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Step-constrained self-avoiding walks on finite grids



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ABSTRACT

The study of self-avoiding walks (SAWs) on integer lattices has been an area of active research for several decades. In this paper, we investigate the number of SAWs between two diagonally opposite corners in a finite rectangular subgraph of the integer lattice, subject to certain constraints. In the two-dimensional case, we provide an explicit formula for the number of SAWs of a prescribed length, restricted to three-step directions. In addition, we develop an algorithm that produces faster computational results than the explicit formula. For some special cases, we present detailed counts of the SAWs in question. For rectangular grid graphs of higher dimensions, we provide a formula to count the number of SAWs that are exactly two steps longer than the shortest walks.

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1. Introduction

A self-avoiding walk (SAW) on a graph is a walk that never visits the same vertex more than once. The study of self-avoiding walks originates from statistical physics, where they serve as simplified lattice models for linear polymers in dilute solutions [19]. Understanding the enumeration and asymptotic behavior of SAWs provides insights into polymer configurations, critical exponents, and universality classes in phase transitions. Consequently, SAWs have become a fundamental combinatorial object in both mathematics and physics. SAWs have been studied most extensively on the integer lattice \mathbb{Z}^d . Determining the number of SAWs of a given length starting from the origin has been an open problem for decades. However, numerous results have been achieved under certain specific constraints and concerning the asymptotic behavior of SAWs. A comprehensive overview of the topic can be found in the book by Madras and Slade [16].

In this paper, we investigate the number of SAWs on finite rectangular subgraphs of \mathbb{Z}^d , with restrictions on the step directions and the length of the walks. We focus exclusively on SAWs that start from the origin and end at the opposite corner in a rectangular grid. Determining the number of such SAWs of a prescribed length is an open problem. However, there are results under certain constraints and concerning the asymptotic behavior of SAWs in rectangular grids (see, e.g., [1,5,6,10,15,17,25]).

Consider a d -dimensional *rectangular grid graph* in \mathbb{Z}^d determined by a given vector $\mathbf{n} = (n_1, n_2, \dots, n_d)$ with positive components. The set of vertices in this subgraph consists of all vectors $\mathbf{v} = (v_1, v_2, \dots, v_d)$ that satisfy $\mathbf{0} \leq \mathbf{v} \leq \mathbf{n}$ (componentwise partial order). Alternatively, the set of vertices can be described as the Cartesian product of finite intervals: $\prod_{i=1}^d \{0, 1, \dots, n_i\}$. In this graph, two distinct vertices $\mathbf{u} = (u_1, u_2, \dots, u_d)$ and $\mathbf{v} = (v_1, v_2, \dots, v_d)$ are connected by an edge if they differ in exactly one coordinate by 1. Formally, $\sum_{i=1}^d |u_i - v_i| = 1$. We say that the edge $\{\mathbf{u}, \mathbf{v}\}$ of a walk on a rectangular grid is a *wrong step* (or *error step*) if \mathbf{u} precedes \mathbf{v} in the vertex sequence of the walk but $\mathbf{v} < \mathbf{u}$, that is, the vertex \mathbf{v} is closer to the origin than the vertex \mathbf{u} . Obviously, a shortest path between the origin and the opposite corner of the grid does not include wrong steps. We denote the number of wrong steps in a SAW by w .

In Section 2, we will examine walks on two-dimensional rectangular grids, where only three out of the four possible step directions are allowed. They are up (\uparrow), left (\leftarrow), and right (\rightarrow). Naturally, the step type that can be excluded must be a wrong step; otherwise, the opposite corner cannot be reached from the origin. Among the two wrong steps, we exclude the down step, as most sources in the literature traditionally discuss SAWs that move up and sideways, but not down. Following the terminology of [4,14,21,26], we will refer to these walks as *up-side self-avoiding walks* (up-side SAWs). In the literature, this concept also appears as a partially directed self-avoiding walk (see, e.g., [3,7,22]) or ENW walk (East–North–West, see, e.g., [9,18]). One such walk is illustrated by Fig. 1. In the figures, we denote the wrong steps by (red) arrows.

Up-side SAWs attract attention not only due to their combinatorial tractability compared to unrestricted SAWs, but also because of their practical relevance. The directional

2. Up-side SAWs crossing an $n \times m$ grid

Let n and m be two positive integers, and fix a planar rectangular grid of size $n \times m$. It is a simple task to determine the total number of up-side SAWs that cross this grid. (Similar arguments appear elsewhere, e.g., in [3,23].) The following proposition provides this number.

Proposition 2.1. *Let $T_{n,m}$ denote the number of up-side self-avoiding walks traversing the $n \times m$ rectangular grid from the origin to the vertex (n, m) . Then*

$$T_{n,m} = (n + 1)^m.$$

Proof. There is a straightforward bijection between the set of up-side SAWs crossing the $n \times m$ rectangular grid and the set

$$\mathcal{L}_{n,m} := \{(l_1, l_2, \dots, l_m) \in \mathbb{Z}^m : 0 \leq l_i \leq n\}.$$

In each up-side SAW, there are exactly m up steps. Associate with each up-side SAW the sequence $(l_1, l_2, \dots, l_m) \in \mathbb{Z}^m$, where l_i is the first coordinate of the starting vertex of the i -th upward step in the given SAW for all $1 \leq i \leq m$. For example, Fig. 2 shows the SAW corresponding to the sequence $(1, 6, 3, 4, 7, 5, 7)$.

Clearly

$$|\mathcal{L}_{n,m}| = (n + 1)^m,$$

which completes the proof. \square

We also want to count the number of up-side SAWs with a fixed length on an $n \times m$ rectangular grid. This task is turning out to be significantly more challenging than counting the total number of up-side SAWs. In this context, previous work by Nkwanta and Shapiro [18] counts up-side SAWs with a predetermined length but does not require the SAWs to terminate at the vertex (n, m) . The study of Gao and Chen [9] considers SAWs that do terminate at (n, m) , but does not enforce that the steps of the SAWs remain within the interior of the rectangle. Therefore, our result provides a different perspective and contributes to the existing literature.

Since the number of upward steps is preset by the height of the rectangle (m), the length of an up-side SAW is determined by specifying the number of leftward steps (wrong steps), as the number of rightward steps equals the number of leftward steps plus n . We fix the number of wrong steps, denoted by w . It is easy to see that w does not exceed $n \cdot \lfloor m/2 \rfloor$.

We denote the number of up-side SAWs containing exactly w wrong steps by $T_{n,m}^{(w)}$. For example, consider a 3×3 grid with $w = 1$ wrong step. In this case, we obtain 18 possible walks, that is, $T_{3,3}^{(1)} = 18$, as illustrated in Fig. 3.

2.1. Explicit form

We present an explicit form for $T_{n,m}^{(w)}$ assuming $1 \leq w \leq n \cdot \lfloor m/2 \rfloor$ for given n and m . Note that if w exceeds the previous upper bound, then there exists no SAW with only horizontal wrong steps.

Suppose now that w is fixed. Then we split w into k packages of consecutive left error steps \leftarrow in all possible ways. One such a decomposition is $w = i_1 + i_2 + \dots + i_k$ (cf. condition C(5)). Clearly, $1 \leq k \leq w$, but $\lceil w/n \rceil \leq k \leq m - 1$ must also hold (cf. C(3) and C(2)). Put $k_1 = \max(1, \lceil w/n \rceil)$ and $k_2 = \min(w, m - 1)$. Then we choose horizontal lines $y = y_1, y = y_2, \dots, y = y_k$ in order to place the wrong step packages i_1, i_2, \dots, i_k (cf. C(2)). If the beginning of the j th package i_j is $M_j(x_j, y_j)$, then x_j satisfies C(3), and for $M_{j+1}(x_{j+1}, y_{j+1})$ C(4) holds. The choice of (y_1, y_2, \dots, y_k) , and then the consecutive recordings of $(x_1, y_1), (x_2, y_2), \dots, (x_k, y_k)$ happen again in all possible ways. Finally, the error-free paths between the packages are counted (details can be found in the proof).

In accordance with the above, when we compute the number of SAWs, then the following conditions must hold:

- C(1). Each horizontal line $y = y_j$ ($0 \leq y_j \leq m$) used for horizontal steps in the $n \times m$ grid can be used for either correct right steps or left wrong steps. Moreover, the two boundary lines $y = 0$ and $y = m$ are only for moving right.
- C(2). The locations of the lines for wrong steps are $1 \leq y_1 < \dots < y_k \leq m - 1$.
- C(3). If the starting point of the j -th error package ($1 \leq j \leq k$) with $i_j \geq 1$ wrong steps is (x_j, y_j) , then $1 \leq i_j \leq x_j \leq n$.
- C(4). If $y_{j+1} = y_j + 1$, then $x_{j+1} = x_j - i_j$; otherwise, $x_{j+1} \geq x_j - i_j$.
- C(5). The equation $w = i_1 + i_2 + \dots + i_k$ holds for the positive integers i_1, i_2, \dots, i_k .

These properties will be applied in presenting the theorem as the corresponding summations are based on them. We remark that the description before C(1), C(2), ..., C(5) plays a guiding role of the proof.

For convenience, conditions C(3) and C(4) together are denoted by C(3,4).

Theorem 2.2. For any positive integers n, m and w , where $1 \leq w \leq n \cdot \lfloor m/2 \rfloor$, the number of SAWs from the origin to the point (n, m) with exactly w left wrong steps is

$$T_{n,m}^{(w)} = \sum_{k=k_1}^{k_2} \sum_{\text{all } C(5)} \sum_{\text{all } C(2)} \sum_{\text{all } C(3,4)} \prod_{j=0}^k \binom{(x_{j+1} - x_j) + (y_{j+1} - y_j) + i_j - 2 + \delta_{y_{j+1}, y_j+1}}{x_{j+1} - x_j + i_j} \tag{1}$$

where $\delta_{u,v}$ is 1 if $u = v$ and 0 otherwise.

Proof. The proof essentially relies on the explanation before conditions C(1), C(2), ..., C(5), and the following easy observation.

Consider an $n \times m$ grid. Clearly, the number of lattice paths from (a_1, b_1) to (a_2, b_2) with only right steps (\rightarrow) and up steps (\uparrow) is given by the binomial coefficient

$$\binom{(a_2 - a_1) + (b_2 - b_1)}{a_2 - a_1} = \binom{a_2 + b_2 - a_1 - b_1}{a_2 - a_1}.$$

Assume that the j th left wrong step package ($1 \leq j \leq k$) begins at point M_j having coordinates (x_j, y_j) and length i_j . Additionally, we put $i_0 = 0$, $x_0 = 0$, and $y_0 = -1$ to represent the starting point of the lattice, further $x_{k+1} = n$, $y_{k+1} = m + 1$ to represent the end point with $i_{k+1} = 0$.

The path between the starting point $(0, 0)$ and the destination point (n, m) can be considered as a composition of $k + 1$ sub-paths. More precisely, a given path can be decomposed into $k + 1$ distinct sub-paths defined between the points $(x_j - i_j, y_j + 1)$ and $(x_{j+1}, y_{j+1} - 1)$ for $0 \leq j \leq k$. At this point, for any sub-path we need to distinguish two cases as follows.

Case 1.

Suppose that the vertical distance between two left wrong packages is at least 2, i.e., $y_{j+1} - y_j \geq 2$ for some $j \in \{0, 1, \dots, k\}$. Hence, $\delta_{y_{j+1}, y_j+1} = 0$.

- The number of grid paths from $(x_0, y_0 + 1) = (0, 0)$ to $(x_1, y_1 - 1)$ is given, via $i_0 = 0$, by (see Fig. 4a)

$$\begin{aligned} \binom{x_1 + (y_1 - 1) - x_0 - (y_0 + 1)}{x_1 - x_0} &= \binom{(x_1 - x_0) + (y_1 - y_0) + i_0 - 2}{x_1 - x_0 + i_0} \\ &= \binom{x_1 + y_1 - 1}{x_1}. \end{aligned}$$

- For any j ($1 \leq j \leq k - 1$) the number of grid paths from $(x_j - i_j, y_j + 1)$ to $(x_{j+1}, y_{j+1} - 1)$ is (see in Fig. 4c)

$$\binom{x_{j+1} - (x_j - i_j) + y_{j+1} - 1 - (y_j + 1)}{x_{j+1} - (x_j - i_j)} = \binom{(x_{j+1} - x_j) + (y_{j+1} - y_j) + i_j - 2}{x_{j+1} - x_j + i_j}.$$

- When $j = k$, as we move from $(x_k - i_k, y_k + 1)$ to (n, m) it has

$$\binom{n - (x_k - i_k) + m - (y_k + 1)}{n - x_k + i_k} = \binom{(x_{k+1} - x_k) + (y_{k+1} - y_k) + i_k - 2}{x_{k+1} - x_k + i_k}$$

possibility (see Fig. 4b).

Subsequently, all the three sub-cases (to get from one wrong package to the next one) have the same form for describing the cardinality of the possible sub-paths. Recall that the value of δ is zero now.

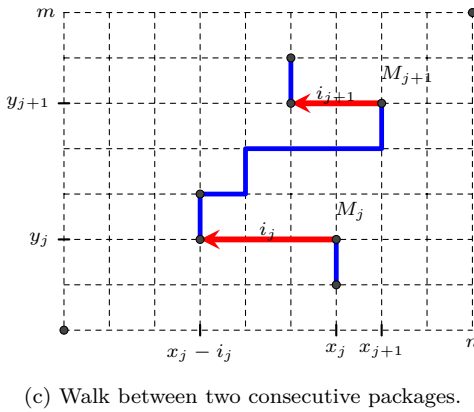
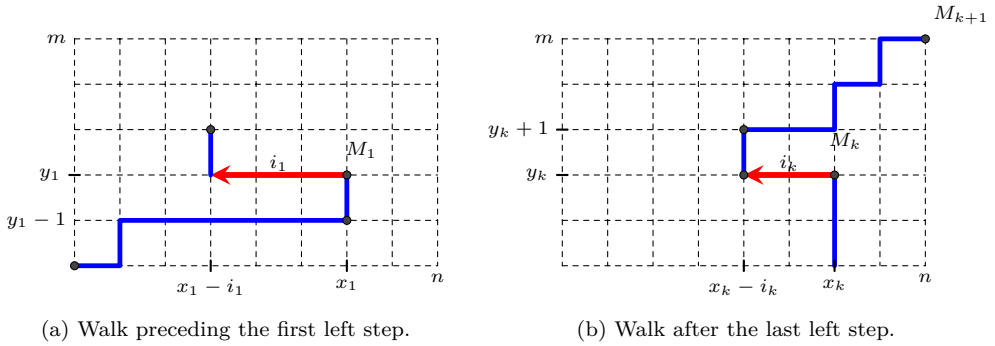


Fig. 4. Walks in different subcases in Case 1.

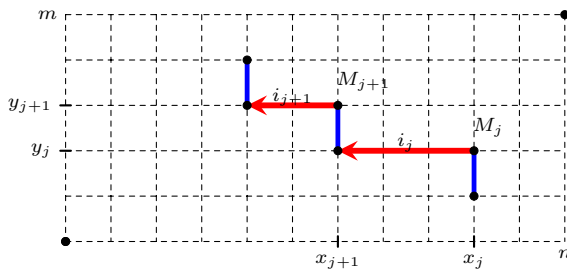


Fig. 5. Walk with a vertical distance between two back steps equal to 1 in Case 2.

Case 2. If the vertical distance between two packages of left wrong steps equals 1, i.e., $y_{j+1} = y_j + 1$ for some $0 \leq j \leq k$, then $x_{j+1} = x_j - i_j$ must hold. In this case, we have only one grid path (see Fig. 5). The two necessary up steps $y_j \uparrow (y_j + 1)$ and $(y_{j+1} - 1) \uparrow y_{j+1}$, after and before the corresponding left wrong packages, respectively, are coincided. Hence, we need the correction term $\delta_{y_{j+1}, y_{j+1}}$, which is now 1. Formally,

$$\binom{x_{j+1} - (x_j - i_j) + y_{j+1} - 1 - (y_j + 1) + \delta_{y_{j+1}, y_{j+1}}}{x_{j+1} - (x_j - i_j)} = \binom{0}{0} = 1.$$

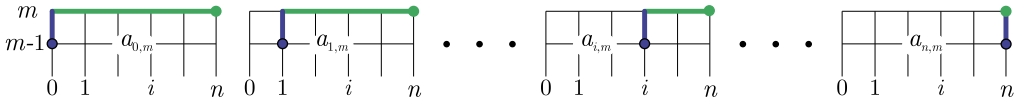


Fig. 6. Types of last sub-walks, they have no wrong steps.

Summary. Thus, considering all the SAWs with fixed triples (x_j, y_j, i_j) , according to the two cases above, the total number of grid paths from $(0, 0)$ to (n, m) can be given by the product

$$\prod_{j=0}^k \binom{(x_{j+1} - x_j) + (y_{j+1} - y_j) + i_j - 2 + \delta_{y_{j+1}, y_j+1}}{x_{j+1} - x_j + i_j}. \tag{2}$$

In order to finish the proof we sum over the product of binomial coefficients (2) for all $1 \leq i_j \leq x_j \leq n$ and $x_j - i_j \leq x_{j+1}$ with the extra situation given in the condition C(4), and then for all $1 \leq y_1 < \dots < y_k \leq m - 1$, and then for all $i_1 + i_2 + \dots + i_k = w$, and finally for all $1 \leq k \leq w$. These conditions have already been enlightened before and in C(1), C(2), ..., C(5), at the beginning of this subsection. \square

Note that for $w = 1$ we obtain

Corollary 2.3. For $n \geq 1$ and $m \geq 2$, we have

$$T_{n,m}^{(1)} = \sum_{y_1=1}^{m-1} \sum_{x_1=1}^n \binom{x_1 + y_1 - 1}{x_1} \binom{n + m - x_1 - y_1}{n - x_1 + 1}.$$

This double sum is equal to the final conclusion of Remark 1 in [17], and it simplifies $n \binom{n+m}{n+2}$ according to Lemma 1 of [17].

2.2. Recursive algorithm

In this section, we provide a system of recurrence relations for our problem and solve this system for the cases $n = 1$, $n = 2$, and $n = 3$. We give a recurrence relation for $T_{n,m}^{(w)}$ in the variables w and m .

We consider an up-side self-avoiding walk with endpoint (n, m) and w wrong steps. The last sub-walk of any SAW from horizontal grid line $m - 1$ can be completed in $n + 1$ different ways as Fig. 6 illustrates all the cases. The last sub-walk cannot contain any wrong steps. The m th upward step of the SAW could be on the vertical grid line $0, 1, \dots, n$. We denote a walk by type $a_{i,m}$ if the last upward step is on the vertical grid line i , where $i \in \{0, 1, \dots, n\}$. The types indicate on which vertical grid line a walk steps up between the horizontal grid lines $m - 1$ and m .

Let $a_{i,m}^w$ denote the number of up-side SAWs with w wrong steps, where the m th upward step is on the vertical line i . We can initial that $a_{0,0}^0 = 1$ and $a_{i,0}^0 = 0$ for $i \neq 0$,

obviously, generally, for $m \geq 0$, $a_{i,m}^0 = \binom{i+m-1}{m-1}$. Moreover, let $a_{i,m}^w = 0$ for all $0 > w$ and $w > n \lfloor m/2 \rfloor$. Then

$$T_{n,m}^{(w)} = \sum_{i=0}^n a_{i,m}^w, \quad \text{for all } 0 \leq m \text{ and } 0 \leq w \leq n \lfloor m/2 \rfloor. \tag{3}$$

Now, we determine the items $a_{i,m}^w$ recursively over primary m and secondary w . For recurrence, if $m = 1$, then $w = 0$, and if $m \geq 2$, then Fig. 7 illustrates all the possibilities of the sub-walks from horizontal grid line $m - 1$ to m . For example, see the second row from top to bottom in Fig. 7. The m th upward step on vertical grid line 1 can be reached from the $(m - 1)$ -th upward step on lines $0, 1, \dots, i, \dots, n$ by steps right and left on horizontal grid line $m - 1$. If $i > 1$, then the $i - 1$ horizontal steps are wrong steps.

Summarizing and formalizing the insights gained from the visual representation, we obtain the complete system of recurrences.

Theorem 2.4. *The number of up-side self-avoiding walks with w left wrong steps on an $n \times m$ grid is given by the system of the recurrence relations in the variables w and m .*

$$\begin{aligned} a_{0,m}^w &= a_{0,m-1}^w + a_{1,m-1}^{w-1} + a_{2,m-1}^{w-2} + \dots + a_{i,m-1}^{w-i} + \dots + a_{n,m-1}^{w-n}, \\ a_{1,m}^w &= a_{0,m-1}^w + a_{1,m-1}^w + a_{2,m-1}^{w-1} + \dots + a_{i,m-1}^{w-i+1} + \dots + a_{n,m-1}^{w-n+1}, \\ &\vdots \\ a_{i,m}^w &= a_{0,m-1}^w + a_{1,m-1}^w + a_{2,m-1}^w + \dots + a_{i,m-1}^{w-i+i} + \dots + a_{n,m-1}^{w-n+i}, \\ &\vdots \\ a_{n,m}^w &= a_{0,m-1}^w + a_{1,m-1}^w + a_{2,m-1}^w + \dots + a_{i,m-1}^w + \dots + a_{n,m-1}^w, \end{aligned} \tag{4}$$

shortly

$$a_{i,m}^w = \sum_{k=0}^i a_{k,m-1}^w + \sum_{k=i+1}^n a_{k,m-1}^{w-k+i}, \quad \text{for } i \in \{0, 1, \dots, n\},$$

with the notation $[k > i] = 1$ if $k > i$, and $= 0$ otherwise,

$$a_{i,m}^w = \sum_{k=0}^n a_{k,m-1}^{w-(k-i)[k>i]}, \quad \text{for } i \in \{0, 1, \dots, n\},$$

where $0 \leq n, 1 \leq m, 0 \leq w \leq n \lfloor m/2 \rfloor$ and

$$T_{n,m}^{(w)} = a_{n,m}^w = \sum_{k=0}^n a_{k,m-1}^w \tag{5}$$

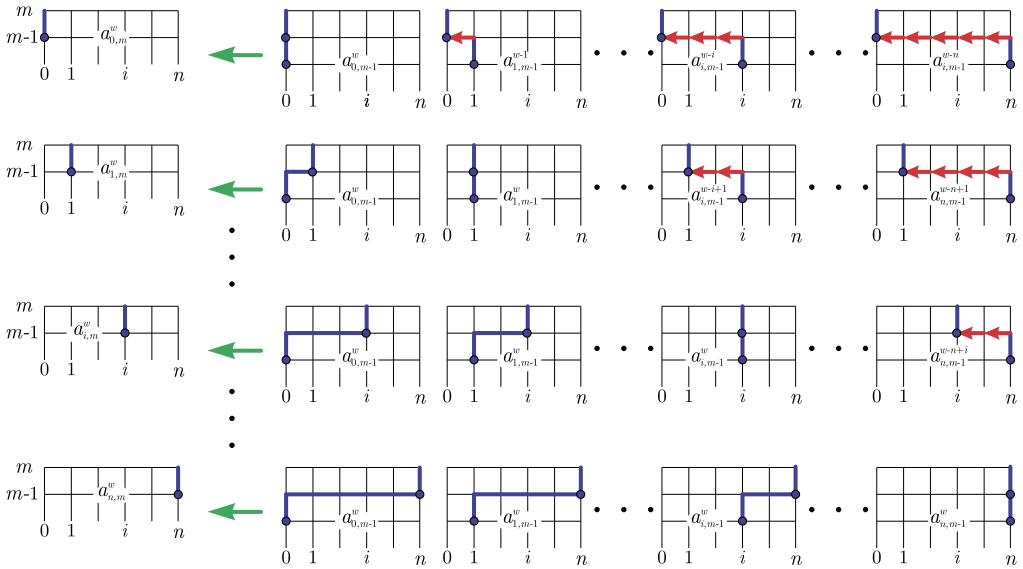


Fig. 7. Base of the system of recurrences, all the possibilities of the sub-walks from horizontal grid line $m - 1$ to m .

with initial values $a_{i,m}^w = 0$ for all $0 > w$ and $w > n \lfloor m/2 \rfloor$, $a_{i,m}^0 = \binom{i+m-1}{m-1}$ for $m \geq 0$, $a_{i,1}^0 = 1$ for $0 \leq i \leq n$.

For the calculations of the values $T_{n,m}^{(w)}$ in the case of small variables, based on Theorem 2.4 we give an algorithm. The input data of Algorithm 1 are n and m_{max} , the outputs are $T_{n,m}^{(w)}$ for all $0 \leq m \leq m_{max}$.

In following sub-sequences, we solve the system (4) for the cases $n = 1$, $n = 2$, and $n = 3$ what we checked with Algorithm 1. Our method solving the system (4) can be continued for larger n as well. For general case we give some conjectures in Section 4.

Algorithm 1 Up-side self-avoiding walk from Theorem 2.4.

Input: $n \geq 0, m_{max} \geq 0$

Output: $T_{n,m}^{(w)}$

$i \in \{0, 1, 2, \dots, n\}, m \in \{0, 1, 2, \dots, m_{max}\}$

$a_{i,m}^0 \leftarrow \binom{i+m-1}{m-1}$

▷ main variables
▷ initialize for $w = 0$

$a_{i,m}^w \leftarrow 0$ for $w < 0$ and for $w > n \lfloor m_{max}/2 \rfloor$

▷ initialize for out of range

for $w = 1$ to $n \lfloor m_{max}/2 \rfloor$ **do**

for $m = 1$ to m_{max} **do**

for $i = 0$ to n **do**

$a_{i,m}^w = \sum_{k=0}^i a_{k,m-1}^w + \sum_{k=i+1}^n a_{k,m-1}^{w-j+1}$

▷ from Equations (4) and Fig. 7

end for

end for

end for

for $w = 0$ to $n \lfloor m_{max}/2 \rfloor$ **do**

for $m = 0$ to m_{max} **do**

$T_{n,m}^{(w)} = \sum_{k=0}^n a_{k,m}^w$

▷ from Equation (5) and Fig. 6

end for

end for

Table 1
Triangle \mathcal{T}_1 .

$m \setminus w$	0	1	2	3	4
0	1				
1	2				
2	3	1			
3	4	4			
4	5	10	1		
5	6	20	6		
6	7	35	21	1	
7	8	56	56	8	
8	9	84	126	36	1

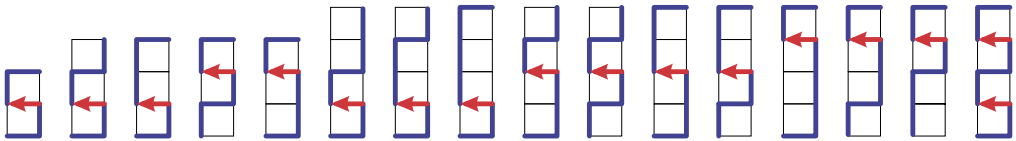


Fig. 8. Walks with wrong steps on 1×2 , 1×3 , and 1×4 grids.

2.2.1. Example for $1 \times m$ grid

In this part, we give some solution for the case $n = 1$. We solve the system of recurrences (4) and give a recurrence equation for $T_{1,m}^{(w)}$.

Theorem 2.5. *The number of up-side self-avoiding walks with w left wrong steps on an $(1 \times m)$ grid is given for $1 \leq m$ and $0 \leq w \leq \lfloor m/2 \rfloor$ by*

$$T_{1,m}^{(w)} = 2T_{1,m-1}^{(w)} - T_{1,m-2}^{(w)} + T_{1,m-2}^{(w-1)} \tag{6}$$

with the initial values $T_{1,0}^{(0)} = 1$ and boundary conditions $T_{1,m}^{(-1)} = T_{1,2w-1}^{(w)} = T_{1,2w-2}^{(w)} = 0$ for all $-1 \leq m$ and $0 \leq w$.

We arrange the values of $T_{1,m}^{(w)}$ in triangular shape \mathcal{T}_1 , where the w th entry of row m (up to down) is equal to $T_{1,m}^{(w)}$ (see Table 1). In additional, the walk with wrong steps on 1×2 , 1×3 , and 1×4 grids are illustrated in Fig. 8. Compare their numbers with the corresponding entries in the table.

Proof. Apply Theorem 2.4 for $n = 1$ the reduced system coming from (4) is

$$\begin{aligned} a_{0,m}^w &= a_{0,m-1}^w + a_{1,m-1}^{w-1}, \\ a_{1,m}^w &= a_{0,m-1}^w + a_{1,m-1}^w. \end{aligned} \tag{7}$$

Subtract the second row of (7) from the first, then

$$a_{0,m}^w = a_{1,m}^w + a_{1,m-1}^{w-1} - a_{1,m-1}^w.$$

Table 2
Triangle \mathcal{T}_2 .

$m \setminus w$	0	1	2	3	4	5	6	7	8
0	1								
1	3								
2	6	2	1						
3	10	10	7						
4	15	30	31	4	1				
5	21	70	105	36	11				
6	28	140	294	184	76	6	1		
7	36	252	714	696	396	78	15		
8	45	420	1554	2160	1666	566	141	8	1

Substituting its shifted versions in values m by -1 into the second row of (7), after some simplifications we have

$$a_{1,m}^w = 2a_{1,m-1}^w - a_{1,m-2}^w + a_{1,m-2}^{w-1}. \tag{8}$$

Since $T_{1,m}^{(w)} = a_{0,m}^w + a_{1,m}^w = a_{1,m+1}^w = 2a_{1,m}^w - a_{1,m-1}^w + a_{1,m-1}^{w-1} = 2T_{1,m-1}^{(w)} - T_{1,m-2}^{(w)} + T_{1,m-2}^{(w-1)}$, the proof is complete. \square

Remark 2.6. According to Proposition 2.1, the row sum sequence of triangle \mathcal{T}_1 is the sequence $(2^m)_{m=0}^\infty$ (A000079 in [24]). Thus, the number of up-side self-avoiding walks with at most only left wrong steps on an $(1 \times m)$ grid is $T_{1,m} = 2^m$ ($m \in \mathbb{N}$).

Remark 2.7. For entries of row m at position w , we obtain

$$\binom{m}{2w} + \binom{m}{2w+1} = \binom{m+1}{2w+1}.$$

2.2.2. Example for $2 \times m$ grid

In this part, we provide a solution for the case $n = 2$. First, using the system of recurrences (4), we arrange the values of $T_{2,m}^{(w)}$ in a triangular shape, denoted by \mathcal{T}_2 , where the w -th entry of row m (from top to bottom) is equal to $T_{2,m}^{(w)}$ (see Table 2). This triangle appears in OEIS [24] as A120907.

We give the reduced system of recurrence sequences (4) and a recurrence equation for $T_{2,m}^{(w)}$.

Theorem 2.8. The number of upside self-avoiding walks with w left wrong steps on an $(2 \times m)$ grid is given for $m \geq 1$ and $0 \leq w \leq 2\lfloor m/2 \rfloor$ by

$$T_{2,m}^{(w)} = 3T_{2,m-1}^{(w)} - 3T_{2,m-2}^{(w)} + T_{2,m-3}^{(w)} + 2T_{2,m-2}^{(w-1)} - 2T_{2,m-3}^{(w-1)} + T_{2,m-2}^{(w-2)} + T_{2,m-3}^{(w-2)} \tag{9}$$

with the initial values $T_{2,0}^{(0)} = 1$ and boundary conditions $T_{2,m}^{(-i)} = T_{2,2\lfloor w/2 \rfloor - j}^{(w)} = 0$ when $i \in \{1, 2\}$, $j \in \{1, 2, 3\}$ for any $m \geq -2$ and $w \geq 0$.

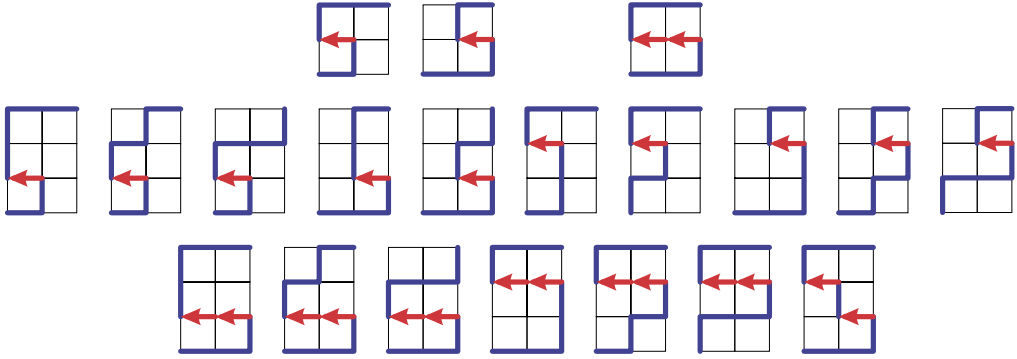


Fig. 9. Walks with wrong steps on 2×2 and 3×2 grids.

Proof. Apply Theorem 2.4 for $n = 2$, the reduced system coming from (4) is

$$\begin{aligned}
 a_{0,m}^w &= a_{0,m-1}^w + a_{1,m-1}^{w-1} + a_{2,m-1}^{w-2}, \\
 a_{1,m}^w &= a_{0,m-1}^w + a_{1,m-1}^{w-1} + a_{2,m-1}^{w-1}, \\
 a_{2,m}^w &= a_{0,m-1}^w + a_{1,m-1}^w + a_{2,m-1}^w.
 \end{aligned}
 \tag{10}$$

Subtract the last row of (10) from the others, then

$$\begin{aligned}
 a_{0,m}^w &= a_{2,m}^w - a_{1,m-1}^w - a_{2,m-1}^w + a_{1,m-1}^{w-1} + a_{2,m-1}^{w-2}, \\
 a_{1,m}^w &= a_{2,m}^w - a_{2,m-1}^w + a_{2,m-1}^{w-1}.
 \end{aligned}
 \tag{11}$$

Substituting the shifted versions of term $a_{1,m}^w$ in values m and w by -1 into the first row of (11), after some simplifications we have

$$a_{0,m}^w = a_{2,m}^w - 2a_{2,m-1}^w + a_{2,m-2}^w + a_{2,m-1}^{w-1} - 2a_{2,m-2}^{w-1} + a_{2,m-1}^{w-2} + a_{2,m-2}^{w-2}.
 \tag{12}$$

Substituting the shifted versions of terms $a_{1,m}^w$ and $a_{0,m}^w$ into the last row of (10), and simplifying, finally it leads to

$$a_{2,m}^w = 3a_{2,m-1}^w - 3a_{2,m-2}^w + a_{2,m-3}^w + 2a_{2,m-2}^{w-1} - 2a_{2,m-3}^{w-1} + a_{2,m-2}^{w-2} + a_{2,m-3}^{w-2}.$$

The initial values are clear, see, i.e., Fig. 9.

Since $T_{2,m}^{(w)} = a_{0,m}^w + a_{1,m}^w + a_{2,m}^w = a_{2,m+1}^w$, the proof is complete. \square

Remark 2.9. According to Proposition 2.1, the row sum sequence of triangle \mathcal{T}_2 is the sequence $(3^m)_{m=0}^\infty$, (A000244 in [24]). Thus, the number of up-side self-avoiding walks with at most only left wrong steps on an $(2 \times m)$ grid is $T_{2,m} = 3^m$ ($m \in \mathbb{N}$).

Table 3
Triangle \mathcal{T}_3 .

$m \setminus w$	0	1	2	3	4	5	6	7	8	9
0	1									
1	4									
2	10	3	2	1						
3	20	18	16	10						
4	35	63	78	65	10	4	1			
5	56	168	288	320	120	56	16			
6	84	378	876	1275	810	469	176	21	6	1
7	120	756	2304	4302	4000	2926	1456	378	120	22

2.2.3. Example for $3 \times m$ grid

Theorem 2.10. *The number of up-side self-avoiding walks with w wrong steps on an $(3 \times m)$ grid is given for $m \geq 1$ and $0 \leq w \leq 3\lfloor m/2 \rfloor$ by*

$$T_{3,m}^w = 4T_{3,m-1}^w - 6T_{3,m-2}^w + 4T_{3,m-3}^w - T_{3,m-4}^w + 3T_{3,m-2}^{w-1} - 6T_{3,m-3}^{w-1} + 3T_{3,m-4}^{w-1} + 2T_{3,m-2}^{w-2} - 3T_{3,m-4}^{w-2} + T_{3,m-2}^{w-3} + 2T_{3,m-3}^{w-3} + T_{3,m-4}^{w-3} \tag{13}$$

with the initial values $T_{3,0}^{(0)} = 1$ and boundary conditions $T_{3,m}^{(-i)} = 0$ when $i \in \{1, 2, 3\}$, $T_{3,2\lceil w/3 \rceil - j}^{(w)} = 0$ when $j \in \{1, 2, 3, 4\}$ for any $m \geq -3$ and $w \geq 0$.

The terms $T_{3,m}^{(w)}$ construct the triangle \mathcal{T}_3 illustrated in Table 3.

Proof. The proof is similar to the previous two examples. From the system (4) we have

$$\begin{aligned} a_{0,m}^w &= a_{0,m-1}^w + a_{1,m-1}^{w-1} + a_{2,m-1}^{w-2} + a_{3,m-1}^{w-3}, \\ a_{1,m}^w &= a_{0,m-1}^w + a_{1,m-1}^w + a_{2,m-1}^{w-1} + a_{3,m-1}^{w-2}, \\ a_{2,m}^w &= a_{0,m-1}^w + a_{1,m-1}^w + a_{2,m-1}^w + a_{3,m-1}^{w-1}, \\ a_{3,m}^w &= a_{0,m-1}^w + a_{1,m-1}^w + a_{2,m-1}^w + a_{3,m-1}^w. \end{aligned} \tag{14}$$

Substitute the last row from the others then the new system is

$$\begin{aligned} a_{0,m}^w &= a_{3,m}^w - a_{1,m-1}^w + a_{1,m-1}^{w-1} - a_{2,m-1}^w + a_{2,m-1}^{w-2} - a_{3,m-1}^w + a_{3,m-1}^{w-3}, \\ a_{1,m}^w &= a_{3,m}^w - a_{2,m-1}^w + a_{2,m-1}^{w-1} - a_{3,m-1}^w + a_{3,m-1}^{w-2}, \\ a_{2,m}^w &= a_{3,m}^w - a_{3,m-1}^w + a_{3,m-1}^{w-1}. \end{aligned}$$

Substitute the last row into the first two we have

$$\begin{aligned} a_{0,m}^w &= -a_{1,m-1}^w + a_{1,m-1}^{w-1} + a_{3,m}^w - 2a_{3,m-1}^w + a_{3,m-2}^w - a_{3,m-2}^{w-1} + a_{3,m-1}^{w-2} - a_{3,m-2}^{w-2} \\ &\quad + a_{3,m-1}^{w-3} + a_{3,m-2}^{w-3}, \\ a_{1,m}^w &= a_{3,m}^w - 2a_{3,m-1}^w + a_{3,m-2}^w + a_{3,m-1}^{w-1} - 2a_{3,m-2}^{w-1} + a_{3,m-1}^{w-2} + a_{3,m-2}^{w-2}. \end{aligned}$$

Again substitute $a_{1,m}^w$ from last row into the first we gain

$$a_{0,m}^w = a_{3,m}^w - 3a_{3,m-1}^w + 3a_{3,m-2}^w - a_{3,m-3}^w + a_{3,m-1}^{w-1} - 4a_{3,m-2}^{w-1} + 3a_{3,m-3}^{w-1} + a_{3,m-1}^{w-2} - 2a_{3,m-3}^{w-2} + a_{3,m-1}^{w-3} + a_{3,m-2}^{w-3}.$$

Finally, combine them with the last row of (14) we have

$$a_{3,m}^w = 4a_{3,m-1}^w - 6a_{3,m-2}^w + 4a_{3,m-3}^w - a_{3,m-4}^w + 3a_{3,m-2}^{w-1} - 6a_{3,m-3}^{w-1} + 3a_{3,m-4}^{w-1} + 2a_{3,m-2}^{w-2} - 3a_{3,m-4}^{w-2} + a_{3,m-2}^{w-3} + 2a_{3,m-3}^{w-3} + a_{3,m-4}^{w-3}. \quad \square$$

Remark 2.11. According to Proposition 2.1, the row sum sequence of triangle \mathcal{T}_3 is $(4^m)_{m=0}^\infty$, (A000302 in [24]). Thus, the number of up-side self-avoiding walks with at most only left wrong steps on an $(3 \times m)$ grid is $T_{3,m} = 4^m$ ($m \in \mathbb{N}$).

Remark 2.12. Summarize the coefficients from the recurrence equations (6), (9), (13) we find an interesting pattern of them what we shall show and discuss in Subsection 4.1 as a conjectures for the coefficients of recurrences of upside SAWs.

3. One wrong arbitrarily directed step in d -dimension

We focus only on $w = 1$ wrong step and do not consider the cases $w \geq 2$. Paper [17] showed how difficult was to extend the result related to $w = 1$ for $w = 2$ in 2-dimension, so here we omit studying any case of larger w .

Let $d \geq 2$ be an integer. Consider the lattice \mathbb{Z}^d . Assume that we want to construct paths from the origin $(0, 0, \dots, 0)$ to the non-negative vertex (n_1, n_2, \dots, n_d) in “Manhattan style” but with exactly 1 error step. Put $n = n_1 + n_2 + \dots + n_d$.

For fixed distinct positive integers i, j and k we define

$$\varepsilon_\ell = \begin{cases} 2, & \text{for } \ell = i \\ -2, & \text{for } \ell = j \\ 0, & \text{otherwise,} \end{cases} \quad \delta_\ell = \begin{cases} 2, & \text{for } \ell = i \\ -1, & \text{for } \ell = j, k \\ 0, & \text{otherwise.} \end{cases} \quad (15)$$

Here we assume that $1 \leq i, j, k \leq d$.

Theorem 3.1. *The number of paths from $(0, 0, \dots, 0)$ to (n_1, n_2, \dots, n_d) on a $n_1 \times n_2 \times \dots \times n_d$ grid with one error step is given by*

$$\sum_{i=1}^d n_i \left[\sum_{\substack{j=1 \\ j \neq i}}^d \binom{n}{n_1 + \varepsilon_1, n_2 + \varepsilon_2, \dots, n_d + \varepsilon_d} + 2 \sum_{\substack{1 \leq j < k \leq d \\ j \neq i, k \neq i}} \binom{n}{n_1 + \delta_1, n_2 + \delta_2, \dots, n_d + \delta_d} \right]. \quad (16)$$

Note that a multinomial coefficient is considered to be 0 if at least one lower index is negative.

Proof. We follow the proof of Theorem 2 in [17]. Assume that the axes of the Cartesian system are x_1, x_2, \dots, x_d . Fix a direction, say it is parallel to the axis x_i . Suppose that the only error step occurs in the opposite direction to x_i . We distinguish two cases.

Case 1: When the direction of the ultimate step before the wrong step and the next step after the wrong one coincide (*homogeneous case*).

Let this other direction be given by x_j ($i \neq j$). We prove that there exists a bijection between the walks with one error step on an $n_1 \times n_2 \times \dots \times n_d$ grid and the *inner* x_i -steps of the error-free walks on an

$$n_1 \times \dots \times (n_i + 2) \times \dots \times (n_j - 2) \times \dots \times n_d$$



grid. An x_i -step is called *inner* if it is neither the first nor the last step in the direction x_i . Since the number of the error-free walks, under the conditions above is

$$\begin{aligned} & \binom{n_1 + \dots + (n_i + 2) + \dots + (n_j - 2) + \dots + n_d}{n_1, \dots, (n_i + 2), \dots, (n_j - 2), \dots, n_d} \\ &= \binom{n}{n_1, \dots, (n_i + 2), \dots, (n_j - 2), \dots, n_d}, \end{aligned}$$

each has n_i inner steps. Thus, we obtain

$$n_i \binom{n}{n_1, \dots, (n_i + 2), \dots, (n_j - 2), \dots, n_d}$$

possibilities in one case.

Now consider an error-free walk on an $n_1 \times \dots \times (n_i + 2) \times \dots \times (n_j - 2) \times \dots \times n_d$ grid, and take an arbitrary inner x_i -step \rightarrow (write S_{x_i} for it). It splits the walk into two parts, they are denoted by \mathcal{P}_1 and \mathcal{P}_2 . Replace S_{x_i} by a 2-dimensional domino  such that the domino lies in the plane spanned by the directions x_i and x_j , further \mathcal{P}_1 and \mathcal{P}_2 now connects to the lower left and upper right corner of the domino, respectively, on an $n_1 \times \dots \times (n_i + 2) \times \dots \times n_j \times \dots \times n_d$ grid. In other words, the replacement of \rightarrow (S_{x_i}) by  increases the size of the grid by two units in direction x_j . Then reflect the domino around its left “vertical” skirt. The top right corner of the original domino will now be the top left corner of the mirrored domino. We will then join a copy of \mathcal{P}_2 to this domino, which will continue from there. This manipulation decreases the size of the grid by two units in direction x_i . The operations ensure the only wrong x_i -step on a resulted $n_1 \times n_2 \times \dots \times n_d$ grid, and \mathcal{P}_1 and \mathcal{P}_2 appear in the new walk in the two opposite ends of the error domino. It is clear that the starting x_i -step must be inner, otherwise the procedure fails. It is clear that distinct error-free walks with distinct inner x_i -steps lead to distinct walks with one error step since the location of $S_{x_i}(t)$ determines the location

of the error step, and if S_{x_i} is common in two error-free walks, then they differ in either \mathcal{P}_1 or \mathcal{P}_2 .

Using the notation of ε_ℓ in (15), the contribution of first case to the number of SAWs with one error step is



$$\sum_{i=1}^d n_i \sum_{\substack{j=1 \\ j \neq i}}^d \binom{n}{n_1 + \varepsilon_1, n_2 + \varepsilon_2, \dots, n_d + \varepsilon_d}.$$

Case 2: When the direction of the ultimate step before the wrong step and the next step after the wrong are distinct (*inhomogeneous case*).

Let the two other directions be denoted by x_j (before) and x_k (after), where $i \neq j$, $i \neq k$, $j \neq k$. We prove that there exists a bijection between the walks with one error step on an $n_1 \times n_2 \times \dots \times n_d$ grid and the *inner* x_i -steps of the error-free walks on an

$$n_1 \times \dots \times (n_i + 2) \times \dots \times (n_j - 1) \times \dots \times (n_k - 1) \times \dots \times n_d$$

grid. Essentially we can follow the way of Case 1, therefore we describe only the differences.

Fixing an inner x_i -step \rightarrow , now we replace it by a 3-dimensional unit cube  (in the previous case the replacement was ) according to the directions x_i , x_j and x_k . The direction x_i corresponds to the middle horizontal unit segment drawn on the cube, while the vertical segment is belonging to the direction x_j . Consequently, the initial lengths $n_j - 1$ and $n_k - 1$ is increased by 1 unit. On the other hand, the length $n_i + 2$ is reduced to n_i when we reflect the cube to the hyperplane given by the left vertical side (in this situation) of the cube. Now we have

$$n_i \binom{n}{n_1, \dots, (n_i + 2), \dots, (n_j - 1), \dots, (n_k - 1), \dots, n_d} \tag{17}$$

possibilities for an error free walk in the initial grid. Note that the order x_k , x_i , and x_j gives also the number of possibilities (17). Thus, we have, using (15)

$$\sum_{i=1}^d n_i \cdot 2 \sum_{\substack{1 \leq j < k \leq d \\ j \neq i, k \neq i}} \binom{n}{n_1 + \delta_1, n_2 + \delta_2, \dots, n_d + \delta_d}$$

SAWs with one error step in total in this case.

Summarizing Cases 1 and 2, it leads to the statement of the theorem immediately. \square

Consider formula (16) if $d = 2$. Now the second inner sum vanishes, while the first one admits $\binom{n}{n_1+2, n_2-2}$ or $\binom{n}{n_1-2, n_2+2}$. Consequently, the total sum is

$$n_1 \binom{n}{n_1 + 2, n_2 - 2} + n_2 \binom{n}{n_1 - 2, n_2 + 2}.$$

This is exactly the formula we obtained in Theorem 2 of [17].

For $d = 3$ formula (16) simplifies to (16) given in

Corollary 3.2. *The number of paths with one error step on a $n_1 \times n_2 \times n_3$ grid is given by*

$$\begin{aligned} n_1 & \left[\binom{n}{n_1 + 2, n_2 - 2, n_3} + \binom{n}{n_1 + 2, n_2, n_3 - 2} + 2 \binom{n}{n_1 + 2, n_2 - 1, n_3 - 1} \right] \\ & + n_2 \left[\binom{n}{n_1 - 2, n_2 + 2, n_3} + \binom{n}{n_1, n_2 + 2, n_3 - 2} + 2 \binom{n}{n_1 - 1, n_2 + 2, n_3 - 1} \right] \\ & + n_3 \left[\binom{n}{n_1 - 2, n_2, n_3 + 2} + \binom{n}{n_1, n_2 - 2, n_3 + 2} + 2 \binom{n}{n_1 - 1, n_2 - 1, n_3 + 2} \right]. \end{aligned}$$

Another important specific case is when the rectangular grid we consider is in a d -dimensional cube.

Corollary 3.3. *Assume that $n_1 = n_2 = \dots = n_d = N \geq 1$. Then expression (16) of Theorem 3.1 simplifies the form*

$$\gamma(N, d) := \frac{d(d-1)((d-1)N-1)N^2(dN)!}{(N+1)(N+2)(N!)^d}. \tag{18}$$

Using the Stirling’s approximation $N! \sim (N/e)^n \sqrt{2\pi N}$, the asymptotic formula for $\gamma(N, d)$ is

$$\gamma(N, d) \sim \frac{(d-1)((d-1)N-1)d^{dN+3/2}}{(2\pi N)^{(d-1)/2}},$$

which leads to $\gamma(N, 3) \sim (2/\pi) \cdot 3^{3N+3/2} = (6\sqrt{3}/\pi) \cdot 3^{3N}$.

3.1. Examples

For $d = 3$ and for $N = 1, \dots, 4$ the formula (18) returns with

$$\gamma(1, 3) = 6, \quad \gamma(2, 3) = 540, \quad \gamma(3, 3) = 22680, \quad \gamma(4, 3) = 776160,$$

respectively.

Case $(\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3) = (\mathbf{1}, \mathbf{1}, \mathbf{1})$.

Now only the third terms of the packages are nonzero. We have

$$2 \binom{3}{3, 0, 0} + 2 \binom{3}{0, 3, 0} + 2 \binom{3}{0, 0, 3} = 6.$$

Case $(\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3) = (\mathbf{2}, \mathbf{2}, \mathbf{2})$.

Each nine terms are “living”! Because of the symmetry, we count only the first package, which is

$$2 \left[\binom{6}{4,0,2} + \binom{6}{4,2,0} + 2 \binom{6}{4,1,1} \right] = 2 [15 + 15 + 2 \cdot 30] = 180.$$

Thus, the correct answer is $3 \times 180 = 540$.

Case $(\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3) = (\mathbf{3}, \mathbf{3}, \mathbf{3})$.

Similar treatment gives

$$3 \left[\binom{9}{5,1,3} + \binom{9}{5,3,1} + 2 \binom{9}{5,2,2} \right] = 3 [504 + 504 + 2 \cdot 756] = 7560,$$

hence we totally have $3 \times 7560 = 22680$.

4. Discussion and Future Work

In this article, we dealt with the up-side self-avoiding walk on $n \times m$ grids. We gave explicit and recursive forms. We have to mention, that Khalid and Prellberg [12] examined similar problems. They gave generating functions for directed paths and solved a similar system of recurrence equations with the help of the Jacobi-Trudy formula. We offer this paper to the readers to study, and we think that in a new article, it is worth determining the generating functions for our examples with a similar method.

Now we give some very interesting conjectures.

4.1. Some conjectures for the coefficients of recurrences of upside SAWs

We recognized in Section 2.2 that the coefficients of the recurrence relations for $n = 1, \dots, 6$ have an interesting pattern. In the following, we show these properties. Perhaps in a new paper these conjectures become a general theorem.

Summarize the coefficients from the rearranged recurrence equations (6), (9), (13), and the non-mentioned cases $n = 4, 5, 6$ to the form

$$T_{n,m}^w - \sum_{i=0}^{n+1} \sum_{j=0}^n C_{i,j} T_{n,m-i}^{w-j} = 0$$

for the coefficients $C_{i,j}$ we obtain Fig. 10 and 11.

After studying the figures more closely, we can discover some rules. For examples,

- the absolute values of the borders of figures contain the rows $n + 1$, n , and $n - 1$ of Pascal’s triangle (blue) and the first n natural numbers (green). More precisely,

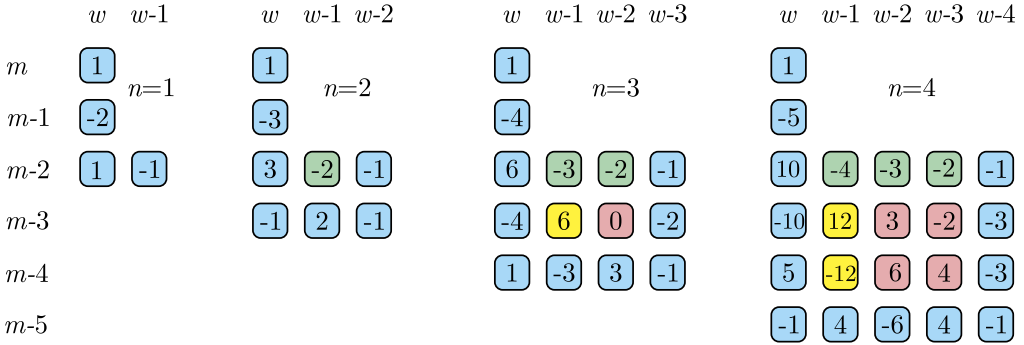


Fig. 10. Coefficients and their positions in the cases of $n = 1, \dots, 4$.

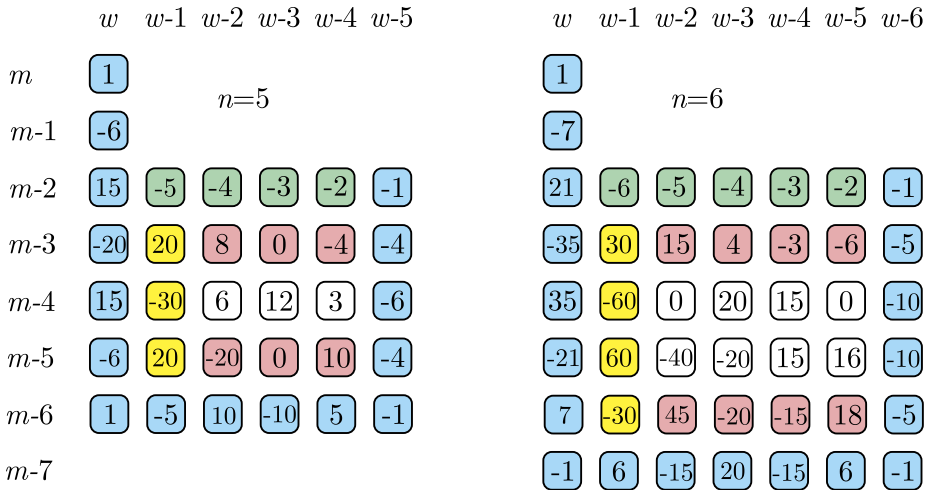


Fig. 11. Coefficients and their positions in the cases of $n = 5$ and $n = 6$.

$$C_{0,j} = \left((-1)^j \binom{n+1}{j} \right)_{j=0}^{n+1}, C_{i,n+1} = \left((-1)^{i+n+1} \binom{n}{i} \right)_{i=0}^n, C_{n,j}$$

$$= \left(-\binom{n-1}{j-2} \right)_{j=2}^{n+1},$$

and $C_{i,2} = (-1)^n_{i=1}^{n+1-i}$;

- the items of the second columns (yellow) are

$$C_{1,j} = \left((-1)^{j+1} n \binom{n-1}{j-2} \right)_{j=3}^n;$$

- the rest items of the second and the last but one rows (pink) are

$$C_{i,3} = ((n+1-i)(n+1-2i))_{i=2}^{n-1} \quad \text{and} \quad C_{i,n} = \left((-1)^{n-i} (n+1-2i) \binom{n}{i} \right)_{i=2}^{n-1}.$$

We think as a conjecture that the above observations are true for bigger n (we checked up to $n = 10$) and we think that there are a general rule for all the items of the coefficients of the recurrences, but we have not yet discovered them.

CRedit authorship contribution statement

The authors contributed equally to this manuscript. All authors read and approved the final manuscript.

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Declaration of generative AI and AI-assisted technologies in the writing process

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