Total domination polynomials of graphs

Jiuhua Hu\textsuperscript{a}, Erfang Shan\textsuperscript{b}, Shaohui Wang\textsuperscript{a,c,*}, Chunxiang Wang\textsuperscript{d}, Bing Wei\textsuperscript{a}

\textsuperscript{a}. Department of Mathematics, The University of Mississippi, University, MS 38677, USA
\textsuperscript{b}. School of Management, Shanghai University, Shanghai 200444, P.R.China
\textsuperscript{c}. Computer Science and Mathematics Department, Adelphi University Garden City, NY 11530, USA
\textsuperscript{d}. School of Mathematics and Statistics, Central China Normal University Wuhan, 430079, P.R. China

Abstract

Given a graph $G$, a total dominating set $D_t$ is a vertex set that every vertex of $G$ is adjacent to some vertices of $D_t$ and let $d_t(G, i)$ be the number of all total dominating sets with size $i$. The total domination polynomial, defined as $D_t(G, x) = \sum_{i=1}^{\mid V(G) \mid} d_t(G, i)x^i$, recently has been one of the considerable extended research in the field of domination theory. In this paper, we obtain the vertex-reduction and edge-reduction formulas of total domination polynomials. As consequences, we give the total domination polynomials for paths and cycles. Additionally, we determine the sharp upper bounds of total domination polynomials for trees and characterize the corresponding graphs attaining such bounds. Finally, we use the reduction-formulas to investigate the relations between vertex sets and total domination polynomials in $G$.

Keywords: Total dominating set; Total domination polynomial; Recurrence relation

\footnote{The first and third authors are partially supported by the Summer Graduate Research Assistantship Program of Graduate School, the second author is partially supported by the National Nature Science Foundation of China (Grant No.11171207).
*Corresponding authors: J. Hu (e-mail: jhu2@go.olemiss.edu), E. Shan (e-mail: efshan@shu.edu.cn), S. Wang (e-mail: swang4@go.olemiss.edu), C. Wang (wexiang@mailccnu.edu.cn), B. Wei (e-mail: bwei@olemiss.edu).}


1 Introduction

Throughout this paper \( G = (V, E) \) is a finite simple undirected graph with vertex set \( V = V(G) \) and edge set \( E = E(G) \). Let \( |V| \) denote the order of \( G \). Especially, \( G = \phi \) or \( V = \phi \) if \( |V| = 0 \). For any \( v \in V(G) \), \( N_G(v) = \{w \in V(G) : vw \in E(G)\} \) is the open neighborhood of \( v \) and \( N_G[v] = N_G(v) \cup \{v\} \) is the closed neighborhood of \( v \) in \( G \). If \( N_G(v) = \phi \), then \( v \) is called an isolated vertex. The set of vertices adjacent in \( G \) to a vertex subset \( S \subseteq V(G) \) is the open neighborhood \( N_G(S) \) of \( S \), \( N_G[S] = N_G(S) \cup S \) is the closed neighborhood of \( S \) and \( G - S \) is a subgraph induced by \( V(G) - S \). For \( u \in V(G) \), \( G/u \) is the contracted graph by the removal of \( u \) and the addition of edges between any pair of non-adjacent neighbors of \( u \), \( G \ominus u \) or \( G \ominus u \oplus v \) represents a subgraph induced by \( V(G) - N_G[u] \) or \( V(G) - N_G[u] - N_G[v] \) respectively. In particular, we set \( G - u \ominus v = (G - u) \ominus v \) and \( G - e \ominus u = (G - e) \ominus u \). A vertex is said to be a pendant vertex if its open neighborhood contains exactly one vertex. The neighbor of a pendant vertex is called a supporting vertex. A graph \( F \) is called a forest if it has no cycles. When \( F \) contains only one component, we say \( F \) is a tree. For graphs \( G_1, G_2, G_1 \cup G_2 \) is called the union graph of \( G_1 \) and \( G_2 \) with vertex set \( V(G_1) \cup V(G_2) \) and edge set \( E(G_1) \cup E(G_2) \), \( G_1 \vee G_2 \) is called the join graph of \( G_1 \) and \( G_2 \) with vertex set \( V(G_1) \cup V(G_2) \) and edge set \( E(G_1) \cup E(G_2) \cup \{uv : u \in V(G_1) \) and \( v \in V(G_2) \} \). In \([4,8]\), the 2-corona of a graph \( G \) is defined by the graph of order \( 3|V(G)| \) obtained by attaching a path of length 2 to each vertex of \( G \) such that the resulting paths are vertex disjoint. Let \( S_n, T_n \) be the star, tree of order \( n \).

A vertex set \( D_t \) of a graph \( G \) is a total dominating set \([11]\) if every vertex of \( V(G) \) is adjacent to some vertices of \( D_t \). Let \( \gamma_t(G) \) be the minimum size of total dominating sets, \( \mathcal{D}_t(G, i) \) be the set of all total dominating sets of size \( i \) and set \( d_t(G, i) = |\mathcal{D}_t(G, i)| \). The total domination polynomial \([14]\), defined as \( D_t(G, x) = \sum_{i=1}^{|V(G)|} d_t(G, i) x^i \), is one of the extended research-area of the domination theory. The domination polynomial was studied recently by several authors, see \([2, 3, 6, 9, 10, 11, 13]\).

The following equalities, which are easy to check by the concepts, are very useful in calculating total domination polynomials of graphs.

**Proposition 1** Let \( G, P_n \) and \( C_n \) be a graph, a path and a cycle with \( n \) vertices. Then

(i) \( D_t(G, x) \neq 0 \) if and only if \( G \) has no isolated vertices.

(ii) The number of supporting vertices of \( G \) is \( n - d_t(G, n - 1) \).
(iii) \[ D_t(G, x) = D_t(G_1, x)D_t(G_2, x), \] where \( G = G_1 \cup G_2 \).

(iv) \[ D_t(P_1, x) = 0, D_t(P_2, x) = x^2, D_t(P_3, x) = x^3 + 2x^2, D_t(P_4, x) = x^4 + 2x^3 + x^2. \]

(v) \[ D_t(C_3, x) = x^3 + 3x^2, D_t(C_4, x) = x^4 + 4x^3 + 4x^2, D_t(C_5, x) = x^5 + 5x^4 + 5x^3, D_t(C_6, x) = x^6 + 6x^5 + 9x^4. \]

The following proposition is due to Cockayne et al. (1980) and Brigham et al. (2000).

**Proposition 2** \[5, 11\] If \( G \) is a connected graph of order \( n \geq 3 \), then \( 2 \leq \gamma_t(G) \leq 2n/3 \), the right equality holds if and only if \( G \) is \( C_3, C_6 \) or 2-corona.

In general, it is very hard to find the total domination number (polynomial) of a graph and determine the solutions of related extremal problems. A plenty of properties of domination number are explored, see \[1, 7, 8, 15, 16\]. However, only a few classes of graphs with exact determination of the coefficients have been appeared in the literature. Vijayan and Kumar \[14\](2012) obtained some properties of total domination polynomials for cycles. Chaluvaraju et al. \[4\](2014) presented some basic properties of total domination polynomials and graph operations of the union and join of graphs. However, the vertex and edge reduction formulas, which are very important tools to investigate the properties of graph polynomials, are still unknown for total domination polynomials.

This article not only obtains recurrence relations of total domination polynomials for graph operations, but also digs out some interesting results on extremal problems and the characterization of graphic structures using the total domination polynomials of a graph. The main results of this study are detailed below.

1. We present the vertex-reduction and edge-reduction formulas of total domination polynomials in Theorems 1 and 3. As consequences, Theorems 2 and 4 give the recurrence relations for total domination polynomials of paths and cycles.

2. We obtain the sharp upper bounds of total domination polynomials for trees and characterize the corresponding graphs attaining such bounds in Theorem 5, which is a classic type of extremal problems.

3. Using the reduction-formulas, we investigate the values of total domination polynomials at \( x = -1 \) in Theorems 6 and 7. Our results indicate that the number of all total dominating sets of even size and that of odd size can differ by at most 1 for the forest.

4. A direct relation between the vertices of degree 2 and the coefficients of total domina-
tion polynomials is given in Theorem 8.

2 Reduction-formulas of total domination polynomials

In this section, we determine the vertex-reduction and edge-reduction formulas of total domination polynomials. For any graph $G$, let $W \subseteq V(G)$ and $C_W$ be a statement on $W$. Denote \( D_t(G, x)\{C_W\} \) to be the generating function for the number of total dominating sets of $G$ under the condition $C_W$:

\[
D_t(G, x)\{C_W\} = \sum_{N_G[W] = V(G)} \varphi(W) x^{|W|}, \text{ where } \varphi(W) = \begin{cases} 1, & \text{if } C_W \text{ holds for } W, \\ 0, & \text{otherwise.} \end{cases}
\]

For instance, if $w \in V(G)$, then $D_t(G, x)\{w \notin W\}$ represents the total domination polynomial generated by all total domination sets $W$ of $G$ with $w \notin W$. Also, define a new identity function $1_{G \ominus u \ominus v}$ as follows: For the vertices $u, v \in V(G)$,

\[
1_{G \ominus u \ominus v} = \begin{cases} 1, & \text{if } G \ominus u \ominus v = \phi, \\ D_t(G \ominus u \ominus v, x), & \text{if } G \ominus u \ominus v \neq \phi. \end{cases}
\]

**Theorem 1** For any connected graph $G$ and $u \in V(G)$,

\[
D_t(G, x) = D_t(G - u, x) + xD_t(G/u, x) - (1 + x)D_t(G/u, x)\{N_G(u) \cap W = \emptyset\} + \sum_{v \in N_G(u)} x^2 1_{G \ominus u \ominus v}.
\]

**Proof.** We first consider the case when the total dominating set $W$ does not contain $u$. Then $W$ is a total dominating set of $G$ if and only if $N_G(u) \cap W \neq \phi$ and $W$ is a total dominating set of $G - u$. Thus,

\[
D_t(G, x)\{u \notin W\} = D_t(G - u, x)\{N_G(u) \cap W \neq \phi\}. \tag{1}
\]

Also, when $W$ is a total domination set of $G - u$, $W$ is also a total domination set of $G/u$ since $G - u$ is a subgraph by the definition of $G - u$ and $G/u$; Conversely, if $W$ is a total domination set of $G/u$ and $N_G(u) \cap W = \phi$, then $W$ is still a total domination set of $G - u$. Thus,

\[
D_t(G - u, x)\{N_G(u) \cap W = \phi\} = D_t(G/u, x)\{N_G(u) \cap W = \phi\}. \tag{2}
\]
By (1) and (2), we can get that,
\[ D_t(G, x)\{u \notin W\} \overset{(1)}{=} D_t(G - u, x)\{N_G(u) \cap W \neq \phi\} \]
\[ \overset{(2)}{=} D_t(G - u, x) - D_t(G/u, x)\{N_G(u) \cap W = \phi\}. \quad (3) \]

Now we consider the case when the total dominating set \(W\) contains \(u\). Then \(N_G(u) \cap W \neq \phi\). If \(|N_G(u) \cap W| = 1\), say \(v \in N_G(u) \cap W\), and \(|N_{G - u}(v) \cap W| = 0\), then either \(G \ominus u \ominus v = \phi\) or \(W - \{u, v\}\) is a total dominating set of \(G \ominus u \ominus v\). We have
\[ D_t(G, x)\{u \in W, N_G(u) \cap W = \{v\}, |N_{G - u}(v) \cap W| = 0\} \]
\[ = \begin{cases} x^2, & \text{if } G \ominus u \ominus v = \phi, \\ x^2D_t(G \ominus u \ominus v, x), & \text{if } G \ominus u \ominus v \neq \phi. \end{cases} = x^21_{G \ominus u \ominus v}. \quad (4) \]

If \(N_G(u) \cap W = \{v\}\) and \(|N_{G - u}(v) \cap W| \geq 1\), then \(W - u\) is also a total dominating set of \(G/u\). Also, for any total dominating set \(W'\) of \(G/u\), we have \(W' \cup \{u\}\) is a total dominating set of \(G\). Thus,
\[ D_t(G, x)\{u \in W, N_G(u) \cap W = \{v\}, |N_{G - u}(v) \cap W| \geq 1\} \]
\[ = xD_t(G/u, x)\{N_G(u) \cap W = \{v\}, |N_{G/u}(v) \cap W| \geq 1\}. \quad (5) \]

Similarly, if \(|N_G(u) \cap W| \geq 2\), then \(W - u\) is a total dominating set of \(G/u\) and for any total dominating set \(W'\) of \(G/u\), then \(W' \cup \{u\}\) is a total dominating set of \(G\). Thus,
\[ D_t(G, x)\{u \in W, |N_G(u) \cap W| \geq 2\} = xD_t(G/u, x)\{|N_G(u) \cap W| \geq 2\}. \quad (6) \]

Furthermore, for the total dominating set \(W\) of \(G\), if \(v \in N_G(u)\) and \(N_{G/u}(v) \cap W = \phi\), then \(d_G(u) = d_G(v) = 1\) and \(uv \in E(G)\), that is, \(v\) is an isolated vertex of \(G/u\). Thus, \(W\) is not a total dominating set of \(G/u\), that is,
\[ D_t(G/u, x)\{N_G(u) \cap W = \{v\}, |N_{G/u}(v) \cap W| = 0\} = 0. \quad (7) \]

For \(G/u\), we can obtain that
\[ D_t(G/u, x) - D_t(G - u, x)\{|N_G(u) \cap W| = 0\} \]
\[ \overset{(2)}{=} D_t(G/u)\{|N_G(u) \cap W| \geq 1\} \]
\[ \overset{(7)}{=} \sum_{v \in N_G(u)} D_t(G/u, x)\{N_G(u) \cap W = \{v\}, |N_{G/u}(v) \cap W| \geq 1\} \]
\[ + D_t(G/u, x)\{|N_G(u) \cap W| \geq 2\}. \quad (8) \]
Also, by (4)-(8) and \( v \in N_G(u) \), one can obtain that

\[
D_t(G, x) \{ u \in W \} = D_t(G, x) \{ u \in W, |N_G(u) \cap W| = 1 \} + D_t(G, x) \{ u \in W, |N_G(u) \cap W| \geq 2 \}
\]

\[
= \sum_{v \in N_G(u)} D_t(G, x) \{ u \in W, N_G(u) \cap W = \{ v \} \} + D_t(G, x) \{ u \in W, |N_G(u) \cap W| \geq 2 \}
\]

\[
= \sum_{v \in N_G(u)} D_t(G, x) \{ u \in W, N_G(u) \cap W = \{ v \} \}, |N_G(v) \cap W| = 1 \} + D_t(G, x) \{ u \in W, |N_G(u) \cap W| \geq 2 \}
\]

\[
= \sum_{v \in N_G(u)} \left[ x^21_{G \oplus u \oplus v} + xD_t(G/u, x) \{ N_G(u) \cap W = \{ v \} \}, |N_G(u) \cap W| \geq 2 \} + xD_t(G/u, x) \{ |N_G(v) \cap W| = 1 \} \right]
\]

\[
= \sum_{v \in N_G(u)} x^21_{G \oplus u \oplus v} + x[D_t(G/u, x) - D_t(G - u, x) \{ |N_G(u) \cap W| = 0 \}].
\]

Finally, combining (3) and the above equality, we can obtain that

\[
D_t(G, x) = D_t(G, x) \{ u \in W \} + D_t(G, x) \{ u \notin W \}
\]

\[
= D_t(G - u, x) +xD_t(G/u, x) - (1 + x)D_t(G/u, x) \{ N_G(u) \cap W = \emptyset \}
\]

\[
+ \sum_{v \in N_G(u)} x^21_{G \oplus u \oplus v}
\]

and Theorem 1 is true.  \( \square \)

By Theorem 1, we can get the following corollary.

**Corollary 1.1** For any connected graph \( G \), if either (i) there exist two vertices \( u, v \in V(G) \) such that \( N_G[v] \subseteq N_G[u] \) or (ii) there exists a supporting vertex \( w \in N_G(u) \), then

\[
D_t(G, x) = D_t(G - u, x) +xD_t(G/u, x) + \sum_{v \in N_G(u)} x^21_{G \oplus u \oplus v}.
\]

**Proof.** Let \( W \subseteq V(G) \) such that \( N_G(u) \cap W = \emptyset \). For (i), since \( v \) cannot be dominated by \( W \), then \( D_t(G/u, x) \{ N_G(u) \cap W = \emptyset \} = 0 \). For (ii), we know that any supporting vertex \( w \) must belong to any total dominating set \( W' \) of \( G \). Otherwise, the pendant vertices adjacent to \( w \) can not be dominated by \( W' \). Thus, \( D_t(G/u, x) \{ N_G(u) \cap W = \emptyset \} = 0 \). Hence, by Theorem 1, we have Corollary 1.1 is true.  \( \square \)

Apply Corollary 1.1 to a path \( P_n = v_1v_2\ldots v_n \) with \( n \geq 5 \). Let \( u = v_2, v \in N_{P_n}(u) = \{ v_1, v_3 \} \), by Proposition 1(i) and (iii), we can get the recurrence relation of paths below.

**Theorem 2** Let \( P_n \) be a path of order \( n \geq 5 \),

\[
D_t(P_n, x) = xD_t(P_{n-1}, x) + x^2D_t(P_{n-3}, x) + x^2D_t(P_{n-4}, x).
\]
As an immediate consequence, we give the total domination polynomials of paths as follows.

**Corollary 2.1** Let $P_n$ be a path of order $n \geq 1$,

$$D_t(P_n, x) = \begin{cases} \frac{2x^n}{x+4} + p(n), & \text{if } n = 4m, \\ -\frac{(x^2+3x)\sqrt{x} - 1}{x+4} + p(n), & \text{if } n = 4m + 1, \\ -\frac{2x^2}{x+4} + p(n), & \text{if } n = 4m + 2, \\ \frac{(x^2+3x)\sqrt{x} + 1}{x+4} + p(n), & \text{if } n = 4m + 3, \end{cases}$$

where $p(n) = \frac{(x+2-\sqrt{x^2+4x})(x-\sqrt{x^2+4x})n + (x+2+\sqrt{x^2+4x})(x+\sqrt{x^2+4x})n}{2^{n+1}(x+4)}$.

**Proof.** If $n = 1, 2, 3, 4$, by Proposition 1(iv), Corollary 2.1 is true. If $n \geq 5$, the characteristic polynomial of the recursion of Theorem 2 is $\lambda^4 - x\lambda^3 - x^2\lambda - x^2 = 0$ with roots $\lambda_1 = \sqrt{-x}$, $\lambda_2 = -\sqrt{-x}$, $\lambda_3 = \frac{x+\sqrt{x(x+4)}}{2}$, $\lambda_4 = \frac{x-\sqrt{x(x+4)}}{2}$. Hence,

$$D_t(P_n, x) = \alpha_1(x)\lambda_1^n + \alpha_2(x)\lambda_2^n + \alpha_3(x)\lambda_3^n + \alpha_4(x)\lambda_4^n$$

with $\alpha_1(x), \alpha_2(x), \alpha_3(x)$ and $\alpha_4(x)$ not dependent on $n$. Using the initial conditions in Proposition 1(iv), we can form a system of equations for $i = 1, 2, 3, 4$, $D_t(P_i, x) = \alpha_1(x)\lambda_1^i + \alpha_2(x)\lambda_2^i + \alpha_3(x)\lambda_3^i + \alpha_4(x)\lambda_4^i$. By solving this system, we get that $\alpha_1(x) = \frac{2+(x+3)\sqrt{-x}}{2(x+4)}$, $\alpha_2(x) = \frac{2-(x+3)\sqrt{-x}}{2(x+4)}$, $\alpha_3(x) = \frac{x+2+\sqrt{x(x+4)}}{2(x+4)}$, $\alpha_4(x) = \frac{x+2-\sqrt{x(x+4)}}{2(x+4)}$.

Thus, by $D_t(P_n, x) = \alpha_1(x)\lambda_1^n + \alpha_2(x)\lambda_2^n + \alpha_3(x)\lambda_3^n + \alpha_4(x)\lambda_4^n$ and setting $n = 4m + i$ with $i = 0, 1, 2, 3$ respectively, we have Corollary 2.1 is true. \[\square\]

**Theorem 3** For any connected graph $G$ and $e = uv \in E(G)$,

$$D_t(G, x) = D_t(G-e, x) + x^21_{G\ominus u\ominus v} + (1+x)[D_t(G-e\ominus u, x)\{v \in W\} + D_t(G-e\ominus v, x)\{u \in W\}]$$

**Proof.** Let $W$ be a total dominating set of $G$, we will consider the cases that whether $u, v \in W$ or not as follows.

**Case 1.** $\{u, v\} \subseteq W$.

If $|N_G(u) \cap W| \geq 2$ and $|N_G(v) \cap W| \geq 2$, then $W$ is also a total dominating set of $G - e$; If $|N_G(u) \cap W| = 1$ and $|N_G(v) \cap W| = 1$, that is, $N_G(u) \cap W = \{v\}$ and $N_G(v) \cap W = \{u\}$, then $W - \{u, v\}$ is a total dominating set of $G \ominus u \ominus v$ unless $G \ominus u \ominus v = \phi$; If $|N_G(u) \cap W| = 1$ and $|N_G(v) \cap W| \geq 2$, then $W - \{u\}$ is a total dominating set of $G - e \ominus u$; If $|N_G(u) \cap W| \geq 2$ and $|N_G(v) \cap W| = 1$, then $W - \{v\}$ is a total dominating set of $G - e \ominus v$. 

7
Hence, if $G \ominus u \ominus v \neq \phi$, then $D_t(G, x)\{\{u, v\} \subseteq W\} = D_t(G - e, x)\{\{u, v\} \subseteq W\} + x^2 D_t(G \ominus u \ominus v, x) + x D_t(G - e \ominus u, x)\{v \in W\} + x D_t(G - e \ominus v, x)\{u \in W\}$; If $G \ominus u \ominus v = \phi$, then $D_t(G, x)\{\{u, v\} \subseteq W\} = D_t(G - e, x)\{\{u, v\} \subseteq W\} + x^2 + x D_t(G - e \ominus u, x)\{v \in W\} + x D_t(G - e \ominus v, x)\{u \in W\}$.

**Case 2.** $\{u, v\} \cap W = \phi$.

Then $W$ is also a total dominating set of $G - e$, that is, $D_t(G, x)\{\{u, v\} \cap W = \phi\} = D_t(G - e, x)\{\{u, v\} \cap W = \phi\}$.

**Case 3.** $u \in W, v \notin W$.

Since $W$ is a total dominating set of $G$, $N_G(v) \cap W \neq \phi$. If $|N_G(v) \cap W| \geq 2$, then $W$ is also a total dominating set of $G - e$; If $N_G(v) \cap W = \{u\}$, then $W$ is a total dominating set of $G - e \ominus v$. Hence, we have $D_t(G, x)\{u \in W, v \notin W\} = D_t(G - e, x)\{u \in W, v \notin W, W \cap N_{G-e}(v) \neq \phi\} + D_t(G - e \ominus v, x)\{u \in W\}$.

**Case 4.** $u \notin W, v \in W$.

Similar to Case 3, we have $D_t(G, x)\{u \notin W, v \in W\} = D_t(G - e, x)\{v \in W, u \notin W, W \cap N_{G-e}(u) \neq \phi\} + D_t(G - e \ominus u, x)\{v \in W\}$.

Finally, we have
\[
D_t(G, x) = D_t(G, x)\{\{u, v\} \subseteq W\} + D_t(G, x)\{\{u, v\} \cap W = \phi\} + D_t(G, x)\{u \in W, v \notin W\} + D_t(G, x)\{u \notin W, v \in W\} = D_t(G - e, x) + x^2 1_{G \ominus u \ominus v} + (1 + x)[D_t(G - e \ominus u, x)\{v \in W\} + D_t(G - e \ominus v, x)\{u \in W\}]
\]
and Theorem 3 is true.

By applying Theorems 2 and 3, we can obtain the recurrence relations of total domination polynomials for cycles.

**Theorem 4** For any cycle $C_n = v_1 v_2 \cdots v_n v_1$ with $n \geq 7$,
\[
D_t(C_n, x) = x D_t(C_{n-1}, x) + x^2 D_t(C_{n-3}, x) + x^2 D_t(C_{n-4}, x).
\]

**Proof.** Let $P_n = C_n - e = v_1 v_2 \cdots v_n$, where $e = v_1 v_n$. We begin with the proof by Claim 1.

**Claim 1.** $D_t(P_n, x)\{v_n \in W\} = x D_t(P_{n-1}, x)\{v_{n-1} \in W\} + x^2 D_t(P_{n-3}, x)\{v_{n-3} \in W\} + x^2 D_t(P_{n-4}, x)\{v_{n-4} \in W\}$.

**Proof of Claim 1.** For $i \geq 1$, let $S_0 = \{W : W \in D_t(P_n, i), v_n \in W\}$, $S_1 = \{W_1 \cup \{v_n\} : W_1 \in D_t(P_{n-1}, i-1), v_{n-1} \in W_1\}$, $S_2 = \{W_2 \cup \{v_n, v_{n-1}\} : W_2 \in D_t(P_{n-3}, i-2), v_{n-3} \in W_2\}$
and \( S_3 = \{ W_3 \cup \{ v_n, v_{n-1} \} : W_3 \in D_t(P_{n-4}, i-2), v_{n-4} \in W_3 \} \). Now it is enough to show that \( S_0 = S_1 \cup S_2 \cup S_3 \).

It is obvious that \( S_1 \cup S_2 \cup S_3 \subset S_0 \). Conversely, choose any \( W \in S_0 \). The definition of total dominating set yields that \( v_{n-1} \in W \). If \( v_{n-2} \in W \), set \( W_1 = W - \{ v_n \} \), that is, \( W_1 \in D_t(P_{n-1}, i-1) \) and \( W_1 \cup \{ v_n \} \subset S_1 \). If \( v_{n-2} \notin W \) and \( v_{n-3} \in W \) and therefore set \( W_2 = W - \{ v_n, v_{n-1} \} \), that is, \( W_2 \in D_t(P_{n-3}, i-2) \) and \( W_2 \cup \{ v_n, v_{n-1} \} \subset S_2 \). If \( v_{n-2} \notin W \) and \( v_{n-3} \notin W \), then \( v_{n-4} \in W \) and therefore set \( W_3 = W - \{ v_n, v_{n-1}, v_{n-3} \} \), that is, \( W_3 \in D_t(P_{n-4}, i-2) \) and \( W_3 \cup \{ v_n, v_{n-1}, v_{n-3} \} \subset S_3 \). Thus, \( S_0 \subset S_1 \cup S_2 \cup S_3 \). Hence, \( D_t(P_n, x)\{ v_n \in W \} = xD_t(P_{n-1}, x)\{ v_{n-1} \in W \} + x^2 D_t(P_{n-3}, x)\{ v_{n-3} \in W \} + x^2 D_t(P_{n-4}, x)\{ v_{n-4} \in W \} \) and Claim 1 is true.

By Theorems 2, 3 and Claim 1, we have
\[
D_t(C_n, x) \quad \text{Theorem 3} \quad D_t(P_n, x) + x^2 D_t(P_{n-4}, x) + (1 + x)(D_t(C_n - e - v_1 - v_2, x)\{ v_n \in W \})
= D_t(P_n, x) + x^2 D_t(P_{n-4}, x) + 2(1 + x)D_t(P_{n-2}, x)\{ v_1 \in W \}
\quad \text{Theorem 2}
= [xD_t(P_{n-1}, x) + x^2 D_t(P_{n-3}, x) + x^2 D_t(P_{n-4}, x)]
\quad \text{Simplify}
+ x^2[xD_t(P_{n-5}, x) + x^2 D_t(P_{n-7}, x) + x^2 D_t(P_{n-8}, x)]
\quad \text{Simplify}
+ 2(1 + x)[xD_t(P_{n-3}, x)\{ v_1 \in W \} + x^2 D_t(P_{n-5}, x)\{ v_1 \in W \}]
\quad \text{Simplify}
+ x^2 D_t(P_{n-6}, x)\{ v_1 \in W \}
\quad \text{Claim 1}
= xD_t(P_{n-1}, x) + x^2 D_t(P_{n-5}, x) + 2(1 + x)D_t(P_{n-3}, x)\{ v_1 \in W \}
+ x^2 D_t(P_{n-3}, x) + x^2 D_t(P_{n-7}, x) + 2(1 + x)D_t(P_{n-5}, x)\{ v_1 \in W \}
+ x^2 D_t(P_{n-4}, x) + x^2 D_t(P_{n-8}, x) + 2(1 + x)D_t(P_{n-6}, x)\{ v_1 \in W \}
\quad \text{Thus, Theorem 4 is true.}

As a direct consequence, we obtain the total domination polynomials of cycles below.

**Corollary 4.1** For any cycle \( C_n \) with \( n \geq 3 \) vertices, \( D_t(C_n, x) = \begin{cases} 2(-x)^n + q(n), & \text{if} \quad n = 2m, \\ q(n), & \text{if} \quad n = 2m + 1, \end{cases} \)
where \( q(n) = \frac{(x - \sqrt{x^2 + 4x})^n + (x + \sqrt{x^2 + 4x})^n}{2^n} \).

**Proof.** If \( n = 3, 4, 5 \) or \( 6 \), by Proposition 1(i), Corollary 4.1 is true. If \( n \geq 7 \), the characteristic polynomial of the recursion of Theorem 4 is \( \lambda^4 - x\lambda^3 - x^2\lambda - x^2 = 0 \) with roots
\[ \lambda_1 = \sqrt{-x}, \lambda_2 = -\sqrt{-x}, \lambda_3 = \frac{x + \sqrt{x(x+4)}}{2}, \lambda_4 = \frac{x - \sqrt{x(x+4)}}{2}. \] Thus, \[ D_t(C_n, x) = \alpha_1(x)\lambda_1^n + \alpha_2(x)\lambda_2^n + \alpha_3(x)\lambda_3^n + \alpha_4(x)\lambda_4^n \]

with \( \alpha_1(x), \alpha_2(x), \alpha_3(x) \) and \( \alpha_4(x) \) not dependent on \( n \). Using the initial conditions in Proposition 1(ii), we form a system of equations for \( i = 3,4,5,6, \) \( D_t(C_i, x) = \alpha_1(x)\lambda_i^1 + \alpha_2(x)\lambda_i^2 + \alpha_3(x)\lambda_i^3 + \alpha_4(x)\lambda_i^4. \) By solving this system, we get \( \alpha_1(x) = \alpha_2(x) = \alpha_3(x) = \alpha_4(x) = 1. \)

Thus, by \( D_t(C_n, x) = \lambda_1^n + \lambda_2^n + \lambda_3^n + \lambda_4^n \) and setting \( n = 2m + i \) with \( i = 0,1 \), we have Corollary 4.1 is true. \[ \square \]

### 3 On total domination polynomials of special graphs

In this section, we obtain the sharp upper bounds of the coefficients of total domination polynomials for trees and characterize the corresponding graphs attaining such bounds.

**Theorem 5** Let \( T_n \) be a tree in \( T_n \) that is a class of trees with \( n \) vertices.

(i) \( d_t(T_n, i) \leq \binom{n-1}{i-1} \) and the equality holds if and only if \( T_n = S_n \).

(ii) There is no tree \( T' \) in \( T_n \) such that \( d_t(T_n, i) \geq d_t(T', i) \) for each \( i \geq 2 \).

**Proof.** If \( n = 0,1 \), then \( D_t(T_n, x) = 0 \), that is, Theorem 5(i) is true. Next we only consider the case that \( n \geq 2 \). By Proposition 2, \( \gamma_t(T_n) \geq 2 \) and it is easy to see that \( d_t(S_n, i) = \binom{n-1}{i-1} \). Let \( r \) be the number of supporting vertices of \( T_n \). Since \( n \geq 2 \), then \( r \geq 1 \). By \( \binom{n-1}{i-1} \leq \binom{n-1}{i-1} \), we obtain that \( S_n \) attains the maximal value for all the coefficients. Thus, (i) is true.

Now we will prove (ii) by the contradiction. Assume that \( T_1 \) attains the minimal value at all of the coefficients. By Proposition 1(ii), we have \( d_t(T_1, n-1) = n-r \). Since \( d_t(T_1, n-1) \) attains the minimal value, then \( r \) is as big as possible. Thus, \( r = \lfloor \frac{n}{2} \rfloor \), that is, \( d_t(T_1, n-1) = n-\lfloor \frac{n}{2} \rfloor = \lceil \frac{n}{2} \rceil \). On the other hand, since \( D_t(G, x) = \sum_{i=\gamma_t(G)} d_t(G, i)x^i \) and in order to obtain that every coefficient is as small as possible, then we would need that \( \gamma_t \) is as big as possible. By Proposition 2, choose a tree \( T_2 \) such that \( \gamma_t(T_2) = \lfloor \frac{2n}{3} \rfloor \). Thus, \( d_t(T_2, \lfloor \frac{2n}{3} \rfloor - 1) = 0 \).

Since \( T_1 \) contains only two types of vertices: \( V_p \) and \( V_s \), where \( V_p \) and \( V_s \) are the sets of all pendant vertices and supporting vertices of \( T_1 \) respectively, then every vertex of \( V_p \cup V_s \) is dominated by some supporting vertices. Otherwise, \( T_1 \) is not a connected graph. Thus, \( \gamma_t(T_1) = \lfloor \frac{n}{2} \rfloor \) and \( d_t(T_1, \lfloor \frac{2n}{3} \rfloor - 1) > 0 = d_t(T_2, \lfloor \frac{2n}{3} \rfloor - 1) \), a contradiction with the choice of \( T_1 \). Therefore, Theorem 5(ii) is true. \[ \square \]
By setting $x = 1$, $D_t(G, 1)$ is the number of all total domination sets in $G$. Togethering with Theorem 5, we have the following corollary.

**Corollary 5.1** Let $T_n$ be a class of trees with $n$ vertices, then $S_n$ contains maximal number of total domination sets in $T_n$.

By Corollary 2.1 and the proof of Theorem 5, we can obtain the special values of total domination polynomials on certain graphs when $x = -1$.

**Theorem 6** Let $S_n, P_n$ be a star and a path with $n$ vertices. Then

(i) $D_t(S_n, -1) = 1$;

(ii) $D_t(P_{n_0}, -1) = D_t(P_{n_2}, -1) = D_t(P_{n_3}, -1) = D_t(P_{n_5}, -1) = 1$, $D_t(P_{n_1}, -1) = D_t(P_{n_4}, -1) = 0$, where $n_i = i (\text{mod } 6)$ and $i = 0, 1, ..., 5$.

**Proof.** (i) Since $\gamma_t(S_n) = 2$ and $D_t(S_n, -1) = \sum_{i=2}^{n} d_t(S_n, -1)(-1)^i = \sum_{i=2}^{n} \binom{n-1}{i-1}(-1)^i$, then let $j = i - 1$, we have

$$D_t(S_n, -1) = \sum_{j=1}^{n-1} \binom{n-1}{j}(-1)^{j+1} = (-1)[\sum_{j=1}^{n-1} \binom{n-1}{j}(-1)^j] = (-1)[\sum_{j=0}^{n-1} \binom{n-1}{j}(-1)^j - \binom{n-1}{0}(-1)^0] = (-1)[(1 - 1)^{n-1} - 1] = 1.$$

For (ii), by Corollary 2.1 and setting $x = -1$, we have $D_t(P_{n}, -1) = \frac{2+\cos(\frac{2\pi}{3})-\sqrt{3}\sin(\frac{2\pi}{3})}{3}$. Let $n_i = 6m + i$ with $m \geq 0$ and $i = 0, 1, ..., 5$, one can obtain that

$$D_t(P_{n_0}, -1) = D_t(P_{n_2}, -1) = D_t(P_{n_3}, -1) = D_t(P_{n_5}, -1) = \frac{2+\cos(4m\pi)-\sqrt{3}\sin(4m\pi)}{3} = 1,$$

$$D_t(P_{n_1}, -1) = D_t(P_{n_4}, -1) = \frac{4\sin^2(2m\pi)}{3} = 0,$$

$$D_t(P_{n_2}, -1) = \frac{2+\sqrt{3}\cos(\frac{k-4m}{3})\pi+\cos(\frac{4(3k+8m)/3}{3})\pi}{3} = 1.$$

Thus, Theorem 6 is true. \hfill \square

From Theorem 6, we see that $D_t(S_n, -1) = 1$ and $0 \leq D_t(P_n, -1) \leq 1$. In general, Theorem 7 shows that the number of all total dominating sets of even size and that of odd size for any forest can differ by at most 1.

**Theorem 7** Let $F_n$ be any forest with $n$ vertices, then $D_t(F_n, -1) \in \{0, 1\}$

**Proof.** By Proposition 1(iii), we will only need to consider $F_n$ as a tree. If $n = 0, 1$, then $D_t(F_n, -1) = 0$ and Theorem 7 is true. If $n = 2, 3$, then $F_n$ is a path. By Proposition 1(iv), we have $D_t(F_n, -1) = 1$ and the proof is done.
Now we will prove it by induction on \( n \geq 4 \). For \( n = 4 \), either \( F_n \) is a path \( P_4 \) or a star \( S_4 \). Also, by Theorem 6, we have \( D_t(P_4, -1) = 0 \) and \( D_t(S_4, -1) = 1 \). Next assume that \( D_t(F_s, -1) \in \{0, 1\} \) with \( s < n \) and consider \( F_n \). Choose \( u \) to be any pendant vertex of \( F_n \) and set \( v \in N(u) \). By Theorem 1, we have

\[
D_t(F_n, -1) = D_t(F_n - u, -1) - D_t(F_n / u, -1) + \sum_{v \in N_G(u)} 1_{G \supseteq u \subseteq v} D_t(F_n / u, -1) + \sum_{v \in N_G(u), G \supseteq u \subseteq v = \phi} 1 D_t(G \supseteq u \subseteq v, -1) - 1.
\]

Since \( F_n \) is a tree and \( u \) is a pendant vertex, then \( F_n - u = F_n / u \), that is, \( D_t(F_n - u, -1) = D_t(F_n / u, -1) \). For \( G \supseteq u \subseteq v = \phi \), we have \( D_t(F_n, -1) = 1 \); for \( G \supseteq u \subseteq v \neq \phi \), we can obtain that \( G \supseteq u \subseteq v \) must have at least one components \( B_i \geq 1 \). If one of the components is an isolated vertex, by Proposition 1(i) and (iii), one can obtain that \( D_t(F_n, -1) = 0 \). If every component \( B_i \) is a tree with at least two vertices, by the induction hypothesis, we have \( D_t(B_i, -1) \in \{0, 1\} \). Thus, by Proposition 1(iii), we have \( D_t(G \supseteq u \subseteq v, -1) = \prod_{i \geq 1} D_t(B_i, -1) \in \{0, 1\} \) for all the cases. Therefore, Theorem 7 is true. \( \square \)

The following result gives the relation between vertex set of degree 2 and coefficients of total domination polynomials.

**Theorem 8** If \( G \) is a connected graph of order \( n \), then the number of vertices of degree 2 is at least \( \binom{n}{2} - \binom{r}{2} - r(n - r) - d_t(G, n - 2) \), where \( r \) is the number of supporting vertices in \( G \).

**Proof.** Let \( L_0 = \{v : d(v) = 2 \text{ and none of } N(v) \text{ is a supporting vertex}\} \), that is, \( |L_0| \) is at most the number of vertices of degree 2. It is enough to show that \( d_t(G, n - 2) = \binom{n}{2} - \binom{r}{2} - r(n - r) - |L_0| \). Now we use "a pair" to give another representation of \( L_0 \). Set \( L = \{\{v_1, v_2\} : \text{there exists } v \in V(G) \text{ such that } N_G(v) = \{v_1, v_2\} \text{ and none of } v_1, v_2 \text{ is a supporting vertex}\} \), then \( |L| = |L_0| \). Next, for any vertices \( v_1, v_2 \) of \( V(G) \), we define

\[
L_1 = \{V(G) - \{v_1, v_2\} : \text{there exists } v \in V(G) \text{ such that } N_G(v) = \{v_1, v_2\}\},
\]

\[
L_2 = \{V(G) - \{v_1, v_2\} : \text{at least one of } v_1, v_2 \text{ is a supporting vertex}\},
\]

\[
T = \{V(G) - \{v_1, v_2\} : V(G) - \{v_1, v_2\} \text{ is not a total dominating set of } G\}.
\]

Then \( |L| = |L_1| - |L_2| \) and \( |L_2| = \binom{r}{2} + r(n - r) \). Now we first show Claim 2.

**Claim 2.** \( T = L_1 \cup L_2 \).

**Proof of Claim 2.** Clearly, \( L_1 \cup L_2 \subseteq T \). Next we will show that \( T \subseteq L_1 \cup L_2 \). Take \( W = V(G) - \{v_1, v_2\} \in T \) and since \( W \) is not a total dominating set of \( G \), by the definition
of total dominating set, there exists \( u \in V(G) \) such that \( N_G(u) \subseteq \{v_1, v_2\} \). If \( u \in W \), then \( d_G(u) \leq 2 \). When \( d_G(u) = 2 \), then \( N_G(u) = \{v_1, v_2\} \), that is, \( W \in L_1 \). When \( d_G(u) = 1 \), then \( u \) is a pendant vertex. Without loss of generality, set \( N_G(u) = \{v_1\} \), that is, \( v_1 \) is a supporting vertex and \( W \in S_2 \). We know \( |W| = n - 2 \), if \( u \notin W \), then \( u \) is either \( v_1 \) or \( v_2 \). Without loss of generality, say \( u = v_1 \). Since \( k = 0 \) and \( N(u) \cap W = \phi \), then \( N_G(u) = v_2 \), that is, \( v_2 \) is a supporting vertex. Thus, \( W \in L_2 \) and Claim 2 is true.

By the definition of total dominating set and Claim 2, we have

\[
d_t(G, n - 2) = \binom{n}{2} - |L_1 \cup L_2| = \binom{n}{2} - (|L_1| + |L_2| - |L_1 \cap L_2|)
\]
\[
= \binom{n}{2} - (\binom{r}{2} + r(n - r)) - (|L_1| - |L_1 \cap L_2|)
\]
\[
= \binom{n}{2} - \binom{r}{2} - r(n - r) - |L_1 - L_2|
\]
\[
= \binom{n}{2} - \binom{r}{2} - r(n - r) - |L|.
\]

Therefore, Theorem 8 is true.

\[\square\]

**References**

[1] H.A. Ahangar, L. Asgharsharghi, S.M. Sheikholeslami, L. Volkmann, Signed mixed Roman domination numbers in graphs. J. Comb. Optim. 32 (2016), no. 1, 299-317.

[2] R. B. Allan, R. Laskar, On domination and independent domination numbers of a graph, Discrete Mathematics, 23 (1978), 73-76.

[3] S. Alikhani, Y. H. Peng, Dominating sets and domination polynomials of cycles, Global Journal of Pure and Applied Mathematics, 4 (2008), 202–210.

[4] B. Chaluvaraju, V. Chaitra, Total domination polynomial of a graph, Journal of Informatics and Mathematical Sciences, 6 (2014), 87-92.

[5] R. C. Brigham, J. R. Carrington, and R. R. Vitray, Connected graphs with maximum total domination number, Journal of Combin. Comput. Combin. Math., 34 (2000), 81-96.

[6] S. T. Hedetniemi, R.C. Laskar, Bibliography on domination in graphs and some basic definitions of domination parameters, Discrete Mathematics, 86 (1990), 257-277.
[7] J.H. Hattingh, E.J. Joubert, Equality in a bound that relates the size and the restrained domination number of a graph. J. Comb. Optim. 31 (2016), no. 4, 1586-1608.

[8] M.A. Henning, V. Naicker, Disjunctive total domination in graphs. J. Comb. Optim. 31 (2016), no. 3, 1090-1110.

[9] M. A. Henning A survey of selected recent results on total domination in graphs, Discrete Mathematics, 309 (2009), 32-63.

[10] D. König, Theorie der Endlichen und Unendlichen Graphen, (Chelsea, New York, 1950).

[11] E. J. Cockayne, R. M. Dawes, and S. T. Hedetniemi, Total domination in graphs, Networks, 10 (1980), 211-219.

[12] T. Kotek, J. Preen, F. Simon, P. Tittmann and M. Trinks, Recurrence relations and splitting formulas for the domination polynomial, Electronic Journal of Combinatorics, 19 (2012), P47.

[13] R. P. Stanley, Acyclic orientations of graphs, Discrete Mathematics, 5 (1973), 171-178.

[14] A. Vijayan, S. S. Kumar, On total domination sets and polynomials of cycles, International Journal of Mathematical Archive, 3 (2012), 1379-1385.

[15] S. Wang, B. Wei, A note on the independent domination number versus the domination number in bipartite graphs, Czechoslovak Mathematical Journal, accepted(2016).

[16] V. Van, H. Jan, Edge criticality in graph domination. Graphs Combin. 32 (2016), no. 2, 801-811.