

RECENT DEVELOPMENTS IN TREE-PRUNING METHODS AND POLYNOMIALS FOR CACTUS GRAPHS AND TREES

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Abstract

The object of this paper is to review the recent developments in tree-pruning methods and characteristic and matching polynomials of spirographs, cacti and trees. The applications of the pruning method to spirographs, Bethe lattices, cactus lattices and Bethe cactus lattices are considered. In each case, the tree-pruning method yields analytical solutions for these graphs.

1. Introduction

Computations of the characteristic and matching polynomials of graphs have been the topic of numerous investigations in recent years [1–40]. A more complete list of references on characteristic polynomials of graphs can be found in a recent review article by Trinajstić [50]. The characteristic and matching polynomials of graphs have many physicochemical applications to a variety of areas ranging from fluid dynamics, quantum chemistry, spectroscopy, chemical kinetics and oscillatory reactions to statistical mechanics.

The evaluation of the characteristic and matching polynomials of graphs was for many years generally regarded as a tedious problem. With the advent of powerful algorithms and computers, it has now become possible to obtain these polynomials for graphs which contain up to 200 vertices. The evaluation of matching polynomials of large graphs containing many fused rings and three-dimensional structures still remains an unsolved problem.

A computer code in Pascal was developed by Ramaraj and the present author [30] to obtain the matching polynomials of graphs and lattices containing a large number of vertices. Although this code can be used to generate the matching polynomials of many graphs, application of this code to real lattices could consume large amounts of computational time due to the possibility of combinatorial explosion.

A fascinating and unsolved problem in statistical physics is the problem of dimer statistics for three-dimensional lattices. The problem is to find the number of ways of placing k dimers (dumbbells) on a lattice containing N points such that any two dimers are placed in a disjoint manner (i.e. two dimers do not have a common vertex in the

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lattice). This problem has many important applications in physics and chemistry. The grand canonical partition function of a lattice gas, the partition function of a system of interacting ferromagnets (the Ising problem), the kinetics and thermodynamics of adsorption of diatomics on surfaces, the enumeration of chemical resonance structures, and the stabilities of ionic crystals can all be shown to be related to the dimer statistics [42–48].

An analytical solution for the complete covering of dimers has been obtained by Temperley and Fisher [53] and Kasteleyn [54] for square lattices. A generating function for the number of ways of placing k dimers on a lattice of N points was called "matching polynomials" by Farrell [55] and Gutman [60], and "z-counting polynomials" by Hosoya [18]. These polynomials have not been obtained even for all two-dimensional lattices. The number of perfect matchings, however, can be obtained using the Pfaffian expansion of the associated directed lattice [42] or by the transfer matrix approach of Onsager [43].

Lattices and graphs with certain special characteristics are candidates for exact analytical solutions. The author [8] showed in 1982 that a powerful method, which he called the tree-pruning method, could be used to generate the characteristic polynomials of tree graphs (connected graphs containing no cycles). This was further expounded by the author and Randić [9] for non-tree graphs containing pending bonds. The author and Randić [10] also showed the use of this method for weighted graphs and trees.

The present author [38] more recently applied the tree-pruning method to the exact lattice statistics of Bethe lattices of any valence and size, including weighted Bethe lattices. Fisher and Essam [46] showed the use of Bethe lattices for percolation and cluster size problems. Although Bethe lattices are not true lattices, since they are mathematical abstractions of true lattices, they serve as useful candidates for exact solutions to many statistical problems. Cayley trees, which are used routinely in many statistical applications, are special cases of Bethe lattices.

In ref. [51], the author showed that the tree-pruning method could also be applied to graphs which he called "spirographs". This term was coined from the name spirocycle, used in organic chemistry for compounds which contain two cycles which share at most one common vertex. The characteristic polynomials of spirographs were shown to be easily derivable using the pruning method.

Hosoya and the author [52] combined the pruning method and the operator technique to obtain the exact lattice statistics and characteristic polynomials of cacti lattices of any length containing rings of any size. Powerful recursive relations were derived using these methods.

As seen from the above survey, there have been many important developments in the area of pruning techniques and graphical polynomials. The objective of this article is to summarize these developments. Section 2 describes the pruning method. Section 3 consists of applications of the pruning method to Bethe lattices. Section 4 comprises the applications of the pruning method to spirographs, while section 5 briefly discusses applications to some cacti lattices.

2. Pruning method

2.1. DEFINITIONS AND PRELIMINARIES

The adjacency matrix of a graph is defined as follows:

$$A_{ij} = \begin{cases} 1 & \text{if the vertices } i \text{ and } j \text{ are connected,} \\ 0 & \text{otherwise.} \end{cases} \quad (1)$$

The secular determinant of the adjacency matrix of a graph is called the characteristic polynomial of the graph. A tree is a connected graph containing no cycles. The non-terminal vertices of a tree (with degree more than 1) can be defined as the roots of the tree. Any tree can be expressed as a product of a quotient tree Q formed by a selected set of roots and the branches resulting from pruning the tree at these selected roots. For example, let us consider the tree in fig. 1. When this tree is pruned, fragments of certain

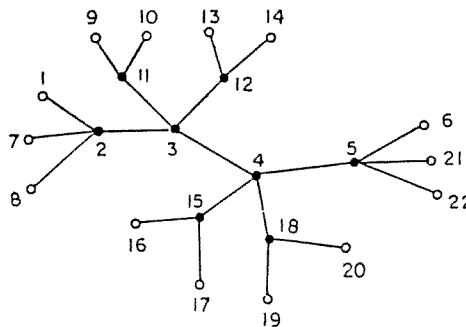


Fig. 1. An NMR tree containing 22 vertices.

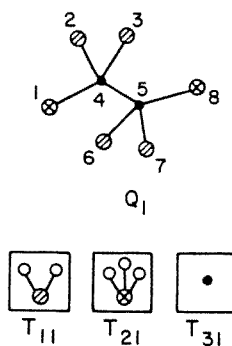


Fig. 2. The quotient tree Q_1 and the fragment types T_{11} , T_{21} and T_{31} generated by pruning the tree of fig. 1.

kinds recur. A collection of such fragments is shown in fig. 2, with the black dots identifying the roots. Let such a branch be denoted T_{ij} , where j stands for the pruning step. Let the characteristic polynomial of branch T_{ij} be H_{ij} . It can be seen that $H_{ij} = h_k = x^k - (k - 1)x^{k-2}$ if T_{ij} contains k vertices. Let the characteristic polynomial of fragments obtained by deleting the root in T_{ij} be denoted $H'_{ij} = h'_k$. It can be easily seen that the characteristic polynomial of $h'_k = x^{k-1}$. The tree in fig. 1 can be pruned at the vertices 2, 11, 12, 15, 5 and 18, resulting in the tree Q_1 shown in fig. 2 and the fragments T_{11} , T_{21} , and T_{31} . If we group all the pruning vertices of the same degree in the unpruned tree in fig. 1 into the same sets, we obtain

$$Y_1 = \{11, 12, 15, 18\}, Y_2 = \{2, 5\}, Y_3 = \{3, 4\}. \tag{2}$$

The tree in fig. 1 can be obtained by attaching each root in the set Y_1 to the root of a copy of the type T_{11} . Such a product was formulated by the author [41], which was called the root-to-root product and can be denoted as $Q \cdot (T_{11}, T_{21}, \dots)$.

The tree-pruning technique provides an elegant solution for the evaluation of characteristic polynomials of trees by contracting the secular determinant of the unpruned tree in terms of the secular determinants of the pruned tree and the branches. Let Q_1 be the quotient tree obtained in the first step of pruning and let T_{11}, T_{21}, \dots be the fragment types. Let q_{ij} be the adjacency matrix of the pruned tree (quotient tree). Define a contracted adjacency matrix of order $m \times m$ if m is the number of vertices in Q by the following recipe:

$$D_{ij} = \begin{cases} -H_{kj}(x) & \text{if } i = j \text{ and } i \in Y_k, \\ +q_{ij}H'_{kj}(x) & \text{if } i \neq j \text{ and } i \in Y_k. \end{cases} \tag{3}$$

It was shown that the characteristic polynomial of the unpruned tree is the determinant of the contracted adjacency matrix.

Let us illustrate this procedure with the tree shown in fig. 1. This tree can be pruned iteratively to a quotient tree containing just two vertices in two successive

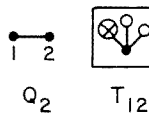


Fig. 3. The quotient tree Q_2 and the fragment type T_{12} obtained by pruning Q_1 in fig. 1.

iterations. The quotient tree and the types generated in the first and second iterations are shown in figs. 2 and 3, respectively. The matrices $D^{(j)}$ and H'_{ij} 's are given by (4)–(6):

$$H_{11} = h_3, \quad H'_{11} = h'_3, \quad H_{21} = h_4, \quad H'_{21} = h'_4, \quad H_{31} = h_1, \quad H'_{31} = 1, \quad (4)$$

$$D^{(12)} = \begin{bmatrix} h_4 & 0 & 0 & -h'_4 \\ 0 & h_3 & 0 & -h'_3 \\ 0 & 0 & h_3 & -h'_3 \\ -1 & -1 & -1 & h_1 \end{bmatrix}, \quad (5)$$

$$D'^{(12)} = \begin{bmatrix} h_4 & 0 & 0 \\ 0 & h_3 & 0 \\ 0 & 0 & h_3 \end{bmatrix}, \quad (6)$$

$$H_{12} = h_3^2 h_4 h_1 - 2h_3 h'_3 h_4 - h_3^2 h'_4, \quad H'_{12} = h_3^2 h_4, \quad (7)$$

$$A^{(2)} = \begin{bmatrix} H_{12} & -H'_{12} \\ -H'_{12} & H_{12} \end{bmatrix}. \quad (8)$$

$\det(A^{(2)}) = H_{12}^2 - H'^2_{12}$, which can be easily seen to be

$$x^{10}(x^6 - 10x^4 + 30x^2 - 28)^2 - x^8(x^6 - 7x^4 + 16x^2 - 12)^2. \quad (9)$$

The advantage of the above pruning method is that it recursively reduces the tree we started with into finally a tiny tree containing just two vertices. Since analytical expressions are known for the characteristic polynomials of branches, the problem of generating the characteristic polynomial of the tree in fig. 1 was reduced to just a 2×2 matrix, which can be evaluated trivially.

In the subsequent sections, we demonstrate the applications of the pruning method to generate polynomials of lattices and cacti.

3. Generating functions for Bethe lattices

A Bethe lattice of valence σ and length n is defined as a tree in which every non-terminal vertex has σ neighbors and there are n bonds from the central vertex to any terminal vertex. Figure 4 illustrates a Bethe lattice of valence 4 and $n = 3$. Let Q_i be the quotient tree generated in the i th step of pruning and T_i be the corresponding fragment type. Let H_i be the characteristic polynomial of type T_i and H'_i be the polynomial obtained after deleting the root (branch point) in T_i ; H_i and H'_i can be obtained recursively. At the n th step of pruning (where n is the length of the lattice), one obtains a simple tree whose polynomial can be obtained easily, and thus the polynomial of the

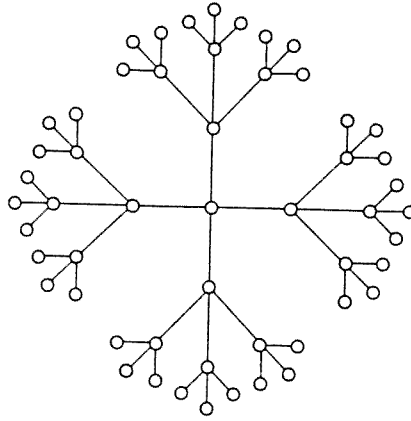


Fig. 4. A Bethe lattice with valence 4 and $n = 3$.

original lattice we started with can be constructed recursively. For a lattice of valence σ at the first iteration, type T_1 would contain one branch point and $(\sigma - 1)$ open vertices. Thus, the characteristic polynomial of T_1 , H_1 , is

$$\begin{aligned} H_1 &= h_\sigma = \lambda^\sigma - (\sigma - 1)\lambda^{\sigma-2}, \\ H'_1 &= \lambda^{\sigma-1}. \end{aligned} \quad (10)$$

At the second iteration, H_2 and H'_2 are expressed in terms of H_1 and H'_1 as

$$\begin{aligned} H_2 &= \lambda H_1^{\sigma-1} - (\sigma - 1)H'_1 H_1^{\sigma-2}, \\ H'_2 &= H_1^{\sigma-1}. \end{aligned} \quad (11)$$

Similarly, H_3 and H'_3 are expressed in terms of H_2 and H'_2 as

$$\begin{aligned} H_3 &= \lambda H_2^{\sigma-1} - (\sigma - 1)H'_2 H_2^{\sigma-2}, \\ H'_3 &= H_2^{\sigma-1}. \end{aligned} \quad (12)$$

Consequently, for any Bethe lattice, the expressions at the i th iteration are related to the ones at the $(i - 1)$ th iteration as

$$\begin{aligned} H_i &= \lambda H_{i-1}^{\sigma-1} - (\sigma - 1)H'_{i-1} H_{i-1}^{\sigma-2}, \\ H'_i &= H_{i-1}^{\sigma-1}. \end{aligned} \quad (13)$$

Finally, at the $(n - 1)$ th iteration, the characteristic polynomial H_{n-1} is

$$\begin{aligned} H_{n-1} &= \lambda H_{n-2}^{\sigma-1} - (\sigma - 1)H'_{n-2}H_{n-2}^{\sigma-2}, \\ H'_{n-1} &= H_{n-2}^{\sigma-1}. \end{aligned} \tag{14}$$

The contracted adjacency matrix of Q_n expressed in terms of H_{n-1} is given by

$$A_{ij} = \begin{cases} H_{n-1} & \text{if } i = j \text{ and } i \in Y_{n-1}, \\ \lambda & \text{if } i = j \text{ and } i \notin Y_{n-1}, \\ -H'_{n-1} q_{ij}^{(n-1)} & \text{if } i \neq j \text{ and } i \in Y_{n-1}, \\ -q_{ij}^{(n-1)} & \text{if } i \neq j \text{ and } i \notin Y_{n-1}, \end{cases} \tag{15}$$

where $q_{ij}^{(n-1)}$ is the adjacency matrix of Q_{n-1} and Y_n is the set of roots (branch points) in Q_{n-1} (there are $\sigma - 1$ vertices in Y_{n-1}). If the open vertex of Q_{n-1} carries the label 1, then the matrix A takes the form

$$A = \begin{bmatrix} \lambda & -1 & -1 & \dots & -1 \\ -H'_{n-1} & H_{n-1} & 0 & \dots & 0 \\ -H'_{n-1} & 0 & H_{n-1} & \dots & 0 \\ & 0 & H_{n-1} & \dots & 0 \\ \vdots & & \vdots & & \\ -H'_{n-1} & 0 & \dots & 0 & \dots & 0 & \dots & H_{n-1} \end{bmatrix}. \tag{16}$$

The determinant of A can be easily seen to be

$$H_n = \lambda H_{n-1}^\sigma - \sigma H'_{n-1} H_{n-1}^{\sigma-1}. \tag{17}$$

The above expression is simply the characteristic polynomial of the Bethe lattice one starts with.

The above method was used to obtain the characteristic polynomials of many Bethe lattices, including the weighted lattices in refs. [38]. Table 1 shows the characteristic (matching) polynomials of Bethe lattices with $n = 3$.

Table 1

The characteristic polynomials of Bethe lattices with $n = 3^*$

σ	Characteristic polynomial
2	$\lambda^7 - 6\lambda^5 + 10\lambda^3 - 4\lambda$
3	$\lambda^{22} - 21\lambda^{20} + 180\lambda^{18} - 816\lambda^{16} + 2112\lambda^{14}$ $- 3120\lambda^{12} + 2432\lambda^{10} - 768\lambda^8$
4	$\lambda^{53} - 52\lambda^{51} + 1224\lambda^{49} - 17,280\lambda^{47}$ $+ 163,350\lambda^{45} - 1,092,528\lambda^{43} + 5,321,700\lambda^{41}$ $- 19,123,128\lambda^{39} + 50,709,969\lambda^{37}$ $- 98,021,340\lambda^{35} + 134,238,060\lambda^{33}$ $- 123,294,312\lambda^{31} + 68,024,448\lambda^{29}$ $- 17,006,112\lambda^{27}$

* $\sigma = 4$ with $n = 3$ is shown in fig. 4.

4. Characteristic polynomials of spirographs

A spirograph can be obtained from simple ring graphs by "joining" a single vertex of one ring to a single vertex of another ring so that the two vertices are fused to become a single vertex in the final coalesced graph.

The resulting single vertex may be called a spiro vertex. Figure 5 shows a spirograph containing four-membered rings. The characteristic polynomials of spirographs can be obtained by pruning the spirograph at the spiral points, as shown by the author in ref. [51].

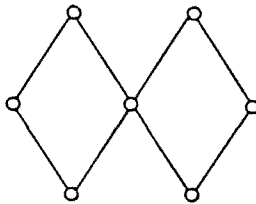


Fig. 5. A spirograph consisting of two 4-membered rings.

The pruning method could be generalized to any spirograph containing n rings. For a linear spirograph which contains n square rings, we obtain the following recursive relations by applying the pruning method. Let h_n denote the polynomial of such a spirograph containing n rings. The following relations can be derived:

Table 2
 Characteristic polynomials of linear spirographs containing hexagons

n	Characteristic polynomial
1	$\lambda^6 - 6\lambda^4 + 9\lambda^2 - 4$
2	$\lambda^{11} - 12\lambda^9 + 50\lambda^7 - 92\lambda^5 + 77\lambda^3 - 24\lambda$
3	$\lambda^{16} - 18\lambda^{14} + 127\lambda^{12} - 456\lambda^{10} + 911\lambda^8 - 1034\lambda^6 + 641\lambda^4 - 188\lambda^2 + 16$
4	$\lambda^{21} - 24\lambda^{19} + 240\lambda^{17} - 1312\lambda^{15} + 4338\lambda^{13} - 9080\lambda^{11} + 12,216\lambda^9 - 10,448\lambda^7 + 5429\lambda^5 - 1536\lambda^3 + 176\lambda$
5	$\lambda^{26} - 30\lambda^{24} + 389\lambda^{22} - 2876\lambda^{20} + 13,490\lambda^{18} - 42,324\lambda^{16} + 91,298\lambda^{14} - 136,944\lambda^{12} + 142,445\lambda^{10} - 100,830\lambda^8 + 46,553\lambda^6 - 12,868\lambda^4 + 1760\lambda^2 - 64$
6	$\lambda^{31} - 36\lambda^{29} + 574\lambda^{27} - 5364\lambda^{25} + 32,795\lambda^{23} - 138,800\lambda^{21} + 419,956\lambda^{19} - 925,160\lambda^{17} + 1,496,871\lambda^{15} - 1,779,076\lambda^{13} + 1,539,598\lambda^{11} - 950,500\lambda^9 + 403,101\lambda^7 - 109,672\lambda^5 + 16,736\lambda^3 - 1024\lambda$
7	$\lambda^{36} - 42\lambda^{34} + 795\lambda^{32} - 8992\lambda^{30} + 67,977\lambda^{28} - 364,190\lambda^{26} + 1,431,467\lambda^{24} - 4,217,420\lambda^{22} + 9,436,331\lambda^{20} - 16,143,846\lambda^{18} + 21,145,865\lambda^{16} - 21,113,992\lambda^{14} + 15,894,747\lambda^{12} - 8,843,410\lambda^{10} + 3,517,489\lambda^8 - 945,996\lambda^6 + 155,632\lambda^4 - 12,672\lambda^2 + 256$
8	$\lambda^{41} - 48\lambda^{39} + 1052\lambda^{37} - 13,976\lambda^{35} + 126,056\lambda^{33} - 819,600\lambda^{31} + 3,982,684\lambda^{29} - 14,803,560\lambda^{27} + 42,737,202\lambda^{25} - 96,770,336\lambda^{23} + 172,806,084\lambda^{21} - 243,777,000\lambda^{19} + 271,009,936\lambda^{17} - 236,160,336\lambda^{15} + 159,286,772\lambda^{13} - 81,642,776\lambda^{11} + 30,884,549\lambda^9 - 8,233,168\lambda^7 + 1,431,120\lambda^5 - 140,032\lambda^3 + 5376\lambda$

$$\begin{aligned}
 h_n &= \lambda^2 h_{n-1} - 4\lambda^2 h'_{n-1}, \\
 h_{n-1} &= \lambda^2 h_{n-2} - 4\lambda^2 h'_{n-2}, \\
 &\vdots \\
 h_2 &= \lambda^2 h_1 - 4\lambda^2 h'_1, \\
 h_1 &= \lambda^4 - 4\lambda^2, \\
 h'_1 &= \lambda^3 - 3\lambda.
 \end{aligned}
 \tag{18}$$

Thus, closed analytical solutions exist for the characteristic polynomials of linear spirographs containing n square rings. Similar recursive relationships can also be derived for many branched and other spirographs. Table 2 shows the characteristic polynomials of spirographs containing hexagons.

5. Characteristic polynomials of cacti lattices

A cactus is thus a special case of a spirograph. One could also form a Bethe cactus. The pruning method was applied to a variety of cacti.

As noted in the introduction, Hosoya and the present author [52] have recently applied a combination of operator and pruning methods to the characteristic and matching polynomials of cactus lattices. We illustrate this application of the pruning

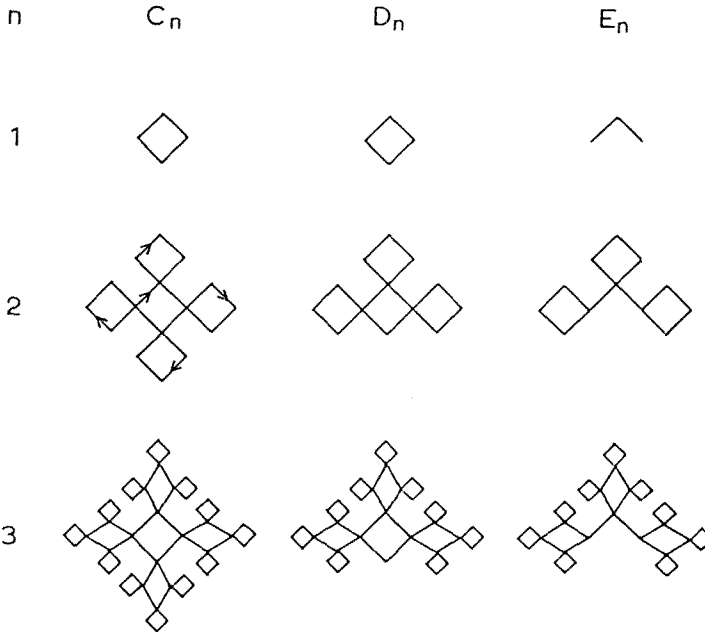


Fig. 6. A Bethe cactus lattice graph.

method with a few lattices. The recursive relation for the characteristic polynomials of a square Bethe cactus (see fig. 6) is given by

$$\begin{aligned}
 C_{n+1} &= D_n^2(D_n^2 - 4E_n^2), \\
 D_{n+1} &= D_n \{ x(D_n^2 - 2E_n^2) - 2D_n E_n \}, \\
 E_{n+1} &= D_n(D_n^2 - 2E_n^2),
 \end{aligned}
 \tag{19}$$

Matching polynomials of Bethe cactus lattices (see fig. 6)		
C_1	$x^4 - 4x^2 + 2$	
D_1	$x^4 - 4x^2 + 2$	
E_1	$x^3 - 3x$	
C_2	$x^{16} - 20x^{14} + 154x^{12} - 592x^{10} + 1224x^8 - 1360x^6 + 768x^4 - 192x^2 + 16$	
E_2	$x^{12} - 14x^{10} + 70x^8 - 156x^6 + 156x^4 - 64x^2 + 8$	
C_3	x^{52}	$- 68x^{50}$
	$2.146x^{48}$	$- 41,808x^{46}$
	$564,176x^{44}$	$- 5,608,944x^{42}$
	$42,660,112x^{40}$	$- 254,428,352x^{38}$
	$1,210,038,944x^{36}$	$- 4,642,068,736x^{34}$
	$14,475,527,136x^{32}$	$- 36,865,992,448x^{30}$
	$76,859,935,360x^{28}$	$- 131,207,699,712x^{26}$
	$183,088,095,744x^{24}$	$- 208,075,950,080x^{22}$
	$191,507,584,256x^{20}$	$- 141,618,212,864x^{18}$
	$83,262,424,576x^{16}$	$- 38,388,748,288x^{14}$
	$13,633,136,640x^{12}$	$- 3,641,827,328x^{10}$
	$708,399,104x^8$	$- 95,731,712x^6$
	$8,343,552x^4$	$- 409,600x^2$
	$8,192$	
D_3	x^{40}	$- 52x^{38}$
	$1,226x^{36}$	$- 17,400x^{34}$
	$166,448x^{32}$	$- 1,138,680x^{30}$
	$5,768,104x^{28}$	$- 22,101,424x^{26}$
	$64,876,080x^{24}$	$- 146,857,536x^{22}$
	$256,821,367x^{20}$	$- 346,124,864x^{18}$
	$357,164,416x^{16}$	$- 279,128,320x^{14}$
	$162,584,960x^{12}$	$- 69,008,384x^{10}$
	$20,678,400x^8$	$- 4,177,920x^6$
	$529,408x^4$	$- 36,864x^2$
	$1,024$	
	x^{39}	$- 50x^{37}$
	$1,132x^{35}$	$- 15,400x^{33}$
	$140,892x^{31}$	$- 919,272x^{29}$
$4,426,488x^{27}$	$- 16,058,032x^{25}$	
$44,414,320x^{23}$	$- 94,189,440x^{21}$	
E_3	$153,239,936x^{19}$	$- 190,488,384x^{17}$
	$179,343,360x^{15}$	$- 126,095,744x^{13}$
	$64,849,792x^{11}$	$- 23,680,256x^9$
	$5,879,040x^7$	$- 927,744x^5$
	$82,432x^3$	$- 3,072x$
Number of vertices N	$C_n: 2(3^n - 1)$	
	$D_n: (3^{n+1} - 1)/2$	
	$E_n: 3(3^n - 1)/2$	

where the symbols C_n, D_n , etc. are illustrated in fig. 6. For a triangular cactus, we obtain

$$\begin{aligned} C_{n+1} &= D_n^3 - 3E_n^2 D_n - 2E_n^3, \\ D_{n+1} &= x(D_n^2 - E_n^2) - 2E_n(D_n + E_n), \\ E_{n+1} &= D_n^2 - E_n^2. \end{aligned} \tag{20}$$

Similar recursive relations could be obtained for any Bethe cactus. By a combination of pruning method and operator technique, Hosoya and the author [52] have obtained the characteristic polynomials and matching polynomials of cactus lattices. An example of a cactus is shown in fig. 6.

As an example, let us illustrate the application of the pruning method to the characteristic polynomial of the Bethe cactus in fig. 6. The matching polynomials of cacti can also be obtained by edge-weighting the lattice, as shown in fig. 7. The

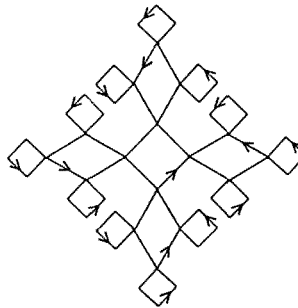


Fig. 7. A directed cactus graph. The characteristic polynomial of this graph is the matching polynomial of the original undirected graph.

characteristic polynomial of the directed lattice in fig. 7 is the matching polynomial if one assigns a weight i in the direction of the arrow and $-i$ in the opposite direction. The matching polynomials of Bethe lattices are shown in table 3. For the matching polynomials of other graphs, see [59].

6. Conclusion

In this paper, we reviewed the recent developments in tree-pruning and operator methods to the exact computations of characteristic and matching polynomials of tree graphs, spirographs, cactus graphs and Bethe lattices. We showed that powerful recursive relations and exact analytical expressions can be obtained through the use of operator and pruning techniques.

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