(G)$ such that $\varphi(G) = H_G(x,y)$, then x and y are not cut vertices.*

Lemma 2.8. *[22] Let x and y be two vertices of graph G and w be a vertex in $N[y]$ such that $\max_{v \in N(y)} H_G(v,y) = H_G(w,y)$ and $d_{N[y]}(w) = k+1$, where $d_{N[y]}(w)$ denotes the degree of vertex w in $N[y]$. Let N be the vertex set of $N[y]$ and G/N be the quotient graph obtained from G by contracting N to a single vertex (also denoted N) and identifying any resulting multiple edges.*

(1) If $N(y) \cap N(w) = \emptyset$, then $H_G(x,y) \le H_{G/N}(x,N) + 1 + 2(e(G) - e(N[y]))$;

(2) If $N(y) \cap N(w) \neq \emptyset$, then $H_G(x,y) \le H_{G/N}(x,N) + \frac{4e(G) - 2e(N[y]) - d(y) + k + 1}{k+2}$,

where $e(G)$ and $e(N[y])$ denote the edge number of G and $N[y]$, respectively.

3. The extremal hitting times on $\mathscr{B}_1^t(n)$ and $\mathscr{B}_2^t(n)$

In this part, we will prove that the upper bound of $\varphi(G)$ can be obtained and the maximal graph can also be obtained whenever $G \in \mathscr{B}_1^t$ or $G \in \mathscr{B}_2^t$.

Theorem 3.1. *Let $G \in \mathscr{B}_1^t(n)$ and $f(n) = n^2 - t^2 + 2n - \frac{22}{3}t - \frac{49}{3}, (t \ge 2, n \ge 15)$. Then*

$$\varphi(G) \le f(n).$$

The equality holds if and only if $G = B_1^t(n)$ and $\varphi(B_1^t(n)) = H_{B_1^t(n)}(x,y)$ is the hitting time from the pendant vertex x in S_t to the pendant vertex y in P_{n-t-3} with root vertex v_1 and $d(x,y) = n - t - 1$.

Proof. By Theorems 2.3, 2.4, 2.5 and Lemma 2.7, we have $H_{B_1^t(n)}(x,y) = n^2 - t^2 + 2n - \frac{22}{3}t - \frac{49}{3}, (t \ge 2, n \ge 15)$, which is the hitting time from the pendant vertex x in S_t to the pendant vertex y in P_{n-t-3} with root vertex v_1 and $d(x,y) = n-t-1$. Let $\phi_1(n) = \max\{\varphi(G) : G \in \mathscr{B}_1^t(n)\}$. Ultimately, we need to prove that $\phi_1(n) = f(n)$. If G is any graph with $\varphi(G) = f(n)$ in $\mathscr{B}_1^t(n)$, then $G = B_1^t(n)$ and $H_{B_1^t(n)}(x,y) = \varphi(G)$, where x and y are all pendant vertices such that $d(x,y) = n-t-1$. To prove the above conclusion, we use induction for n.

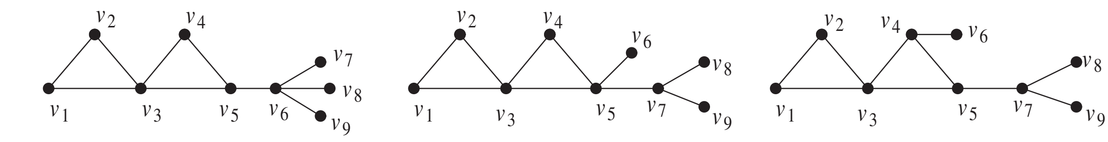
When $n = 9$ and $t = 3$, then $\mathscr{B}_1^3(9)$ contains 51 bicyclic graphs, denoted by $G_9^i, i = 1, \cdots, 51$ (see Figure 4).

Through calculations, we can obtain that

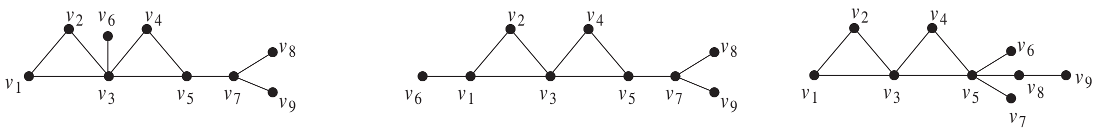
$$
\begin{array}{lll}
\varphi(G_9^1) = H(v_1, v_9) = 40, & \varphi(G_9^2) = H(v_1, v_9) = 42, & \varphi(G_9^3) = H(v_1, v_9) = \dfrac{128}{3}, \\
\varphi(G_9^4) = H(v_1, v_9) = \dfrac{130}{3}, & \varphi(G_9^5) = H(v_6, v_9) = \dfrac{137}{3}, & \varphi(G_9^6) = H(v_1, v_9) = 44, \\
\varphi(G_9^7) = H(v_9, v_7) = 38, & \varphi(G_9^8) = H(v_1, v_9) = \dfrac{140}{3}, & \varphi(G_9^9) = H(v_6, v_9) = \dfrac{151}{3}, \\
\varphi(G_9^{10}) = H(v_1, v_9) = \dfrac{134}{3}, & \varphi(G_9^{11}) = H(v_1, v_9) = \dfrac{136}{3}, & \varphi(G_9^{12}) = H(v_6, v_9) = \dfrac{143}{3}, \\
\varphi(G_9^{13}) = H(v_1, v_9) = 46, & \varphi(G_9^{14}) = H(v_6, v_9) = \dfrac{145}{3}, & \varphi(G_9^{15}) = H(v_6, v_9) = 49, \\
\varphi(G_9^{16}) = H(v_1, v_9) = 34, & \varphi(G_9^{17}) = H(v_5, v_9) = 38, & \varphi(G_9^{18}) = H(v_8, v_7) = \dfrac{125}{3}, \\
\varphi(G_9^{19}) = H(v_4, v_9) = 36, & \varphi(G_9^{20}) = H(v_9, v_8) = \dfrac{115}{3}, & \varphi(G_9^{21}) = H(v_9, v_8) = \dfrac{121}{3}, \\
\varphi(G_9^{22}) = H(v_8, v_7) = 41, & \varphi(G_9^{23}) = H(v_6, v_8) = \dfrac{121}{3}, & \varphi(G_9^{24}) = H(v_1, v_9) = \dfrac{106}{3}, \\
\varphi(G_9^{25}) = H(v_1, v_7) = \dfrac{110}{3}, & \varphi(G_9^{26}) = H(v_1, v_9) = \dfrac{110}{3}, & \varphi(G_9^{27}) = H(v_8, v_7) = \dfrac{137}{3}, \\
\varphi(G_9^{28}) = H(v_1, v_9) = \dfrac{110}{3}, & \varphi(G_9^{29}) = H(v_1, v_9) = \dfrac{112}{3}, & \varphi(G_9^{30}) = H(v_9, v_7) = 45, \\
\varphi(G_9^{31}) = H(v_1, v_9) = 38, & \varphi(G_9^{32}) = H(v_1, v_9) = 40, & \varphi(G_9^{33}) = H(v_9, v_7) = \dfrac{133}{3}, \\
\varphi(G_9^{34}) = H(v_1, v_9) = 28, & \varphi(G_9^{35}) = H(v_5, v_7) = 32, & \varphi(G_9^{36}) = H(v_1, v_9) = \dfrac{57}{2}, \\
\varphi(G_9^{37}) = H(v_5, v_9) = 23, & \varphi(G_9^{38}) = H(v_5, v_9) = \dfrac{91}{3}, & \varphi(G_9^{39}) = H(v_1, v_7) = 33, \\
\varphi(G_9^{40}) = H(v_1, v_9) = 30, & \varphi(G_9^{41}) = H(v_8, v_7) = 36, & \varphi(G_9^{42}) = H(v_1, v_9) = \dfrac{63}{2}, \\
\varphi(G_9^{43}) = H(v_8, v_9) = \dfrac{211}{6}, & \varphi(G_9^{44}) = H(v_5, v_7) = 33, & \varphi(G_9^{45}) = H(v_5, v_8) = \dfrac{95}{3}, \\
\varphi(G_9^{46}) = H(v_9, v_7) = \dfrac{69}{2}, & \varphi(G_9^{47}) = H(v_5, v_8) = \dfrac{97}{3}, & \varphi(G_9^{48}) = H(v_7, v_9) = \dfrac{69}{2}, \\
\varphi(G_9^{49}) = H(v_1, v_8) = 34, & \varphi(G_9^{50}) = H(v_8, v_7) = 37, & \varphi(G_9^{51}) = H(v_1, v_8) = 33.
\end{array}
$$

According to the value of the hitting time of each bicyclic graph calculated as above, we get $\phi_1(9) = \max\{\varphi(G_9^1), \cdots, \varphi(G_9^{51})\} = \varphi(G_9^9) = \frac{151}{3} = f(9)$. So G_9^9 is the only extremely graph of order 9 with 3 pendant vertices in $\mathcal{B}_1^3(9)$ and $d_{G_9^9}(v_6, v_9) = 9 - 3 - 1 = 5$, where x and y are all pendant vertices with $d(x, y) = n - t - 1$.

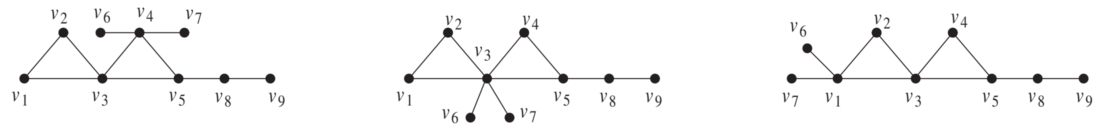
Graphs 1-3:



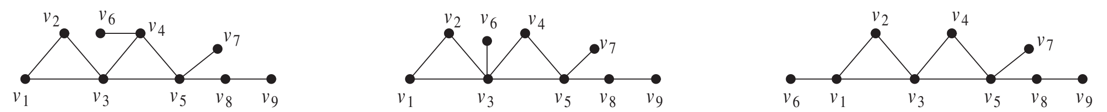
Graphs 4-6:



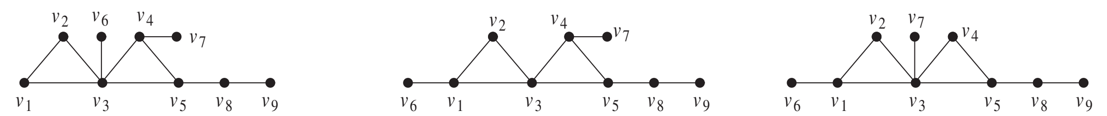
Graphs 7-9:



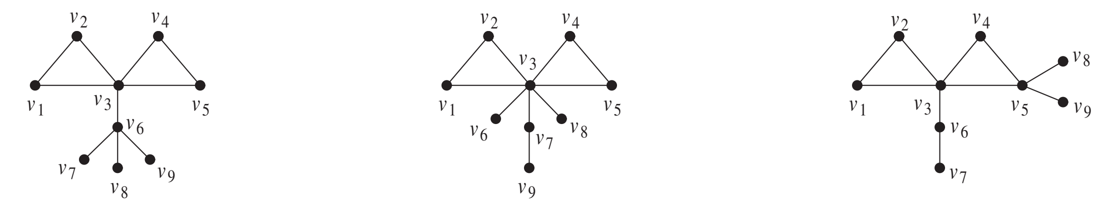
Graphs 10-12:



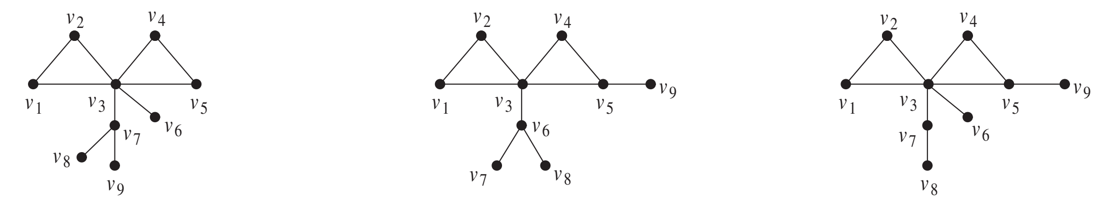
Graphs 13-15:



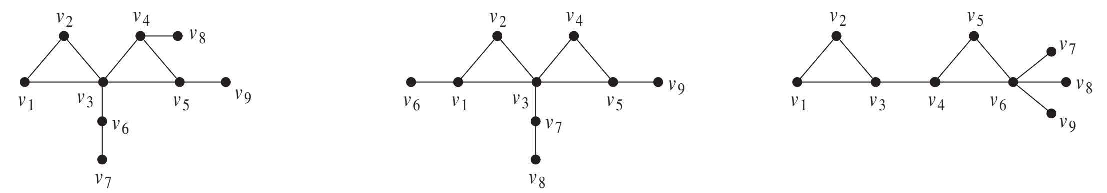
Graphs 16-18:



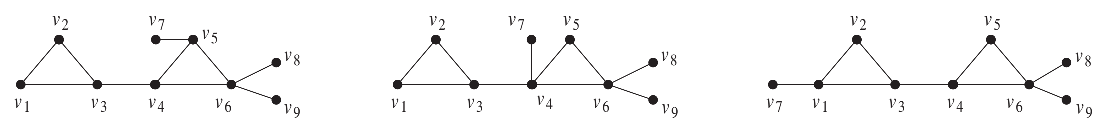
Graphs 19-21:



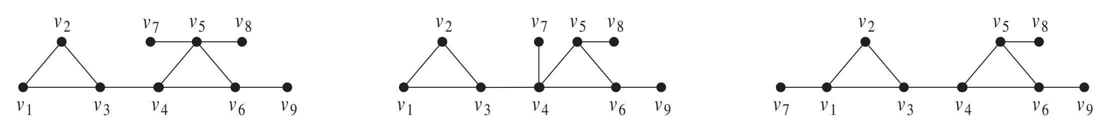
Graphs 22-24:



Graphs 25-27:



Graphs 28-30:



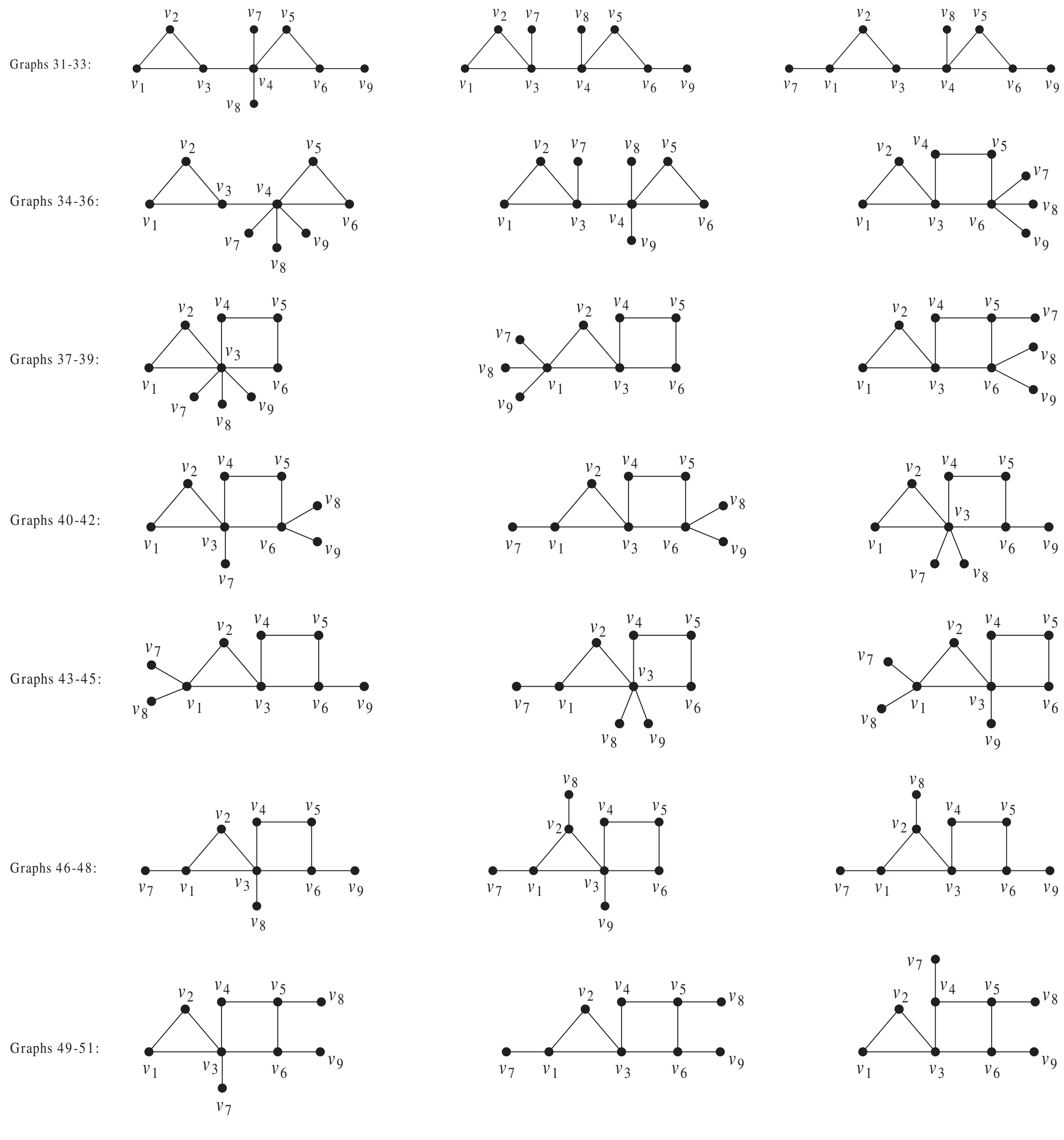


Figure 4: Bicyclic graphs in $\mathcal{B}_1^3(9)$.

We assume that the above conclusion holds for $n-1$. In other words, $\phi_1(n-1) = f(n-1)$. In addition, if G is any graph in $\mathcal{B}_1^t(n-1)$ with $\varphi(G) = f(n-1)$, then $G = B_1^t(n-1)$ and $H_{B_1^t(n-1)}(x, y) = \varphi(G)$, where x and y are all pendant vertices with $d(x, y) = (n-1) - t - 1 = n - t - 2$. Next, we will prove the above conclusion holds for n. Without loss of generality, we assume G is a n-maximal graph in $\mathcal{B}_1^t(n)$ approach $\varphi(G) = \phi_1(n)$. In that way, by the definition of $\varphi(G)$, there exist two vertices x and y in G such that $H_G(x, y) = \varphi(G) = \phi_1(n)$. By Lemma 2.7, y is not a cut vertex in G, we will consider the following two situations below.

Case 1. y is a vertex on the cycle in G with $d(y) = 2$. So there exists a vertex w in $N[y]$ that makes

$\max_{v\in N(y)} H_G(v,y) = H_G(w,y)$ and $d_{N[y]}(w) = k+1$.

Subcase 1.1. $k = 0$. Then $e(N[y]) = 2$, by Lemma 2.8, $N(y) \cap N(w) = \emptyset$ and $H_G(x,y) \le H_{G/N}(x,N) + 1 + 2(e(G) - e(N[y]))$. By substituting numerical values, then $H_G(x,y) \le H_{G/N}(x,N) + 2n - 1$. In addition, G/N is a unicyclic graph with $n-2$ vertices or $G/N \in \mathcal{B}_1^t(n-2)$.

If G/N is a unicyclic graph with $n-2$ vertices. Then by Theorem 2.2, $H_{G/N}(x,N) \le (n-2)^2 - t^2 - \frac{8}{3}t - \frac{7}{3} = n^2 - t^2 - 4n - \frac{8}{3}t + \frac{5}{3}$. So, $H_G(x,y) \le n^2 - t^2 - 2n - \frac{8}{3}t + \frac{2}{3} < f(n)$.

If $G/N \in \mathcal{B}_1^t(n-2)$. Then, $H_{G/N}(x,N) \le (n-2)^2 - t^2 + 2(n-2) - \frac{22}{3}t - \frac{52}{3}$. So, $H_G(x,y) \le (n-2)^2 - t^2 + 2(n-2) - \frac{22}{3}t - \frac{52}{3} + 2n - 1 = n^2 - t^2 - \frac{22}{3}t - \frac{55}{3} < f(n)$.

Subcase 1.2. $k = 1$. Then, $e(N[y]) = 3$. By Lemma 2.8, $N(y) \cap N(w) \ne \emptyset$. Therefore, $H_G(x,y) \le H_{G/N}(x,N) + \frac{4e(G)-2e(N[y])-d(y)+k+1}{k+2} = H_{G/N}(x,N) + \frac{4n-2}{3}$, by substituting numerical values $H_G(x,y) \le n^2 - t^2 - \frac{8}{3}n - \frac{8}{3}t + 1 < f(n)$.

Therefore, if y is a vertex on the cycle in G with $d(y) = 2$, then $\phi_1(n) = \varphi(G) < f(n)$.

Case 2. y is a pendant vertex in G, y has a unique adjacent vertex v. In that way, v must be a cut vertex in G and $G^- := G - y$ is a connected bicyclic graph with $n-1$ vertices and t pendant vertices. By Theorems 2.3 and 2.4, there are $H_G(x,y) = H_G(x,v) + H_G(v,y) = H_{G^-}(x,v) + H_G(v,y)$ and $H_G(v,y) = 2n+1$.

Subcase 2.1. By making inductive assumptions about G^-, $H_{G^-}(x,v) \le \phi_1(n-1) = f(n-1) = \varphi(B_1^t(n-1))$. Therefore, $\phi_1(n) = \varphi(G) = H_G(x,y) = H_{G^-}(x,v) + H_G(v,y) \le f(n-1) + 2n + 1 = f(n)$.

Subcase 2.2. Let both vertices x and y be pendant vertices such that $d(x,y) = n-t-1$. Let v be the unique adjacent vertex of y. By inductive assumption, we have

$$\begin{aligned} \phi_1(n) &\ge \varphi(B_1^t(n)) \ge H_{B_1^t(n)}(x,y) \\ &= H_{B_1^t(n)}(x,v) + H_{B_1^t(n)}(v,y) \\ &= H_{B_1^t(n-1)}(x,v) + 2n + 1 \\ &= f(n-1) + 2n + 1 = f(n). \end{aligned}$$

Therefore, $\phi_1(n) = f(n)$. In addition, G is any graph with n vertices in $\mathcal{B}_1^t(n)$ with $\varphi(G) = \phi_1(n) = f(n)$. All that there are two vertices x and y such that $H_G(x,y) = \varphi(G) = f(n)$, then y must be a pendant vertex. We use v to be the unique adjacent vertex of y, then $G - y$ is a bicyclic graph with $n-1$ vertices in $\mathcal{B}_1^t(n-1)$. By inductive assumption,

$$\begin{aligned} f(n) &= H_G(x,y) = H_G(x,v) + H_G(v,y) \\ &= H_{G-y}(x,v) + 2n + 1 \\ &\le \varphi(G-y) + 2n + 1 \\ &\le f(n-1) + 2n + 1 = f(n). \end{aligned}$$

The above formula indicates that $\varphi(G-y) = H_{G-y}(x,v) = f(n-1)$. By inductive assumption, $G - y$ must be $B_1^t(n-1)$ and v is a pendant vertex in $B_1^t(n-1)$. Therefore, $G = B_1^t(n)$ and $f(n) = \varphi(B_1^t(n)) = H_{B_1^t(n)}(x,y)$, where both x and y are pendant vertices with $d(x,y) = n-t-1$. Therefore, the above conclusion holds for all n. □

Theorem 3.2. *Let $G \in \mathcal{B}_2^t(n)$ and $g(n) = n^2 - t^2 + 2n - 6t - 11$, where $t \ge 2$. Then*

$$\varphi(G) \le g(n).$$

The equation holds if and only if $G = B_2^t(n)$ and $\varphi(B_2^t(n)) = H_{B_2^t(n)}(u,v)$, which is the hitting time from pendant vertex u in S_t with root vertex u_1 to pendant vertex v in P_{n-t-2} with root vertex v_1 and $d(u,v) = n-t$.

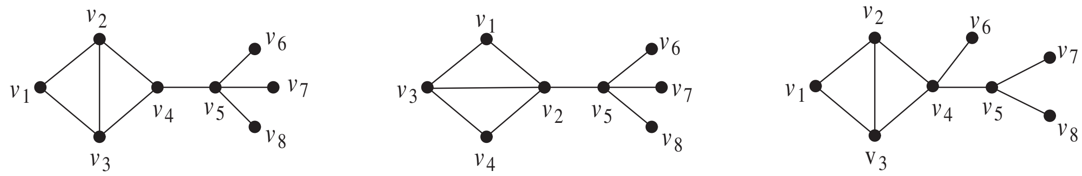
Proof. By Theorems 2.3, 2.4, 2.5, 2.6 and Lemma 2.7, we have $H_{B_2^t(n)}(u,v) = n^2 - t^2 + 2n - 6t - 11$, $(t \ge 2, n \ge 15)$, which is the hitting time from pendant vertex u in S_t with root vertex u_1 to pendant vertex v in P_{n-t-2} with root vertex v_1 and $d(u,v) = n-t$. Let $\phi_2(n) = \max\{\varphi(G) : G \in \mathcal{B}_2^t(n)\}$, we need to prove $\phi_2(n) = g(n) = n^2 - t^2 + 2n - 6t - 11$ and $\varphi(G) = g(n)$ for any graph G, then $G = B_2^t(n)$ and $g(n) = H_{B_2^t(n)}(u,v)$, where both u and v are pendant vertices with $d(u,v) = n-t$. To prove the above results, we use induction for n.

When $n = 8$ and $t = 3$, then $\mathcal{B}_2^3(8)$ contains 46 bicyclic graphs, denoted by G_8^j, $j = 1, \cdots, 46$ (see Figure 5). Through simple calculations,

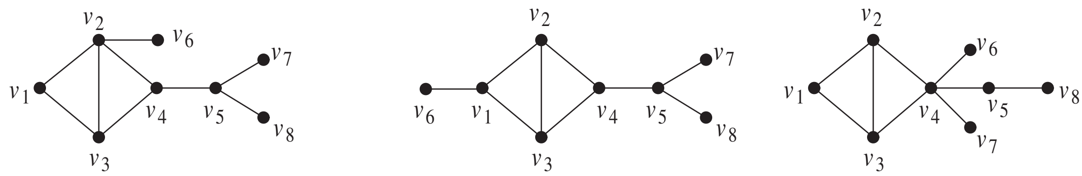
$$\varphi(G_8^1) = H(v_1, v_8) = 33, \quad \varphi(G_8^2) = H(v_3, v_8) = \frac{61}{2}, \quad \varphi(G_8^3) = H(v_1, v_8) = 35,$$
$$\varphi(G_8^4) = H(v_6, v_8) = \frac{145}{4}, \quad \varphi(G_8^5) = H(v_6, v_8) = 38, \quad \varphi(G_8^6) = H(v_1, v_8) = 37,$$
$$\varphi(G_8^7) = H(v_6, v_8) = \frac{153}{4}, \quad \varphi(G_8^8) = H(v_6, v_8) = 40, \quad \varphi(G_8^9) = H(v_6, v_8) = \frac{79}{2},$$
$$\varphi(G_8^{10}) = H(v_6, v_8) = 41, \quad \varphi(G_8^{11}) = H(v_6, v_8) = 42, \quad \varphi(G_8^{12}) = H(v_1, v_8) = \frac{65}{2},$$
$$\varphi(G_8^{13}) = H(v_6, v_8) = \frac{69}{2}, \quad \varphi(G_8^{14}) = H(v_6, v_8) = \frac{69}{2}, \quad \varphi(G_8^{15}) = H(v_1, v_8) = \frac{69}{2},$$
$$\varphi(G_8^{16}) = H(v_5, v_8) = \frac{73}{2}, \quad \varphi(G_8^{17}) = H(v_5, v_8) = \frac{73}{2}, \quad \varphi(G_8^{18}) = H(v_5, v_8) = \frac{151}{4},$$
$$\varphi(G_8^{19}) = H(v_6, v_8) = 37, \quad \varphi(G_8^{20}) = H(v_5, v_8) = \frac{75}{2}, \quad \varphi(G_8^{21}) = H(v_1, v_8) = \frac{266}{11},$$
$$\varphi(G_8^{22}) = H(v_4, v_8) = \frac{233}{11}, \quad \varphi(G_8^{23}) = H(v_4, v_8) = 24, \quad \varphi(G_8^{24}) = H(v_1, v_6) = \frac{282}{11},$$
$$\varphi(G_8^{25}) = H(v_1, v_8) = \frac{280}{11}, \quad \varphi(G_8^{26}) = H(v_7, v_6) = \frac{327}{11}, \quad \varphi(G_8^{27}) = H(v_7, v_6) = \frac{186}{7},$$
$$\varphi(G_8^{28}) = H(v_8, v_6) = 29, \quad \varphi(G_8^{29}) = H(v_6, v_8) = \frac{304}{11}, \quad \varphi(G_8^{30}) = H(v_6, v_8) = \frac{317}{11},$$
$$\varphi(G_8^{31}) = H(v_1, v_8) = \frac{294}{11}, \quad \varphi(G_8^{32}) = H(v_7, v_6) = \frac{258}{11}, \quad \varphi(G_8^{33}) = H(v_5, v_6) = \frac{288}{11},$$
$$\varphi(G_8^{34}) = H(v_6, v_7) = \frac{302}{11}, \quad \varphi(G_8^{35}) = H(v_6, v_8) = \frac{304}{11}, \quad \varphi(G_8^{36}) = H(v_6, v_8) = \frac{317}{11},$$
$$\varphi(G_8^{37}) = H(v_4, v_6) = 26, \quad \varphi(G_8^{38}) = H(v_1, v_8) = 23, \quad \varphi(G_8^{39}) = H(v_4, v_8) = 21,$$
$$\varphi(G_8^{40}) = H(v_6, v_8) = \frac{73}{3}, \quad \varphi(G_8^{41}) = H(v_7, v_6) = 28, \quad \varphi(G_8^{42}) = H(v_8, v_6) = 27,$$
$$\varphi(G_8^{43}) = H(v_6, v_8) = 25, \quad \varphi(G_8^{44}) = H(v_7, v_8) = \frac{77}{3}, \quad \varphi(G_8^{45}) = H(v_6, v_8) = \frac{74}{3},$$
$$\varphi(G_8^{46}) = H(v_6, v_8) = 27.$$

According to the value of the hitting time of each bicyclic graph calculated as above, we have $\phi_2(8) = \max\{\varphi(G) : G \in \mathcal{B}_2^3(8)\} = \varphi(G_8^{11}) = g(8) = 42$ and $d(v_6, v_8) = 8 - 3 = 5$, so the above conclusion holds for $n = 8$.

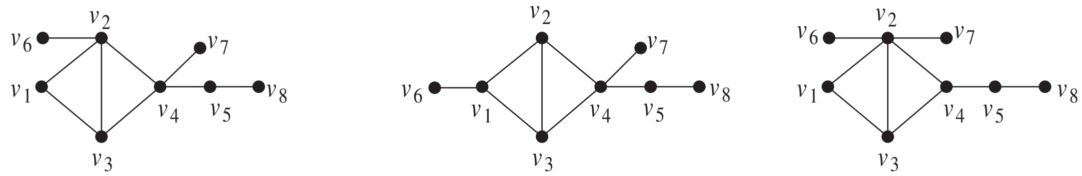
Graphs 1-3:



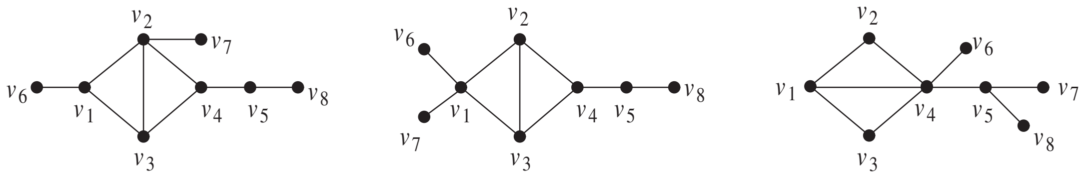
Graphs 4-6:



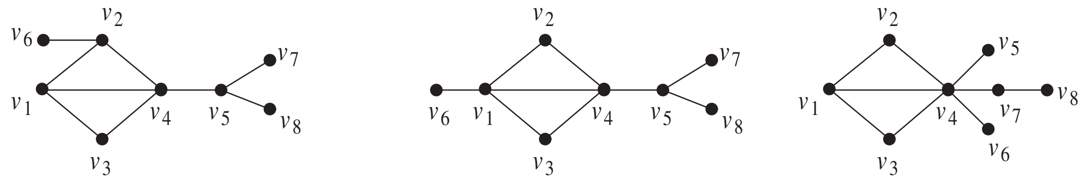
Graphs 7-9:



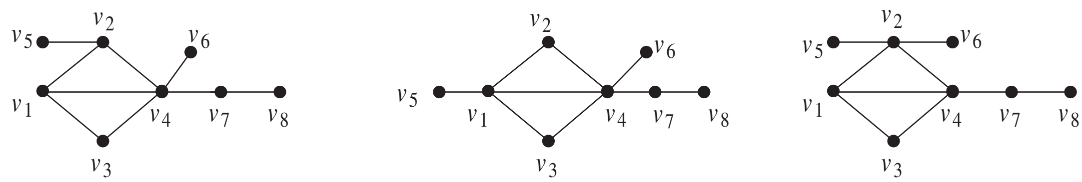
Graphs 10-12:



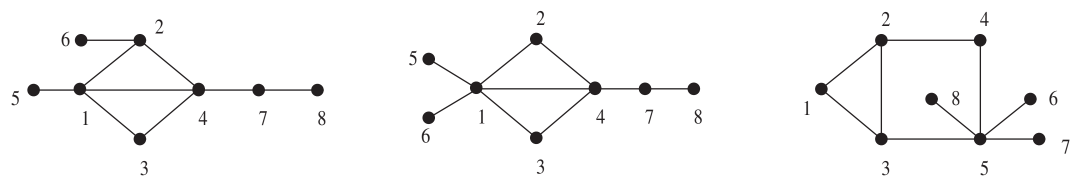
Graphs 13-15:



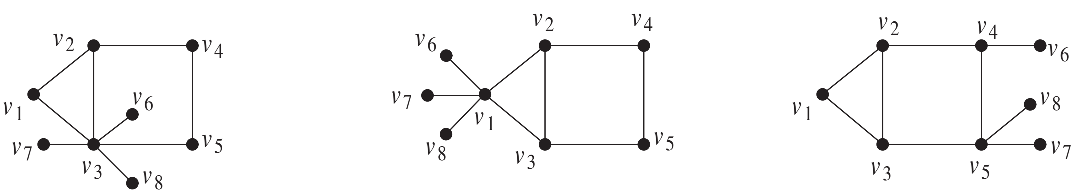
Graphs 16-18:



r a 19-21:



Graphs 22-24:



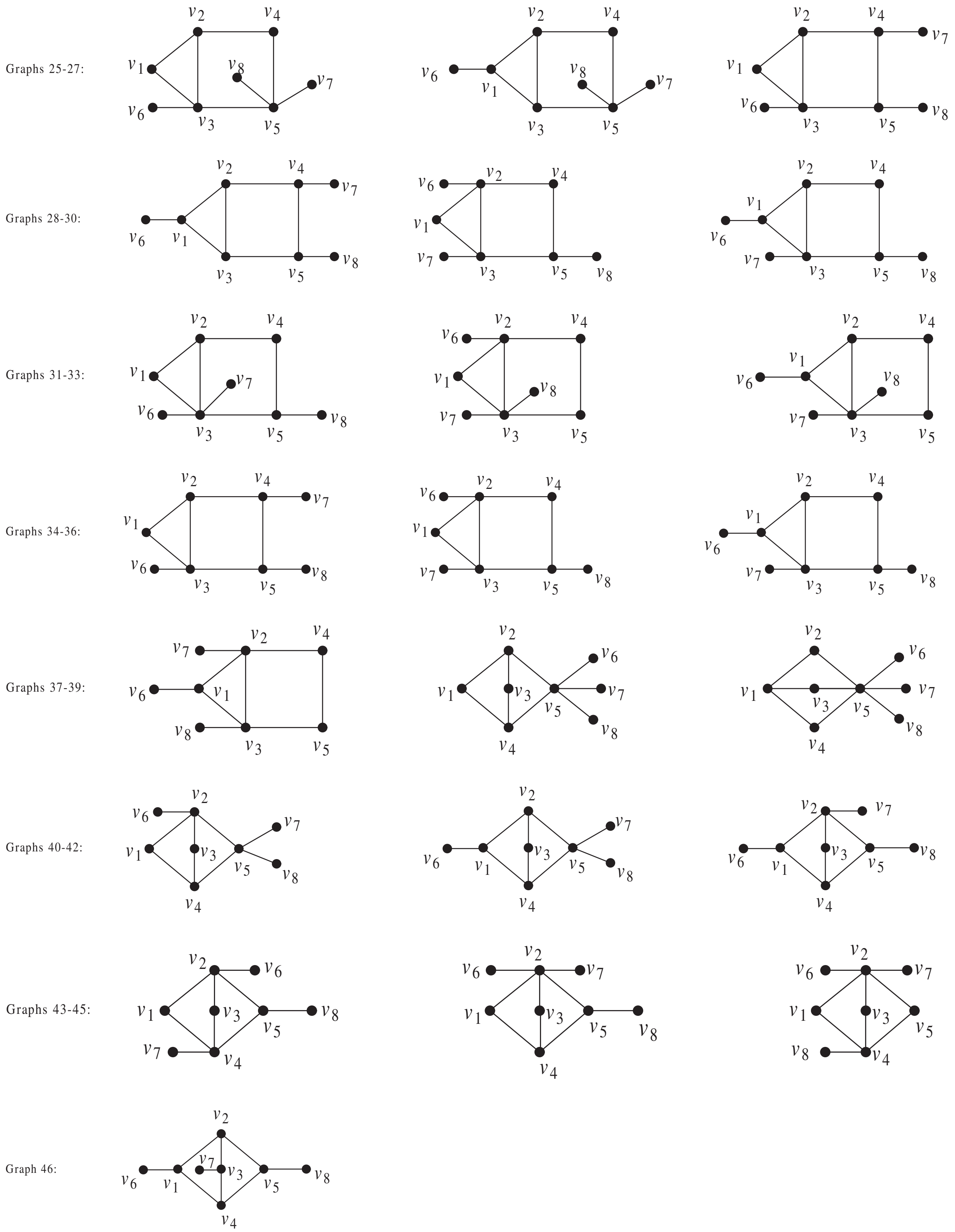


Figure 5: Bicyclic graphs in $\mathcal{B}_2^3(8)$.

Assuming that the above conclusion holds for $n-1$ approach $\phi_2(n-1) = g(n-1)$. In addition, if G is an arbitrary bicyclic graph with $n-1$ vertices and t pendant vertices and $\varphi(G) = \phi_2(n-1)$, then $G = B_2^t(n-1)$ and there are two pendant vertices u and v in $B_2^t(n-1)$ such that $\varphi(B_2^t(n-1)) = H_{B_2^t(n-1)}(u,v) = \phi_2(n-1) = g(n-1)$ and $d(u,v) = n-t$.

Let G be an arbitrary graph with n vertices and t pendant vertices in $\mathcal{B}_2^t(n)$ such that $\varphi(G) = \phi_2(n)$. Now we will prove that $\phi_2(n) = g(n)$, where the equation holds if and only if $G = B_2^t(n)$. In addition, by the definition of $\varphi(G)$, there are two vertices u and v in G such that $H_G(u,v) = \varphi(G) = \phi_2(n)$. By Lemma 2.7, v is not a cut vertex, let w be a vertex in $N[v]$ such that $\max_{z\in N(v)} H_G(z,v) = H_G(w,v)$ and $d_{N[v]}(w) = k+1$. We consider the following two cases.

Case 1. v is a vertex on the cycle with $d(v) = 3$, so we need to consider the following three situations.

Subcase 1.1. $k = 0$. By Lemma 2.8, $N(v) \cap N(w) = \emptyset$, then we have that $e(N[v]) = 3$ or $e(N[v]) = 4$.

Firstly, we discuss the situation of $e(N[v]) = 3$, then there are four situations for G/N, which are $G/N \in \mathcal{B}_2^t(n-3)$, $G/N \in \mathcal{B}_1^t(n-3)$, G/N is a unicyclic graph with $n-3$ vertices or G/N is a tree with $n-3$ vertices.

If $G/N \in \mathcal{B}_2^t(n-3)$, then $H_G(u,v) \le (n-3)^2 - t^2 + 2(n-3) - 6t - 11 + 2n - 3 < g(n)$.

If $G/N \in \mathcal{B}_1^t(n-3)$, then by Theorem 3.1, which can obtain $H_G(u,v) \le (n-3)^2 - t^2 + 2(n-3) - \frac{22}{3}t - \frac{49}{3} + 2n - 3 < g(n)$.

If G/N is a unicyclic graph with $n-3$ vertices, then by Theorem 2.2, which can gain $H_G(u,v) \le (n-3)^2 - t^2 - \frac{8}{3}t - \frac{7}{3} + 2n - 3 < g(n)$.

If G/N is a tree with $n-3$ vertices, then by Theorem 2.1, which can calculate that $H_G(u,v) \le (n-t-3)^2 + 2(n-t-3)(t-1) + 2n - 3 < g(n)$.

Next, if $e(N[v]) = 4$, then there are two situations in that G/N is a unicyclic graph with $n-3$ vertices or G/N is a tree with $n-3$ vertices.

If G/N is a tree with $n-3$ vertices, then by Theorem 2.1, we can gain $H_G(u,v) \le (n-t-3)^2 + 2(n-t-3)(t-1) + 2n - 5 < g(n)$.

If G/N is a unicyclic graph with $n-3$ vertices, then by Theorem 2.2, which can gain $H_G(u,v) \le (n-3)^2 - t^2 - \frac{8}{3}t - \frac{7}{3} + 2n - 5 < g(n)$.

Subcase 1.2. $k = 1$. By Lemma 2.8, we have $N(v) \cap N(w) \ne \emptyset$, then we can obtain that $e(N[v]) = 4$ or $e(N[v]) = 5$.

Firstly, if $e(N[v]) = 4$, then G/N is a unicyclic graph with $n-3$ vertices or G/N is a tree with $n-3$ vertices.

If G/N is a unicyclic graph with $n-3$ vertices, then $H_G(u,v) \le (n-3)^2 - t^2 - \frac{8}{3}t - \frac{7}{3} + \frac{4n-5}{3} < g(n)$.

If G/N is a tree with $n-3$ vertices, then $H_G(u,v) \le (n-t-3)^2 + 2(n-t-3)(t-1) + \frac{4n-5}{3} < g(n)$.

Next, if $e(N[v]) = 5$, then G/N is a tree with $n-3$ vertices. Therefore, $H_G(u,v) \le (n-t-3)^2 + 2(n-t-3)(t-1) + \frac{4n-7}{3} < g(n)$

Subcase 1.3. $k = 2$. By Lemma 2.8, we have $N(v) \cap N(w) \ne \emptyset$, then $e(N[v]) = 5$ and $H_G(u,v) \le H_{G/N}(u,N) + \frac{2n-3}{2}$. In addition, G/N is a tree with $n-3$ vertices, then $H_G(u,v) \le (n-t-3)^2 + 2(n-t-3)(t-1) + \frac{2n-3}{2} < g(n)$.

Case 2. v is a pendant vertex in G, so there exists a unique adjacent vertex z of v in G. Let $G^- = G - v$, then z must be a cut vertex. By Theorem 2.3, we have $H_G(u,v) = H_G(u,z) + H_G(z,v) = H_{G^-}(u,z) + H_G(z,v)$. By Theorem 2.4, $H_G(z,v) = 2n+1$. Firstly, by the inductive hypothesis, we have

$$H_{G^-}(u,z) \le \varphi(G^-) \le \phi_2(n-1) = g(n-1).$$

Therefore,

$$\phi_2(n) = \varphi(G) \le \phi_2(n-1) + 2n + 1 = g(n-1) + 2n + 1 = g(n).$$

In addition, let u_1, u_2 be two vertices in $B_2^t(n)$, $d(u_1) = d(u_2) = 1$ and $d(u_1,u_2) = n-t$. Let w be the unique adjacent vertex of u_2, by inductive assumptions about the definition of $\phi_2(n)$, we have

$$\begin{aligned}
\phi_2(n) &\ge \varphi(B_2^t(n)) \ge H_{B_2^t(n)}(u_1,u_2) \\
&= H_{B_2^t(n)}(u_1,w) + H_{B_2^t(n)}(w,u_2) \\
&= H_{B_2^t(n-1)}(u_1,w) + 2n + 1 \\
&= g(n-1) + 2n + 1 = g(n).
\end{aligned}$$

Therefore, $\phi_2(n) = g(n)$. In addition, $\phi_2(n) = \varphi(B_2^t(n)) = H_{B_2^t(n)}(u_1, u_2) = g(n)$. For an arbitrary graph G with n vertices and t pendant vertices with $\varphi(G) = \phi_2(n) = g(n)$, there exist two vertices u and v such that $H_G(u, v) = \varphi(G) = g(n)$. Based on the above proof, v must be a pendant vertex in G. In addition, z is the only adjacent vertex of v, so $g(n) = H_G(u, v) \le \varphi(G-v)+2n+1 \le g(n-1)+2n+1 = g(n)$, where $\varphi(G-v) = g(n-1)$. By inductive hypothesis, $G - v = B_2^t(n-1)$. Therefore, $G = B_2^t(n)$ and the above conclusion is valid. □

4. Proof of Theorem 1.1

Proof of Theorem 1.1. For the upper bound, by Theorems 3.1 and 3.2 , then

$$\varphi(G) \le n^2 - t^2 + 2n - 6t - 11.$$

This proves that our main result is valid.

By Theorems 3.1 and 3.2, we can draw conclusions that $\varphi(G) \le f(n) = n^2 - t^2 + 2n - \frac{22}{3}t - \frac{49}{3}$ and $\varphi(G) \le g(n) = n^2 - t^2 + 2n - 6t - 11$. By using the subtraction method, i.e., comparing $f(n) - g(n)$ (or $g(n) - f(n)$) with 0, we can obtain $g(n) < f(n)$. Therefore, the upper bound of $\varphi(G)$ is $g(n) = n^2 - t^2 + 2n - 6t - 11$, i.e., the conclusion that Theorem 1.1 can be obtained holds. In addition, we can also obtain the extremal graph of any bicyclic graph with n vertices and t pendant vertices is $B_2^t(n)$ (see Figure 6), which consist of star trees S_t, $K_4 - e$ and a path with the length of $n - t - 3$.

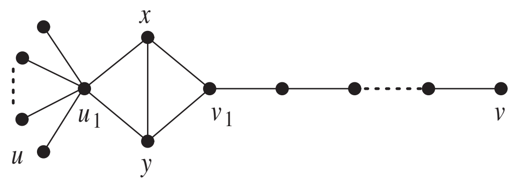


Figure 6: The extremal graph: $B_2^t(n)$.

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