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ZZ Polynomials of Regular m-tier Benzenoid Strips as Extended Strict Order Polynomials of Associated Posets Part 2. Guide to Practical Computation

Johanna Langner[1] **, Henryk A. Witek**[1,2]

[1] *Department of Applied Chemistry and Institute of Molecular Science, National Yang Ming Chiao Tung University, Hsinchu, Taiwan*
[2] *Center for Emergent Functional Matter Science, National Yang Ming Chiao Tung University, Hsinchu, Taiwan*

johanna.langner@arcor.de, hwitek@mail.nctu.edu.tw

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Abstract

We present an algorithm for computing the ZZ polynomial of an arbitrary m-tier regular strip of length n. Our approach is based on the equivalence between the ZZ polynomial $\mathrm{ZZ}(\boldsymbol{S},x)$ of a regular benzenoid strip $\boldsymbol{S}$ and the extended strict order polynomial $\mathrm{E}^{\circ}_{\mathcal{S}}(n,1+x)$ of the corresponding poset $\mathcal{S}$, demonstrated formally in Part 1 of the current series of papers. The process of computing $\mathrm{ZZ}(\boldsymbol{S},x)$ in the form of $\mathrm{E}^{\circ}_{\mathcal{S}}(n,1+x)$ reduces to four, fully automatable steps: (i) Construction of the poset $\mathcal{S}$ corresponding to $\boldsymbol{S}$. (ii) Construction of the Jordan-Hölder set $\mathcal{L}(\mathcal{S})$ of linear extensions of $\mathcal{S}$. (iii) Computing the number $\mathrm{des}(w)$ of descents in each $w \in \mathcal{L}(\mathcal{S})$. ($iv$) Computing the number $\mathrm{fix}_{\mathcal{S}}(w)$ of fixed labels in each $w \in \mathcal{L}(\mathcal{S})$. The ZZ polynomial of $\boldsymbol{S}$ can then be expressed in the following form

$$\mathrm{ZZ}(\boldsymbol{S},x) = \mathrm{E}^{\circ}_{\mathcal{S}}(n,1+x) = \sum_{w\in\mathcal{L}(\mathcal{S})} \sum_{k=0}^{|\mathcal{S}|} \binom{|\mathcal{S}| - \mathrm{fix}_{\mathcal{S}}(w)}{k\ - \mathrm{fix}_{\mathcal{S}}(w)} \binom{n+\mathrm{des}(w)}{k} (1+x)^k ,$$

where $|\mathcal{S}|$ denotes the number of elements in $\mathcal{S}$. Practical applications of the algorithm are illustrated with a few examples. The complete account of ZZ polynomials of regular m-tier benzenoid strips $\boldsymbol{S}$ with $m = 1$–6 computed using the introduced algorithm is presented in Part 3 of the current series of papers.

1 Introduction

Consider a cycle C_H in a two-dimensional hexagonal grid H. We define the *benzenoid* $\boldsymbol{B}$ as a graph consisting of all the vertices and edges of H which lie on C_H and in the interior of C_H. We consider further two types of spanning subgraphs of $\boldsymbol{B}$: Kekulé structures and Clar covers [42]. A *Kekulé structure* K is a spanning subgraph of $\boldsymbol{B}$ in which every component is isomorphic to K_2 (i.e., a complete graph on two vertices). A *Clar cover* C is a spanning subgraph of $\boldsymbol{B}$ in which every component is isomorphic either to K_2 or to C_6 (i.e., a cycle graph with 6 vertices). Let us denote the number of Kekulé structures of $\boldsymbol{B}$ by $\mathcal{K} \equiv \mathcal{K}(\boldsymbol{B})$ and the number of Clar covers of $\boldsymbol{B}$ by $\mathcal{C} \equiv \mathcal{C}(\boldsymbol{B})$. The determination of $\mathcal{K}$ and $\mathcal{C}$ constitutes one of the most important problems in chemical graph theory. The enumeration of Clar covers can be substantially simplified by stratifying the set of Clar covers into strata indexed by their order k, which, for a given C, is defined as the number of C_6 components in C. Denoting by c_k the cardinality of the stratum corresponding to the order k, we immediately have $\mathcal{K} = c_0$ and $\mathcal{C} = c_0 + \cdots + c_{Cl}$, where the number Cl—usually referred to as the *Clar number* of $\boldsymbol{B}$ and naturally bounded from above by $|V(\boldsymbol{B})|/6$—denotes the maximal number of C_6 components that can be accommodated in $\boldsymbol{B}$. The generating function for the sequence $[c_0, c_1, \ldots, c_{Cl}]$

$$\mathrm{ZZ}\left(\boldsymbol{B}, x\right) = \sum_{k=0}^{Cl} c_k x^k, \tag{1}$$

usually referred to as the *Clar covering polynomial*, the *Zhang-Zhang polynomial*, or simply the *ZZ polynomial* of $\boldsymbol{B}$, was introduced into chemical graph theory in 1996 by two Chinese mathematicians, Heping Zhang and Fuji Zhang [80, 81, 83, 85, 86]. It was soon realized that the ZZ polynomial of an arbitrary benzenoid $\boldsymbol{B}$ can be efficiently computed using a recursive decomposition process [21, 45, 83, 85, 86] expressible in the form of a computer algorithm [21, 45], which has been implemented in a number of freely available efficient computer programs (initially ZZCalculator [20,21] and later ZZDecomposer [24,25,90,91]). With these automatized programs, characterization and enumeration of Clar covers of benzenoids containing up to a few thousands of vertices became a routine task [76].

ZZDecomposer played yet another important role in the development of the ZZ polynomial theory: It allowed for the determination and derivation of closed-form ZZ polynomial formulas for whole families of isostructural benzenoids [4,5,41,43,45,80–86], allowing to extend the analogous, heroic effort of computing $\mathcal{K}\left(\boldsymbol{B}\right)$ lead by Cyvin and Gutman some 30 years earlier [11, 29–38, 42, 44]. ZZDecomposer has been used in many applications [19–24, 26, 47, 54, 60, 62, 74–78] to find closed-form formulas for ZZ polynomials of various families of basic catacondensed and pericondensed benzenoids, substantially extending the total body of previously available results. The rapid development of Clar theory stimulated by these discoveries in recent years lead to many new interesting applications and connections to other branches of chemistry, graph theory, and combinatorics [1–6, 8–10, 15–18, 28, 40, 41, 46, 50, 54, 62, 64, 65, 71, 73, 79, 87–89]. A completely new chapter in the research on Clar covers has been opened with the development of the interface theory of benzenoids [52, 53, 55, 56], which showed that the distribution of K_2 and C_6 components in Clar covers of a benzenoid $\boldsymbol{B}$ is governed by a set of simple geometric rules. Assume that $\boldsymbol{B}$ is oriented such that some of its edges are horizontal; then the total number of C_6 components and horizontally oriented K_2 components depends only on the shape of $\boldsymbol{B}$. Likewise, the relative positions of these components are restricted: Between two such components within the same vertical column of hexagons, one will always find exactly one such component in each of the neighbouring hexagon columns. Conversely, specifying the absolute positions within $\boldsymbol{B}$ of the C_6 and horizontal K_2 components of a Clar cover C fully defines C. This observation gives rise to an important strategy for enumerating Clar covers: We may encode every Clar cover of a given benzenoid $\boldsymbol{B}$ as a map indicating the positions of its C_6 and horizontal K_2 components in $\boldsymbol{B}$. The geometric rules governing the number and distribution of the Clar cover components are naturally translated into certain restrictions on the aforementioned maps, enabling us to construct the full set of Clar covers of $\boldsymbol{B}$ in terms of the full set of maps following these restrictions.

In the prequel [58] to this paper we have demonstrated that for a particular class of benzenoids referred to as *regular m-tier strips*, the enumeration of Clar covers can be done in an especially efficient way using concepts borrowed from poset theory. A regular m-tier strip $\boldsymbol{S}$ of length n is defined as follows. Take the previously considered hexagonal grid H, oriented such that some of its edges are horizontal. A *regular 1-tier strip of length n* is a graph obtained by merging n consecutive adjacent hexagons located in the same vertical column of H. A *regular m-tier strip* $\boldsymbol{S}$ is obtained by merging m consecutive regular 1-tier strips located in adjacent columns of H, in such a way that the following two conditions are satisfied: (i) Two adjacent 1-strips differ at each end by $\pm\frac{1}{2}$ hexagon unit. (ii) The first and the last regular 1-tier strips are both of the same length

n [77,78]. This paper gives a detailed, self-contained, step-by-step guide on the practical computation of Zhang-Zhang polynomials of regular strips. Let us summarize here the underlying ideas behind this computational recipe, which are explained in much greater detail in [58]. The special shape of regular m-tier strips translates into especially simple rules governing the maps encoding their Clar covers: For any regular m-tier strip $\boldsymbol{S}$, we may construct a corresponding partially ordered set (poset) $\mathcal{S}$ such that every strictly order-preserving map from an induced subposet Q of $\mathcal{S}$ to $\{1, 2, \ldots, n\}$ corresponds to exactly one Kekulé structure of $\boldsymbol{S}$ with $|Q|$ proper sextets, and consequently (since we may replace any number of the proper sextets by aromatic rings $C_6 =$) to $2^{|Q|}$ Clar covers of $\boldsymbol{S}$. Simultaneously, every Kekulé structure (and Clar cover) is associated with exactly one such strictly order-preserving map from some induced subposet of $\mathcal{S}$ to the set $\{1, 2, \ldots, n\}$. This isomorphism between Kekulé structures and maps enables us to use preexisting tools to enumerate these maps for the poset $\mathcal{S}$, and in the same breath obtain the number of Clar covers of the corresponding regular strip $\boldsymbol{S}$. Specifically, we may compute the Zhang-Zhang polynomial $\mathrm{ZZ}(\boldsymbol{S}, x)$ of a given Kekuléan regular m-tier strip $\boldsymbol{S}$ of length n as the *extended strict order polynomial* $\mathrm{E}^{\circ}_{\mathcal{S}}(n, 1+x)$ of the poset $\mathcal{S}$ corresponding to $\boldsymbol{S}$:

$$\mathrm{ZZ}\,(\boldsymbol{S}, x) = \mathrm{E}^{\circ}_{\mathcal{S}}(n, 1+x). \tag{2}$$

The extended strict order polynomial $\mathrm{E}^{\circ}_{\mathcal{S}}(n, z)$ was introduced in our previous publications [57,58] as a generalization of the Stanley's strict order polynomial $\Omega^{\circ}_{\mathcal{P}}(n)$ [66–68], which enumerates the strictly order-preserving maps $\phi : \mathcal{P} \to \{1, \ldots, n\}$ and can be computed as

$$\Omega^{\circ}_{\mathcal{P}}(n) = \sum_{w \in \mathcal{L}(\mathcal{P})} \binom{n + \mathrm{des}(w)}{|\mathcal{P}|}, \tag{3}$$

where $|\mathcal{P}|$ denotes the cardinality of a poset $\mathcal{P}$, $\mathcal{L}(\mathcal{P})$ denotes the Jordan-Hölder set of linear extensions w of $\mathcal{P}$, and $\mathrm{des}(w)$ is the number of descents in w. Based on this idea, the extended strict order polynomial $\mathrm{E}^{\circ}_{\mathcal{S}}(n, z)$ of the poset $\mathcal{S}$ is defined as

$$\mathrm{E}^{\circ}_{\mathcal{S}}(n, z) = \sum_{\mathcal{P} \subset \mathcal{S}} \Omega^{\circ}_{\mathcal{P}}(n)\, z^{|\mathcal{P}|}, \tag{4}$$

with the summation running over all induced subposets of $\mathcal{S}$. We have demonstrated in [58] that it can be efficiently computed using the following formula

$$\mathrm{E}^{\circ}_{\mathcal{S}}(n, z) = \sum_{w \in \mathcal{L}(\mathcal{S})} \sum_{k=0}^{|\mathcal{S}|} \binom{|\mathcal{S}| - \mathrm{fix}_{\mathcal{S}}(w)}{k \ - \mathrm{fix}_{\mathcal{S}}(w)} \binom{n + \mathrm{des}(w)}{k} z^{k}, \tag{5}$$

where $\mathrm{fix}_{\mathcal{S}}(w)$ denotes the number of fixed labels in the linear extension w of $\mathcal{S}$.

The following sections give step-by-step instructions for the practical computation of Zhang-Zhang polynomials via extended strict order polynomials. This exposition uses as little formal language as possible to highlight the practical aspects of the computations; we believe that the theoretical framework was sufficiently exposed in the preceding publications [57, 58] to justify the course taken here.

2 Computation of ZZ polynomials via posets

The computation of the Zhang-Zhang polynomial $\mathrm{ZZ}(\boldsymbol{S}, x)$ of a regular strip $\boldsymbol{S}$ as an extended strict order polynomial $\mathrm{E}^{\circ}_{\mathcal{S}}(n, 1+x)$ of a corresponding poset $\mathcal{S}$ using Eq. (5) consists of four, fully automatable steps:

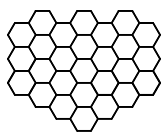
1. Determination of the poset $\mathcal{S}$ corresponding to $\boldsymbol{S}$—see Subsection 2.1.
2. Construction of the full set $\mathcal{L}(\mathcal{S})$ of linear extensions of $\mathcal{S}$—see Subsection 2.2.
3. Counting the number $\mathrm{des}(w)$ of descents for each $w \in \mathcal{L}(\mathcal{S})$—see Subsection 2.3.
4. Counting the number $\mathrm{fix}_{\mathcal{S}}(w)$ of fixed labels for each $w \in \mathcal{L}(\mathcal{S})$—see Subsection 2.3.

Finally, all the precomputed ingredients are substituted into Eq. (5), which, by virtue of Eq. (2), yields the ZZ polynomial of $\boldsymbol{S}$.

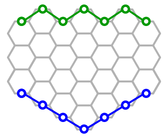
2.1 Constructing the poset $\mathcal{S}$ from a regular strip $\boldsymbol{S}$

The existence of a corresponding poset $\mathcal{S}$ for every Kekuléan strip $\boldsymbol{S}$ has been formally demonstrated in [58] together with an outline of a construction of $\mathcal{S}$; here we give a much simpler, step-by-step recipe for constructing $\mathcal{S}$. Let us start with a four-step graphical representation of the process of creating $\mathcal{S}$ from $\boldsymbol{S}$. Subsequently, we will give an algebraic representation of this process, which is more suitable for developing an associated fully-automatized computer code.

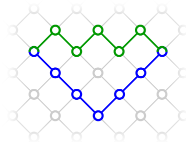
(i) Let $\boldsymbol{S}$ be any regular strip, such as the 7-tier oblate pentagon $D^j(4,3)$ shown on the right. We draw $\boldsymbol{S}$ in such a way that its defining hexagon columns are oriented vertically.



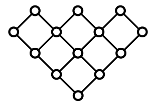
(*ii*) We trace the upper and lower boundaries of $\boldsymbol{S}$ by connecting the centers of the top and bottom horizontal edges of consecutive hexagon columns.



(*iii*) We construct a square grid $\boldsymbol{G}$ rotated by 45°. We embed the upper and lower boundaries of $\boldsymbol{S}$ in $\boldsymbol{G}$ in such a way that the pattern of each boundary is preserved and that the ends of both boundaries coincide.[1]



(*iv*) The Hasse diagram of the poset $\mathcal{S}$ is obtained by choosing all the vertices and edges of $\boldsymbol{G}$ which lie on or below the upper boundary ***and*** on or above the lower boundary.[2]



The Hasse diagram S of $\mathcal{S}$ is interpreted in the following standard way: Its vertices represent the elements of $\mathcal{S}$ and its upward-directed edges, the cover relations in $\mathcal{S}$: If a vertex $s \in V(S)$ is connected to a vertex $t \in V(S)$ by an upwards-directed edge of S, we say that t *covers* s and we write $s \lessdot_{\mathcal{S}} t$. If a vertex $s \in V(S)$ is connected to a vertex $t \in V(S)$ by an upward-directed path in S, we say that s is smaller (in $\mathcal{S}$) than t and we write $s <_{\mathcal{S}} t$. Clearly, specifying only the cover relations $\lessdot_{\mathcal{S}}$ is sufficient to define the partial order $<_{\mathcal{S}}$ (formally, as the transitive closure of $\lessdot_{\mathcal{S}}$). These concepts are illustrated

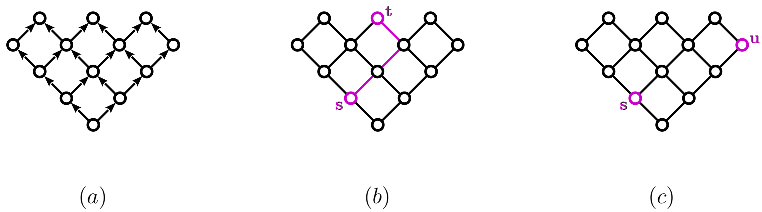


Figure 1. (*a*) The Hasse diagram is a directed graph representation of a poset $\mathcal{S}$: The vertices correspond to the elements of $\mathcal{S}$, and the upward-directed edges to the cover relations in $\mathcal{S}$. (*b*) Two elements s, t stand in the relation $s <_{\mathcal{S}} t$ if there is a monotonously upward-directed path from s to t. (*c*) Two elements s, u are incomparable by $<_{\mathcal{S}}$ if there is no upward-directed path from s to u or *vice versa*.

[1] If it is not possible to make both ends coincide, $\boldsymbol{S}$ is non-Kekuléan. Similarly, if the upper boundary departs more than one square down in G from the lower boundary, $\boldsymbol{S}$ is non-Kekuléan.

[2] If the boundaries cross, the Hasse diagram of $\mathcal{S}$ is disconnected, see e.g. Fig. 2 (*iv*).

in Fig. 1. Practical application of this simple graphical algorithm is illustrated in Fig. 2 for five typical regular strips.

The presented graphical construction of the Hasse diagram of $\mathcal{S}$ corresponding to a regular strip $\boldsymbol{S}$ seems to be the most intuitive. However, with a computer program implementation in mind, it might be advantageous to give an alternative, algebraic representation of the construction process.

To this end, let us first introduce a way of specifying the shape of any regular strip $\boldsymbol{S}$ in a compact form, as a list of letters. As above, ensure that $\boldsymbol{S}$ is oriented such that its

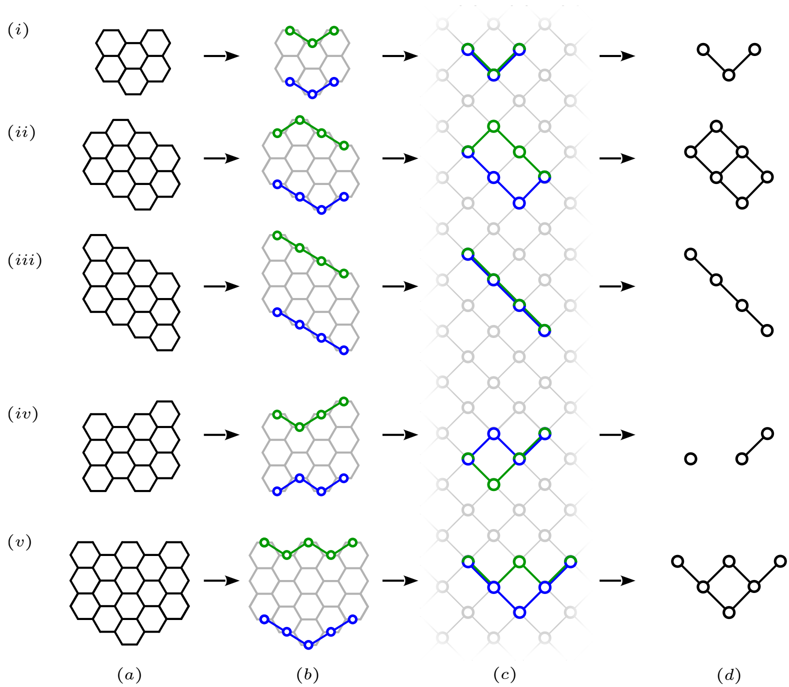


Figure 2. Graphical construction of Hasse diagrams for various regular strips $\boldsymbol{S}$: (i) chevron $Ch(2,2,2)$, (ii) hexagonal flake $O(4,2,2)$, (iii) parallelogram $M(4,3)$, (iv) streamer $\Sigma(2,3,n)$, and (v) prolate pentagon $D^i(3,3)$. Steps of the construction involve: (a) drawing $\boldsymbol{S}$ in vertical orientation, (b) tracing the upper and lower boundary of $\boldsymbol{S}$, (c) embedding the upper and lower boundaries of $\boldsymbol{S}$ in the square grid $\boldsymbol{G}$ in such a way that the pattern of each boundary is preserved and that the ends of both boundaries coincide, and (d) forming the Hasse diagram of $\mathcal{S}$ by selecting all the vertices and edges of $\boldsymbol{G}$ which lie on or below the upper boundary ***and*** on or above the lower boundary.

defining columns run vertically. Then, going from left to right, compare each column i_k to the previous one (i_{k-1}). We know from the definition of regular strips that, on the top and bottom ends, i_k is either half a hexagon longer or shorter than i_{k-1}. We can therefore distinguish four cases:

`W`	(wider)	if i_k	is longer than i_{k-1} on both ends.
`N`	(narrower)	if i_k	is shorter than i_{k-1} on both ends.
`R`	(raised)	if i_k	is longer than i_{k-1} on the top, but shorter on the bottom.
`L`	(lowered)	if i_k	is shorter than i_{k-1} on the top, but longer on the bottom.

Consequently, every regular m-tier strip $\boldsymbol{S}$ of length n can be uniquely represented by its length n and a $(m-1)$-letter sequence of these descriptors, obtained by comparing the shapes of i_k and i_{k-1} for $k = 2, \ldots, m$. For example, the structures (i)–(v) analyzed in Fig. 2 can be uniquely represented by the following pairs: (i) ($[\mathtt{L}, \mathtt{R}]$, $n = 2$), (ii) ($[\mathtt{W}, \mathtt{L}, \mathtt{N}]$, $n = 2$), (iii) ($[\mathtt{L}, \mathtt{L}, \mathtt{L}]$, $n = 3$), (iv) ($[\mathtt{N}, \mathtt{W}, \mathtt{R}]$, $n = 3$), and (v) ($[\mathtt{L}, \mathtt{W}, \mathtt{N}, \mathtt{R}]$, $n = 3$). The 7-tier oblate pentagon $D^j(4, 3)$ discussed in the first example corresponds to ($[\mathtt{W}, \mathtt{L}, \mathtt{W}, \mathtt{N}, \mathtt{R}, \mathtt{N}]$, $n = 3$). These sequences of column shapes are used as the input for Algorithm 1 for constructing the poset $\mathcal{S}$.

Algorithm 1: Construction of the poset $\mathcal{S}$, with its order $<_{\mathcal{S}}$ indicated through the set $\mathcal{C}$ of cover relations.

Data: Sequence *shapes* of length $m - 1$
Result: Poset $\mathcal{S}$ with the set of cover relations $\mathcal{C}$

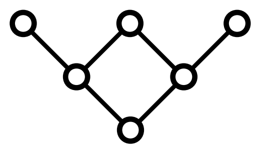
$l_1 := 0;$ `// Boundaries`
$r_1 := 0;$
$\mathcal{S} := \{s_{0,0}\};$ `// Poset`
$\mathcal{C} := \{\};$ `// Set of cover relations`
for $k = 2$ **to** m **do**
  if $shapes_k \in \{\mathtt{W}, \mathtt{L}\}$ **then** $l_k := l_{k-1} - 1$ **else** $l_k := l_{k-1} + 1$;
  if $shapes_k \in \{\mathtt{W}, \mathtt{R}\}$ **then** $r_k := r_{k-1} + 1$ **else** $r_k := r_{k-1} - 1$;
  if $r_k - l_k < -2$ **then return** "Non-Kekuléan strip, no corresponding poset.";
  for $j = l_k$ **to** r_k **by** *2* **do**
    $\mathcal{S} := \mathcal{S} \cup \{s_{k,j}\};$
    if $s_{k-1,j-1} \in \mathcal{S}$ **then** $\mathcal{C} := \mathcal{C} \cup \{s_{k-1,j-1} \lessdot_{\mathcal{S}} s_{k,j}\}$;
    if $s_{k-1,j+1} \in \mathcal{S}$ **then** $\mathcal{C} := \mathcal{C} \cup \{s_{k,j} \lessdot_{\mathcal{S}} s_{k-1,j+1}\}$;
  end
end
return $(\mathcal{S}, \mathcal{C})$;

2.2 Generation of the Jordan-Hölder set $\mathcal{L}(\mathcal{S})$ of $\mathcal{S}$

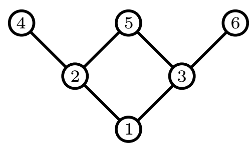
Intuitively speaking, every partial order $\mathcal{S}$ can be extended to a linear order by augmenting $\mathcal{S}$ with a certain number of additional "$s <^*_{\mathcal{S}} t$" relations. Usually, such an extension can be performed in multiple ways, resulting in multiple distinct linear orders compatible with a given partial order $\mathcal{S}$. The set of linear orders that can be generated in this way is referred to as the Jordan-Hölder set $\mathcal{L}(\mathcal{S})$ of $\mathcal{S}$, and a single linear order $w \in \mathcal{L}(\mathcal{S})$ is referred to as a linear extension of $\mathcal{S}$. A linear extension $w \in \mathcal{L}(\mathcal{S})$ of a p-element poset $\mathcal{S}$ is represented as a sequence $w = w_1 w_2 w_3 \dots w_p$ of labels $w_i \in \{1, 2, \dots, p\}$ in the following way: First, we decide on a function $\omega : \mathcal{S} \to \{1, 2, \dots, p\}$ which assigns to each element s of $\mathcal{S}$ a label $\omega(s) \in \{1, 2, \dots, p\}$. It is useful to choose a *natural labeling*, which means that whenever two elements $s, t \in \mathcal{S}$ stand in the relation $s <_{\mathcal{S}} t$, their labels satisfy $\omega(s) < \omega(t)$. Using this labeling, a sequence $w = w_1 w_2 \dots w_p$ now signifies the linear order $\omega^{-1}(w_1) <^*_{\mathcal{S}} \omega^{-1}(w_2) <^*_{\mathcal{S}} \dots <^*_{\mathcal{S}} \omega^{-1}(w_p)$. A linear order $<^*_{\mathcal{S}}$ is compatible with the partial order $<_{\mathcal{S}}$ if for every $s, t \in \mathcal{S}$ with $s <_{\mathcal{S}} t$, we also have $s <^*_{\mathcal{S}} t$. In other words, a sequence w is a linear extension of $\mathcal{S}$ if for every $s, t \in \mathcal{S}$ with $s <_{\mathcal{S}} t$, the label $\omega(s)$ precedes the label $\omega(t)$ in the sequence w.

We believe that it is in the spirit of the current guide to illustrate the introduced theoretical concepts with some elementary examples. The introduced in Subsection 2.1 poset $\mathcal{S}$ corresponding to $D^j(4, 3)$ has as many as 8580 linear extensions and does not constitute a good *elementary* example. Instead, we analyze the linear extensions of the five posets depicted in Fig. 2, which have manageable numbers of linear extensions.

Let us start the analysis on the example of the poset $\mathcal{S}$ corresponding to $D^i(3, n)$ depicted in Fig. 2(v). The first task is to assign labels $\omega(s) \in \{1, 2, \dots, 6\}$ to each element $s \in \mathcal{S}$ in such a way that the mapping $\omega : \mathcal{S} \to \{1, 2, \dots, 6\}$ is a natural labeling.



This can be easily accomplished by labeling the vertices of the corresponding Hasse diagram in the bottom→top direction and (secondarily) in the left→right direction.



Clearly, since ω is a natural labeling, the sequence 123456 is a linear extension. The remaining linear extensions are generated by considering all permutations of the labels that are compatible with the studied poset $\mathcal{S}$. In particular, for any linear extension w of the poset $\mathcal{S}$ associated with $D^i(3,n)$, the following conditions must be satisfied: (i) Since $\omega^{-1}(1) <_{\mathcal{S}} \omega^{-1}(s)$ for all $s \in \mathcal{S}$, the label 1 must precede all other labels. (ii) Since $\omega^{-1}(2) <_{\mathcal{S}} \omega^{-1}(4)$ and $\omega^{-1}(2) <_{\mathcal{S}} \omega^{-1}(5)$, the label 2 must precede labels 4 and 5. (iii) Since $\omega^{-1}(3) <_{\mathcal{S}} \omega^{-1}(5)$ and $\omega^{-1}(3) <_{\mathcal{S}} \omega^{-1}(6)$, the label 3 must precede labels 5 and 6. It is easy to construct all 16 label sequences which satisfy these conditions; they are listed in Eq. (8). We leave it as an exercise to the reader to demonstrate that the Jordan-Hölder sets for the posets $\mathcal{S}$ depicted in Fig. 2(i–iv) are given by: (i) $\mathcal{L}(\mathcal{S}) = \{123, 132\}$, (ii) $\mathcal{L}(\mathcal{S}) = \{123456, 132456, 123546, 132546, 124356\}$, (iii) $\mathcal{L}(\mathcal{S}) = \{1234\}$, and (iv) $\mathcal{L}(\mathcal{S}) = \{123, 213, 231\}$.

Analysis of linear extensions of finite posets has received considerable attention in the literature. Counting linear extensions of a general poset $\mathcal{S}$ was demonstrated to be #P-complete [13]. Several algorithms and strategies for generating linear extensions of non-structured posets were reported over the years [7,12,14,27,39,48,49,51,61,63,70,72]. In our practical investigations, we generate $\mathcal{L}(\mathcal{S})$ using the command `extensions` from Stembridge's poset Maple package [69] for small and medium-size posets $\mathcal{S}$; and for larger posets, we use an in-house written Maple routine counting linear extensions using walks on an auxiliary graph of "compatible" antichains of $\mathcal{S}$. For example, the poset $\mathcal{S}$ associated with $D^i(3,n)$ is represented in the Stembridge's poset Maple package [69] as a set of edges corresponding to the cover relations in $\mathcal{S}$

$$\mathcal{S} = \{[1,2],[1,3],[2,4],[2,5],[3,5],[3,6]\} \tag{6}$$

and the linear extension $w = 123645$ is represented as the list

$$w = [1,2,3,6,4,5]. \tag{7}$$

The complete list of linear extensions produced by the command `extensions`$(\mathcal{S})$ is produced by Maple in the form of a list of lists:

$$\begin{aligned} \mathcal{L}(\mathcal{S}) \;=\; & [\,[\,1,2,3,4,5,6\,],[\,1,2,3,4,6,5\,],[\,1,2,3,5,4,6\,],[\,1,2,3,5,6,4\,], \\ & [\,1,2,3,6,4,5\,],[\,1,2,3,6,5,4\,],[\,1,2,4,3,5,6\,],[\,1,2,4,3,6,5\,], \\ & [\,1,3,2,4,5,6\,],[\,1,3,2,4,6,5\,],[\,1,3,2,5,4,6\,],[\,1,3,2,5,6,4\,], \\ & [\,1,3,2,6,4,5\,],[\,1,3,2,6,5,4\,],[\,1,3,6,2,4,5\,],[\,1,3,6,2,5,4\,]\,] \end{aligned} \tag{8}$$

2.3 Computing the number of descents des(w) and the number of fixed labels fix$_{\mathcal{S}}(w)$ for each linear extension $w \in \mathcal{L}(\mathcal{S})$

In the next step, for each of the linear extension $w \in \mathcal{L}(\mathcal{S})$, we compute its two invariants: the number of descents in w and the number of fixed labels in w. The number of descents, $\mathrm{des}(w)$, is computed directly from the definition of a descent: If two subsequent labels w_i and w_{i+1} in w stand in the relation $w_i > w_{i+1}$, then the index i is called a *descent* of w. The other invariant, $\mathrm{fix}_{\mathcal{S}}(w)$, is somewhat more complicated to compute. The—very inefficient but human-readable—Algorithm 2 determines whether a label w_i is fixed in a linear extension w.

i	w_i	$w_i>w_{i+1}$?	L	P	$\max(L)>\max(P)$?
1	1		$\{\}$	$\{\}$	FALSE
2	3		$\{\}$	$\{p \mid w_p\in\{1\}\}=\{1\}$	FALSE
3	6	TRUE			
4	2		$\{l \mid w_l\in\{6\}\}=\{3\}$	$\{p \mid w_p\in\{1\}\}=\{1\}$	TRUE
5	4		$\{l \mid w_l\in\{6\}\}=\{3\}$	$\{p \mid w_p\in\{1,2\}\}=\{1,4\}$	FALSE
6	5		$\{l \mid w_l\in\{6\}\}=\{3\}$	$\{p \mid w_p\in\{1,2,3\}\}=\{1,2,4\}$	FALSE

Table 1. Application of Algorithm 2 to the labels of the linear extension $w = 136245$: For the label $w_3 = 6$, we find $w_3 > w_4$, which directly returns TRUE. For all other labels, we find $w_i \not> w_{i+1}$, and thus we proceed to computing the sets L and P. For the label $w_4 = 2$, we have $\max(L) > \max(P)$, which returns TRUE; for the remaining labels the algorithm returns FALSE.

Algorithm 2: Is the label w_i fixed in the sequence w?

Data: Poset $\mathcal{S}$, linear extension $w = w_1w_2w_3 \dots w_p$, and an element w_i of w.
Result: TRUE iff w_i is fixed in w.

if $w_i > w_{i+1}$ **then**
  return TRUE;
else
  $L := \{l \mid l < i, w_l > w_i\}$; `// Positions of larger labels`
  $P := \{p \mid \omega^{-1}(w_p) <_{\mathcal{S}} \omega^{-1}(w_i)\}$; `// Positions of necessarily preceding labels`
  if $\max(L) > \max(P)$ **then return** TRUE **else return** FALSE;
end

<table>
<tr><th>Linear extension</th><th>des(w)</th><th>$\mathrm{fix}_{\mathcal{S}}(w)$</th><th>$c_k^{\mathrm{des}(w),\mathrm{fix}_{\mathcal{S}}(w)}$</th></tr>
<tr><td>1 2 3 4 5 6</td><td>$\underline{0}$</td><td>0</td><td>$c_k^{0,0} = \binom{6-\mathbf{0}}{k-\mathbf{0}}\binom{n+\underline{0}}{k}$</td></tr>
<tr><td>1 3 2 4 5 6</td><td rowspan="7">$\underline{1}$</td><td rowspan="6">2</td><td rowspan="6">$c_k^{1,2} = 6\binom{6-\mathbf{2}}{k-\mathbf{2}}\binom{n+\underline{1}}{k}$</td></tr>
<tr><td>1 2 4 3 5 6</td></tr>
<tr><td>1 3 6 2 4 5</td></tr>
<tr><td>1 2 3 5 4 6</td></tr>
<tr><td>1 2 3 4 6 5</td></tr>
<tr><td>1 2 3 5 6 4</td></tr>
<tr><td>1 2 3 6 4 5</td><td rowspan="2">3</td><td rowspan="2">$c_k^{1,3} = \binom{6-\mathbf{3}}{k-\mathbf{3}}\binom{n+\underline{1}}{k}$
$c_k^{2,3} = \binom{6-\mathbf{3}}{k-\mathbf{3}}\binom{n+\underline{2}}{k}$</td></tr>
<tr><td>1 2 3 6 5 4</td><td rowspan="7">$\underline{2}$</td></tr>
<tr><td>1 3 2 5 4 6</td><td rowspan="5">4</td><td rowspan="5">$c_k^{2,4} = 5\binom{6-\mathbf{4}}{k-\mathbf{4}}\binom{n+\underline{2}}{k}$</td></tr>
<tr><td>1 3 2 4 6 5</td></tr>
<tr><td>1 3 6 2 5 4</td></tr>
<tr><td>1 2 4 3 6 5</td></tr>
<tr><td>1 3 2 5 6 4</td></tr>
<tr><td>1 3 2 6 4 5</td><td rowspan="2">5</td><td rowspan="2">$c_k^{2,5} = \binom{6-\mathbf{5}}{k-\mathbf{5}}\binom{n+\underline{2}}{k}$
$c_k^{3,5} = \binom{6-\mathbf{5}}{k-\mathbf{5}}\binom{n+\underline{3}}{k}$</td></tr>
<tr><td>1 3 2 6 5 4</td><td>$\underline{3}$</td></tr>
</table>

Table 2. Zhang-Zhang polynomial of $D^i(3,n)$ from Fig. 2(v) can be computed as $\mathrm{ZZ}(D^i(3,n)) = \sum_{k=0}^{6} c_k\,(1+x)^k$, where $c_k = c_k^{0,0} + c_k^{1,2} + \cdots c_k^{3,5}$ represents the sum $\sum_{w\in\mathcal{L}(\mathcal{S})}\binom{|\mathcal{S}|-\mathrm{fix}_{\mathcal{S}}(w)}{k\ -\mathrm{fix}_{\mathcal{S}}(w)}\binom{n+\mathrm{des}(w)}{k}$. Descents and **fixed labels** are highlighted for each $w \in \mathcal{L}(\mathcal{S})$ and the choice of colors pertains to Algorithm 2.

Let us illustrate in detail the process of computation of both invariants on the example of the linear extension $w = 136245$ of the poset $\mathcal{S}$ depicted in Fig. 2(v) and associated with the prolate pentagon $D^i(3,n)$. There is only one descent in w at $i = 3$ given by $w_3 = 6 > 2 = w_4$; for all remaining positions, $i \neq 3$, we have $w_i < w_{i+1}$, meaning that they are not descents in w. Therefore, $\mathrm{des}(w) = 1$. Computation of $\mathrm{fix}_{\mathcal{S}}(w)$ proceeds by application of Algorithm 2 to each label of w, which leads to the results displayed in Table 1, showing that only the labels 6 and 2 are fixed in w. Therefore, $\mathrm{fix}_{\mathcal{S}}(w) = 2$. Table 2 lists all the linear extensions of the poset $\mathcal{S}$ associated with $D^i(3,n)$ together with their $\mathrm{des}(w)$ and $\mathrm{fix}_{\mathcal{S}}(w)$ invariants. The class of linear extensions corresponding to $(\mathrm{des}(w) = 1, \mathrm{fix}_{\mathcal{S}}(w) = 2)$ consists of 6 linear extensions and the class corresponding to $(\mathrm{des}(w) = 2, \mathrm{fix}_{\mathcal{S}}(w) = 4)$, of 5 linear extensions; the remaining classes all consist of 1 linear extension. The coefficient $\sum_{w\in\mathcal{L}(\mathcal{S})}\binom{|\mathcal{S}|-\mathrm{fix}_{\mathcal{S}}(w)}{k\ -\mathrm{fix}_{\mathcal{S}}(w)}\binom{n+\mathrm{des}(w)}{k}$ in Eq. (5) corresponding to a given set of invariants, $(\mathrm{des}(w), \mathrm{fix}_{\mathcal{S}}(w))$, is denoted as $c_k^{\mathrm{des}(w),\mathrm{fix}_{\mathcal{S}}(w)}$; these coefficients are listed in the last column of Table 2. Substitution of these values into Eq. (5) yields the ZZ polynomial of the prolate pentagon $D^i(3,n)$ in the following form

$$\mathrm{ZZ}(D^i(3,n)) = \sum_{k=0}^{6}\Bigg(\tbinom{6}{k}\tbinom{n}{k} + \Big(6\tbinom{4}{k-2}+\tbinom{3}{k-3}\Big)\tbinom{n+1}{k} + \Big(\tbinom{3}{k-3}+5\tbinom{2}{k-4}+\tbinom{1}{k-5}\Big)\tbinom{n+2}{k}+\tbinom{1}{k-5}\tbinom{n+3}{k}\Bigg)(1+x)^k.$$

In practical investigations, using the same representation of a linear extension w as in Eq. (7), the number $\mathrm{des}(w)$ of descents can be computed using the Maple operator

$$\mathrm{des} := w \to \texttt{nops}(\texttt{select}(x \to x < 0, [\,\texttt{op}(w[\,2\,..\,\texttt{nops}(w)\,]), \texttt{nops}(w)+1\,] - w)) \tag{9}$$

and the number $\mathrm{fix}_{\mathcal{S}}(w)$ of fixed labels in w can be computed for example by the following Maple operator

$$
\begin{aligned}
\mathrm{fix}_{\mathcal{S}} \;:=\; & \texttt{proc}\,(w,\mathcal{S}) \\
& \quad \texttt{local}\; j,k,f := [\,\texttt{op}(w[2\,..\,\texttt{nops}(w)\,]), \texttt{nops}(w)+1\,] - w\texttt{:} \\
& \quad \texttt{for}\; j\; \texttt{from}\; 1\; \texttt{to}\; \texttt{nops}(w)\; \texttt{do} \\
& \quad\quad \texttt{if}\; f[\,j\,] > 0\; \texttt{then} \\
& \quad\quad\quad \texttt{for}\; k\; \texttt{from}\; j-1\; \texttt{to}\; 1\; \texttt{by}\; -1\; \texttt{do} \\
& \quad\quad\quad\quad \texttt{if}\; \texttt{evalb}([\,w[\,k\,], w[\,j\,]\,]\; \texttt{in}\; \mathcal{S})\; \texttt{then break: fi:} \\
& \quad\quad\quad\quad \texttt{if}\; w[\,j\,] < w[\,k\,]\; \texttt{then}\; f[\,j\,] := -k\texttt{: break: fi: od: fi: od:} \\
& \quad \texttt{return}\; \texttt{nops}(\texttt{select}(x \to x < 0, f))\texttt{:} \\
& \texttt{end proc:}
\end{aligned}
\tag{10}
$$

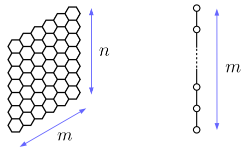
3 Examples of computation of the extended strict order polynomial $\mathrm{E}^{\circ}_{\mathcal{S}}(n, 1+x)$ for various classes of regular benzenoid strips

In the previous section, we have explained in detail the construction of a poset $\mathcal{S}$ for any Kekuléan regular strip $\boldsymbol{S}$ and using it for computing the ZZ polynomial of $\boldsymbol{S}$ in the form of the extended strict order polynomial of $\mathcal{S}$. In this section, we illustrate this process on several examples, producing a number of non-trivial results. In every case, the process starts with a molecular graph of a given regular m-tier benzenoid strip $\boldsymbol{S}$ of length n, and proceeds via construction of the corresponding poset $\mathcal{S}$, generating the set $\mathcal{L}(\mathcal{S})$ of linear extensions of $\mathcal{S}$, finding the invariants $\mathrm{des}(w)$ and $\mathrm{fix}_{\mathcal{S}}(w)$ for each $w \in \mathcal{L}(\mathcal{S})$, and substituting all the ingredients into the working equation

$$\mathrm{ZZ}(\boldsymbol{S},x) = \mathrm{E}^{\circ}_{\mathcal{S}}(n,1+x) = \sum_{w\in\mathcal{L}(\mathcal{S})}\sum_{k=0}^{|\mathcal{S}|}\binom{|\mathcal{S}|-\mathrm{fix}_{\mathcal{S}}(w)}{k\;-\mathrm{fix}_{\mathcal{S}}(w)}\binom{n+\mathrm{des}(w)}{k}(1+x)^k\,. \tag{11}$$

The described above steps constitute a very efficient and straightforward algorithm for determination of ZZ polynomials, providing additionally deep understanding of their internal structure and relative complexity.

Example 1. For any parallelogram $M(m,n)$, the corresponding Hasse diagram is a chain $\boldsymbol{m}$. Thus, $\mathcal{L}(\mathcal{S})$ contains only the one element $w = 123\ldots m$, for which we find $\mathrm{des}(w) = 0$ and $\mathrm{fix}_{\mathcal{S}}(w) = 0$. It follows immediately from Eq. (11) that

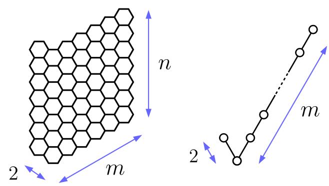


$\boldsymbol{S} = M(m,n)$ $\mathcal{S} = \boldsymbol{m}$

$$\mathrm{ZZ}(M(m,n),x) = \mathrm{E}^{\circ}_{\boldsymbol{m}}(n, 1+x) = \sum_{k=0}^{m} \tbinom{m}{k}\tbinom{n}{k} (1+x)^k ,$$

which reproduces the well-known formula given by Eq. (4) of [23] and agrees with similar formulas given in [43].

Example 2. For a chevron $Ch(2,m,n)$, the corresponding Hasse diagram consists of two chains ($\boldsymbol{m}$ and $\mathbf{2}$), which are merged at their minimal elements. This poset has m linear extensions, each of them in the form of the sequence $1345\ldots(m+1)$ with the label 2 inserted in any position after 1. The linear



$\boldsymbol{S} = Ch(2,m,n)$ $\mathcal{S} = \mathbf{2} \vee \boldsymbol{m}$

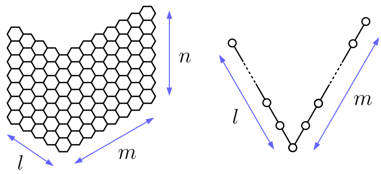
extension $1234\ldots(m+1)$ has 0 descents and 0 fixed labels; the remaining $m-1$ linear extensions have 1 descent and 2 fixed labels that are involved in the descent. Consequently, the ZZ polynomial of a chevron $Ch(2,m,n)$ is given by

$$\mathrm{ZZ}(Ch(2,m,n),x) = \mathrm{E}^{\circ}_{\mathbf{2}\vee\boldsymbol{m}}(n, 1+x) = \sum_{k=0}^{m+1} \left[\tbinom{m+1}{k}\tbinom{n}{k} + (m-1)\tbinom{m-1}{k-2}\tbinom{n+1}{k}\right] (1+x)^k .$$

Similar considerations for a chevron $Ch(3,m,n)$ show that it has 1 linear extension with 0 descents and 0 fixed labels, $2\,(m-1)$ linear extensions with 1 descent and 2 fixed labels, and $\binom{m-1}{2}$ linear extensions with 2 descent and 4 fixed labels. Consequently, the ZZ polynomial of a chevron $Ch(3,m,n)$ is given by

$$\mathrm{ZZ}(Ch(3,m,n),x) = \mathrm{E}^{\circ}_{\mathbf{3}\vee\boldsymbol{m}}(n, 1+x) = \sum_{k=0}^{m+2} \left[\tbinom{m+2}{k}\tbinom{n}{k} + 2(m-1)\tbinom{m}{k-2}\tbinom{n+1}{k} + \tbinom{m-1}{2}\tbinom{m-2}{k-4}\tbinom{n+2}{k}\right] (1+x)^k .$$

Example 3. The two formulas given in Example 2 show a large degree of similarity. It is plausible to make a conjuncture that the generalization of these two formulas to a poset $\mathcal{S} = \boldsymbol{l} \vee \boldsymbol{m}$ with an arbitrary positive integer value of l (i.e., to a general chevron $Ch(l, m, n)$ represented by the poset $\mathcal{S} = \boldsymbol{l} \vee \boldsymbol{m}$) is given by the following expression



$\boldsymbol{S} = Ch(l, m, n)$ $\qquad$ $\mathcal{S} = \boldsymbol{l} \vee \boldsymbol{m}$

$$\mathrm{ZZ}(Ch(l,m,n), x) = \mathrm{E}^{\circ}_{\boldsymbol{l} \vee \boldsymbol{m}}(n, 1+x) = \sum_{k=0}^{m+l-1} \sum_{d=0}^{m+l} \tbinom{l-1}{d} \tbinom{m-1}{d} \tbinom{m+l-1-2d}{k-2d} \tbinom{n+d}{k} (1+x)^k . \quad (12)$$

Indeed, direct, brute-force computation of the ZZ polynomial of $Ch(3, m, n)$ using ZZDecomposer [24, 25, 90, 91] with preselected values of the structural parameters l, m, and n shows that Eq. (12) is correct. Since a closed-form expression for the ZZ polynomial of a general chevron $Ch(l, m, n)$ was reported in the literature (Eq. (16) of [23])

$$\begin{aligned} \mathrm{ZZ}(Ch(l,m,n), x) \;&=\; {}_2F_1\left[\begin{matrix} 1-l, -n \\ 1 \end{matrix} ; 1+x\right] \cdot {}_2F_1\left[\begin{matrix} 1-m, -n \\ 1 \end{matrix} ; 1+x\right] \\ &+ \sum_{k=0}^{n-1} (1+x) \cdot {}_2F_1\left[\begin{matrix} 1-l, -k \\ 1 \end{matrix} ; 1+x\right] \cdot {}_2F_1\left[\begin{matrix} 1-m, -k \\ 1 \end{matrix} ; 1+x\right] \end{aligned} \quad (13)$$

it remains to be demonstrated that these two equations are equivalent. In particular, after expanding the hypergeometric functions in Eq. (13) as binomial sums, it is sufficient to show that for arbitrary positive values of k, l, m, and n the following equality holds

$$\begin{aligned} &\sum_{d=0}^{l-1} \tbinom{l-1}{d} \tbinom{m-1}{d} \tbinom{m+l-1-2d}{k-2d} \tbinom{n+d}{k} \\ = &\sum_{d=0}^{l-1} \tbinom{l-1}{d} \left[\tbinom{n}{d} \tbinom{m-1}{k-d} \tbinom{n}{k-d} + \sum_{j=0}^{n-1} \tbinom{j}{d} \tbinom{m-1}{k-1-d} \tbinom{j}{k-1-d} \right] \end{aligned}$$

in order to prove many interesting properties of linear extensions of the poset $\mathcal{S} = \boldsymbol{l} \vee \boldsymbol{m}$ (which might, alternatively, also be understood through combinatorial considerations):

- The maximal number of descents in linear extensions of $\mathcal{S} = \boldsymbol{l} \vee \boldsymbol{m}$ is $\min(l-1, m-1)$.
- For any linear extension $w \in \mathcal{L}(\boldsymbol{l} \vee \boldsymbol{m})$, we have $\mathrm{fix}_{\mathcal{S}}(w) = 2\,\mathrm{des}(w)$, i.e., labels are fixed only if they are involved in descents.
- The number of linear extensions with d descents and $2d$ fixed labels is $\binom{l-1}{d}\binom{m-1}{d}$.

- The total number of linear extensions for $\mathcal{S} = \boldsymbol{l} \vee \boldsymbol{m}$ is $|\mathcal{L}(\boldsymbol{l} \vee \boldsymbol{m})| = \binom{m+l-2}{l-1}$.

Alternatively, one may demonstrate correctness of Eq. (12) directly by designing combinatorial proofs of the listed facts, based on the number of different ways of monotonic merging of chains $\boldsymbol{l-1}$ and $\boldsymbol{m-1}$.

4 Conclusion

We have presented an algorithm and a practical guide for computing the ZZ polynomial $\mathrm{ZZ}(\boldsymbol{S}, x)$ of an arbitrary regular m-tier benzenoid strip $\boldsymbol{S}$ in the form of the extended strict order polynomial $\mathrm{E}^{\circ}_{\mathcal{S}}(n, 1+x)$ of the corresponding poset $\mathcal{S}$ associated with $\boldsymbol{S}$. The algorithm is based on the equivalence between $\mathrm{ZZ}(\boldsymbol{S}, x)$ and $\mathrm{E}^{\circ}_{\mathcal{S}}(n, 1+x)$ demonstrated in the prequel to this paper [58], and used for the determination of the ZZ polynomials of all regular m-tier strips with $m = 1 - 6$ in the sequel [59]. The presented algorithm is illustrated with several examples to facilitate its use in practice. The algorithm consists of a number of fully automatable steps: generation of the poset $\mathcal{S}$ associated with $\boldsymbol{S}$, constructing the set $\mathcal{L}(\mathcal{S})$ of linear extensions of $\mathcal{S}$, computing the invariants $\mathrm{des}(w)$ and $\mathrm{fix}_{\mathcal{S}}(w)$ for each $w \in \mathcal{L}(\mathcal{S})$, and substituting all the computed ingredients into the generic equation

$$\mathrm{ZZ}(\boldsymbol{S}, x) = \mathrm{E}^{\circ}_{\mathcal{S}}(n, 1+x) = \sum_{w \in \mathcal{L}(\mathcal{S})} \sum_{k=0}^{|\mathcal{S}|} \binom{|\mathcal{S}| - \mathrm{fix}_{\mathcal{S}}(w)}{k \ - \mathrm{fix}_{\mathcal{S}}(w)} \binom{n + \mathrm{des}(w)}{k} (1+x)^{k} . \qquad (14)$$

Application of the algorithm to a sequence of chevrons $Ch(l, m, n)$ resulted in a completely new, simpler form of the ZZ polynomial of a general chevron $Ch(l, m, n)$, given by Eq. (12) (currently as a conjecture). Simultaneously, the analysis revealed (also as conjectures) a number of interesting facts about the linear extensions of a poset $\mathcal{S} = \boldsymbol{l} \vee \boldsymbol{m}$ (i.e., a poset formed from two chains of length $\boldsymbol{l}$ and $\boldsymbol{m}$ by merging them at their minimal elements). We believe that the presented methodology will open a path to more efficient methods of computing ZZ polynomials of general benzenoids, possibly without the actual construction of the entire set $\mathcal{L}(\mathcal{S})$. At the same time, it seems to us that the multiple interesting properties of ZZ polynomials for various classes of benzenoids might provide valuable information about properties of various posets and their linear extensions.

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