Exact Enumeration of Multiple Self-Avoiding Polygons

Richard Shank, Jack Hanke

Abstract

Hong and Oh calculated upper and lower bounds on the number of multiple self-avoiding polygons in the square lattice. These results accompanied 7 distinct tiles that together model multiple ring polymers in physics. We introduce a formula for exact enumeration for these multiple self-avoiding polygons, along with enumeration results on variations on the tile set and rules considered.

1   Introduction

Consider the following 7 unit squares with red symbols on them.
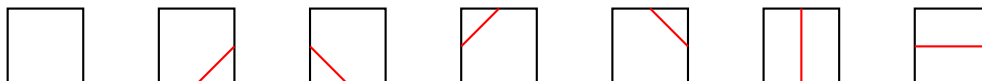

Call these unit squares *mosaic tiles*. Then let an (n, m)-mosaic be an $n \times m$ matrix of mosaic tiles. For example, below is a $(7, 5)$-mosaic.
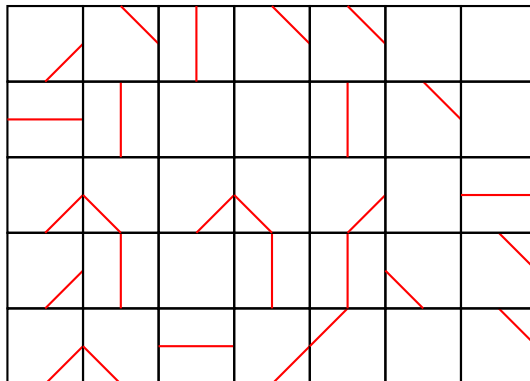
Next, define a *polygon mosaic* as a mosaic in which any pair of mosaic tiles lying immediately next to each other in either the same row or the same column have or do not have connection points simultaneously on their common edge, as well as no connection point on the boundary edges.

Example 1.1. Below is an example of a polygon $(7, 5)$-mosaic that contains 2 polygons, hilighted in gray.
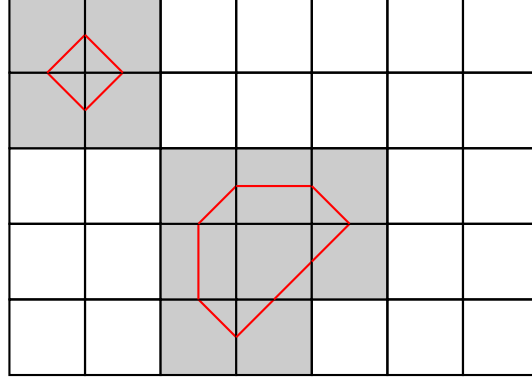
Hong and Oh [HO18, Hong2018] gave the following upper and lower bounds on the number of polygon (n, m)-mosaics $p_{n,m}$, namely

$$2^{n+m-3}\left(\frac{17}{10}\right)^{(n-2)(m-2)} \leq p_{n,m} + 1 \leq 2^{n+m-3}\left(\frac{31}{16}\right)^{(n-2)(m-2)}.$$

The array $p_{n,m} + 1$ is A181245 on the [OEI, OEIS] We give an exact expression for $p_{n,m}$ in Theorem 1. We also introduce and enumerate *messy polygon mosaics*, a variant on the previously studied polygon mosaics.

Theorem 1. *TODO*
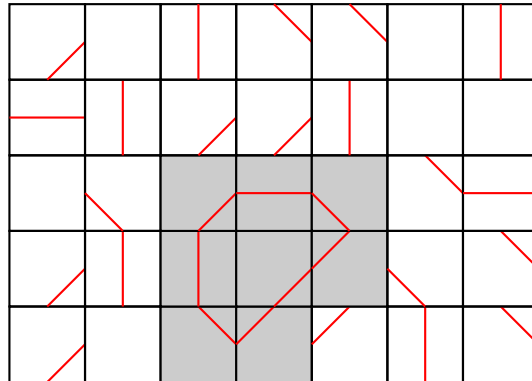
2 Proof of Theorem 1

Proof. TODO $\qquad\qquad\square$

3 Messy Polygon Mosaics

Define a *messy polygon mosaic* as a mosaic that contains at least one self-avoiding polygon, with no restriction on other connection points.

Example 3.1. Below is a messy polygon $(7, 5)$-mosaic with 1 SAP hilighted in gray.

Note that one can also consider creating messy polygon mosaics with the alternate tile set below.

From now on we refer to the different tile sets as the 7-tileset and the 6-tileset respectively. Enumerating messy polygon mosaics under the 7-tileset immediately gives a similar result for the 6-tileset, so we focus on the 7-tileset and give analagous results when necessary.

It turns out that it is easier to enumerate the number of mosaics that *do not* contain a SAP. Therefore, let $t_{n,m}$ be the number of mosaics that do not contain a SAP. Clearly $t_{n,m} = t_{m,n}$. Also from the fact that the smallest SAP is
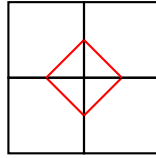
we have that $t_{n,1} = 7^n$, and $t_{2,2} = 7^4 - 1$. What else can be said?

Theorem 2. *TODO verify!!!*

Assume $n \geq m \geq 2$, and define

$$M(2) = \begin{bmatrix} 7^2 & 1 \\ -1 & 1 \end{bmatrix}$$

Then for $m \geq 2$, if

$$M(m) = \begin{bmatrix} M_1 & M_2 \\ M_3 & M_4 \end{bmatrix},$$

then

$$M(m+1) = \begin{bmatrix} 7M_1 & 7M_2 & \frac{1}{7}M_1 & M_2 \\ 7M_3 & 7M_4 & 0M_3 & M_4 \\ -\frac{1}{7}M_1 & 0M_2 & \frac{1}{7}M_1 & 1M_2 \\ M_3 & M_4 & -M_3 & 7M_4 \end{bmatrix},$$

where M_i is a sub-matrix of the block matrix M.

Then for the given m, define the rows and columns of $M(m)$ as

$$M(m) = \begin{bmatrix} c_1 & c_2 & ... & c_{2^{m-1}} \end{bmatrix} = \begin{bmatrix} r_1 \\ r_2 \\ ... \\ r_{2^{m-1}} \end{bmatrix}$$

Then let $L(n) \in \mathbb{R}^{2^{m-1} \times 1}$ so that $L(1) = \vec{0}$ and for $n > 1$ we have

$$L(n) = M(m) \cdot L(n-1) + c_1$$

Then $t_{n,m} = r_1 \cdot (M(m) \cdot L(n-1) + c_1)$.

Theorem 3. *The result is the same for the 6-tileset, except we swap the appearances of a 7 with a 6, namely*

$$M(2) = \begin{bmatrix} 6^2 & 1 \\ -1 & 1 \end{bmatrix}.$$

Then for $m \geq 2$, if

$$M(m) = \begin{bmatrix} M_1 & M_2 \\ M_3 & M_4 \end{bmatrix},$$

then

$$M(m+1) = \begin{bmatrix} 6M_1 & 6M_2 & \frac{1}{6}M_1 & M_2 \\ 6M_3 & 6M_4 & 0M_3 & M_4 \\ -\frac{1}{6}M_1 & 0M_2 & \frac{1}{6}M_1 & 1M_2 \\ M_3 & M_4 & -M_3 & 6M_4 \end{bmatrix},$$

where M_i is a sub-matrix of the block matrix M.
Then for the given m, define the rows and columns of $M(m)$ as

$$M(m) = \begin{bmatrix} c_1 & c_2 & ... & c_{2^{m-1}} \end{bmatrix} = \begin{bmatrix} r_1 \\ r_2 \\ ... \\ r_{2^{m-1}} \end{bmatrix}$$

*Then let $L(n) \in \mathbb{R}^{2^{m-1} \times 1}$ so that $L(1) = \vec{0}$ and for $n > 1$ we have*

$$L(n) = M(m) \cdot L(n-1) + c_1$$

Then $t_{n,m} = r_1 \cdot (M(m) \cdot L(n-1) + c_1)$.

# 4   Proof of Theorem 2

We prove the enumeration result for the 7-tileset. The proof for the 6-tileset is analagous.

Proof. Begin by labelling the vertices of the rectangular lattice as follows. If the vertex is surrounded by an even number of SAPs, color it black. If the vertex is surrounded by an odd number of SAPs, color it green. Using the mosaic from Example 3.1, we get the following labelling.
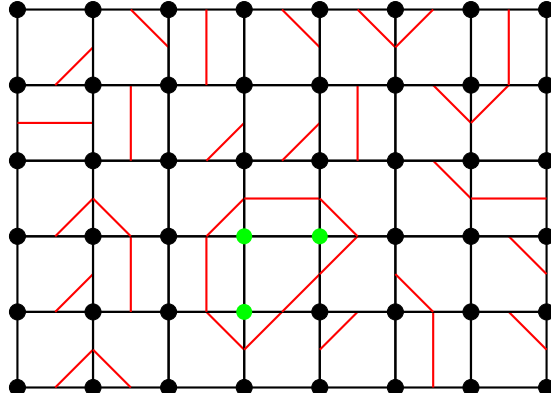
Notice that vertices on the boundary of the lattice will always be black. The associated *parity configuration* for the above mosaic is below.
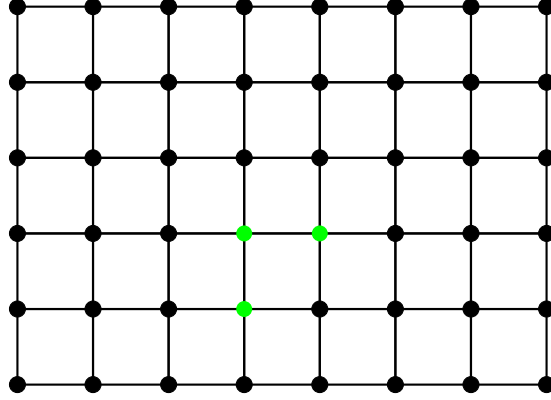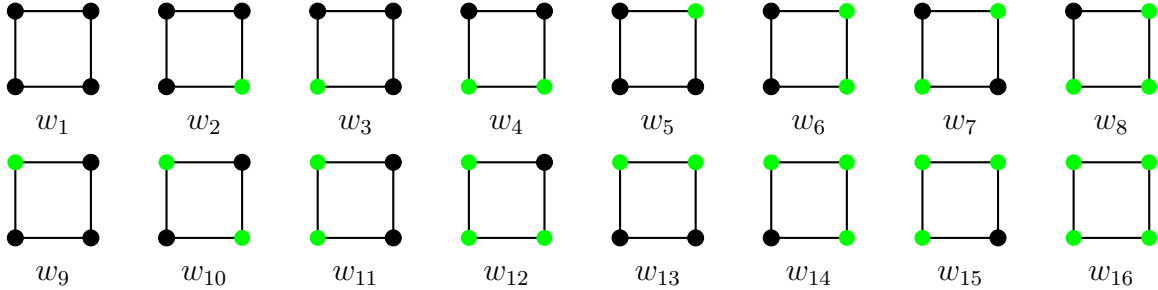

Let $\mathcal{P}(n,m)$ denote all possible parity configurations for an (n,m) rectangular lattice. Clearly $|\mathcal{P}(n,m)| = 2^{(n-1)(m-1)}$. Then let $f(p)$ be a function of a specific parity configuration that retuns the number of possible mosaics that map to p, multiplied by -1 to the number of SAPs specified by p. For example, the above parity configuration specifies only 1 SAP, so $f(p) = -1 * 7^{28}$.

Then one can write

$$t_{n,m} = \sum_{p \in \mathcal{P}(n,m)} f(p).$$

Amazingly, $f(p)$ can be written as a product of some choice of weights $w_1, \ldots, w_{16}$ associated with the following individual *cell-parity configurations*.

One can assign values to $w_1, \ldots, w_{16}$ so that the product for all parity configurations p equals $f(p)$. To find these assignments, first notice that $w_1 = w_{16} = 7$, as these cells do not indicate a specific tile. Similarly, $w_7 = w_{10} = 0$, as these are impossible parity configurations for our tile set. The remaining weights uniquely specify a tile, and so are equal to 1 or -1. But how do we find these assignments?

First notice that we want a weight assignment so that the parity configurations for a given SAP multiply to -1. This means that if there are multiple SAPs in a mosaic, then the product will be positive if there is an even number of SAPs specified, and negative if there is an odd number specified.

Next note the following lemma.

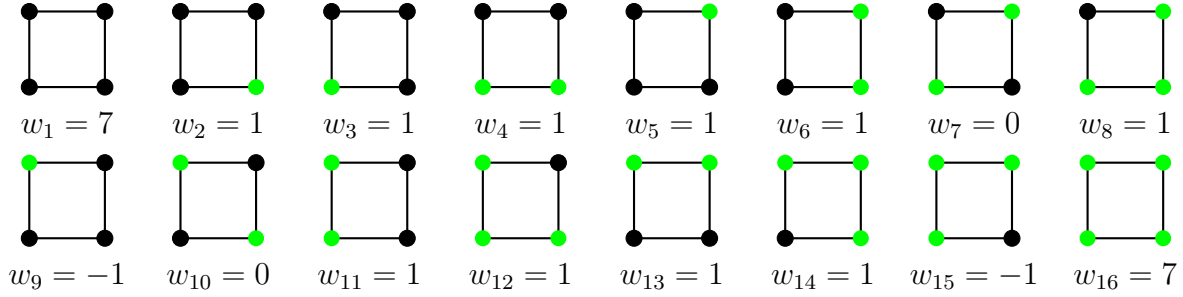**Lemma 4.** *One can construct all larger SAPs from the smallest SAP using a finite set of transformations S.*

Proof. TODO ☐

This is because one can find $w_1, \ldots, w_{16}$ so that the following two constraints hold:

Constraint 5. *The weights associated with the smallest SAP multiply to -1, ie. $w_2 w_3 w_5 w_9 = -1$.*

Constraint 6. *All transformations in S preserve the weight product of a changed SAP.*

Constraint 5 and Constraint 6 amount to a series of constraints on the values of w_i. The derivation for these constraints can be found in the Appendix. Choosing a solution set from these constraints gives the following weights.


| $w_1 = 7$ | $w_2 = 1$ | $w_3 = 1$ | $w_4 = 1$ | $w_5 = 1$ | $w_6 = 1$ | $w_7 = 0$ | $w_8 = 1$ |

| $w_9 = -1$ | $w_{10} = 0$ | $w_{11} = 1$ | $w_{12} = 1$ | $w_{13} = 1$ | $w_{14} = 1$ | $w_{15} = -1$ | $w_{16} = 7$ |

TODO

☐

Theorem 1. *Let the probability that an (n, m)-mosaic does not contain a SAP be denoted $p_{n,m} = \frac{t_{n,m}}{7^{nm}}$. Then the growth rate of the main diagonal $p_{n,n}$ has*

$$\gamma = \lim_{n \to \infty} \frac{p_{n+1,n+1} p_{n-1,n-1}}{p_{n,n}^2} = ?$$

5 Appendix

Flipping the parity of a single vertex in a parity configuration changes the 4 surrounding cells. This creates a constraint on a subset of $w_1, \ldots, w_{16}$.

The flipping of parity of a single vertex can result in 2 distinct types of constraints. Let a constraint of *Type 1* be a parity flip that does not change the number of SAPs in the parity configuration. For example, consider the following flip of the center vertex in the following portion of a parity configuration.
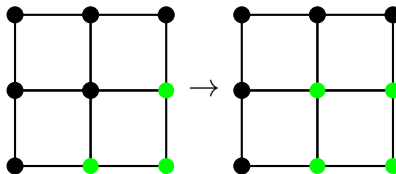
As this does not change the associated number of SAPs in the larger parity configuration, we want this to preserve the sign of the weight product. This gives the following associated constraint.

$$\text{sign}(w_1 w_2 w_5 w_9) = \text{sign}(w_2 w_4 w_6 w_{16}).$$

Now let a constraint of *Type 2* be a parity flip that does change the number of SAPs. For example, consider flipping the center vertex of the following portion of a parity configuration.
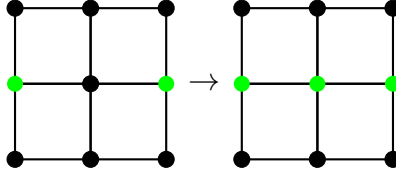
The above transformation corresponds with *either* two distinct SAPs joining into one SAP *or* one SAP splitting into two distinct SAPs. In either case, we want the sign of the product to switch. This corresponds with the following constraint.

$$\text{sign}(w_3 w_2 w_9 w_5) = -\text{sign}(w_4 w_4 w_{13} w_{13}).$$

All Type 1 constraints are as follows.

$$w_1 w_1 w_2 w_3 = w_2 w_3 w_6 w_{11} \qquad w_1 w_1 w_2 w_4 = w_2 w_3 w_6 w_{12} \qquad w_1 w_1 w_4 w_3 = w_2 w_3 w_8 w_{11}$$

$$w_1 w_1 w_4 w_4 = w_2 w_3 w_8 w_{12} \qquad w_1 w_2 w_1 w_5 = w_2 w_4 w_5 w_{13} \qquad w_1 w_2 w_1 w_6 = w_2 w_4 w_5 w_{14}$$

$$w_1 w_2 w_2 w_8 = w_2 w_4 w_6 w_{16} \qquad w_1 w_2 w_4 w_8 = w_2 w_4 w_8 w_{16} \qquad w_3 w_1 w_9 w_1 = w_4 w_3 w_{13} w_9$$

$$w_3 w_1 w_{11} w_1 = w_4 w_3 w_{15} w_9 \qquad w_3 w_1 w_{12} w_3 = w_4 w_3 w_{16} w_{11} \qquad w_3 w_1 w_{12} w_4 = w_4 w_3 w_{16} w_{12}$$

$$w_3 w_2 w_{12} w_8 = w_4 w_4 w_{16} w_{16} \qquad w_1 w_6 w_1 w_5 = w_2 w_8 w_5 w_{13} \qquad w_1 w_6 w_1 w_6 = w_2 w_8 w_5 w_{14}$$

$$w_1 w_6 w_2 w_8 = w_2 w_8 w_6 w_{16} \qquad w_1 w_6 w_4 w_8 = w_2 w_8 w_8 w_{16} \qquad w_3 w_6 w_{12} w_8 = w_4 w_8 w_{16} w_{16}$$

$$w_5 w_9 w_1 w_1 = w_6 w_{11} w_5 w_9 \qquad w_5 w_{13} w_1 w_1 = w_6 w_{15} w_5 w_9 \qquad w_5 w_{14} w_1 w_5 = w_6 w_{16} w_5 w_{13}$$

$$w_5 w_{14} w_1 w_6 = w_6 w_{16} w_5 w_{14} \qquad w_5 w_{14} w_2 w_8 = w_6 w_{16} w_6 w_{16} \qquad w_5 w_{14} w_4 w_8 = w_6 w_{16} w_8 w_{16}$$

$$w_{11} w_1 w_9 w_1 = w_{12} w_3 w_{13} w_9 \qquad w_{11} w_1 w_{11} w_1 = w_{12} w_3 w_{15} w_9 \qquad w_{11} w_1 w_{12} w_3 = w_{12} w_3 w_{16} w_{11}$$

$$w_{11} w_1 w_{12} w_4 = w_{12} w_3 w_{16} w_{12} \qquad w_{11} w_2 w_{12} w_8 = w_{12} w_4 w_{16} w_{16} \qquad w_{11} w_6 w_{12} w_8 = w_{12} w_8 w_{16} w_{16}$$

$$w_{13} w_9 w_1 w_1 = w_{14} w_{11} w_5 w_9 \qquad w_{15} w_9 w_9 w_1 = w_{16} w_{11} w_{13} w_9 \qquad w_{15} w_9 w_{11} w_1 = w_{16} w_{11} w_{15} w_9$$

$$w_{15} w_9 w_{12} w_3 = w_{16} w_{11} w_{16} w_{11} \qquad w_{15} w_9 w_{12} w_4 = w_{16} w_{11} w_{16} w_{12} \qquad w_{13} w_{13} w_1 w_1 = w_{14} w_{15} w_5 w_9$$

$$w_{13} w_{14} w_1 w_5 = w_{14} w_{16} w_5 w_{13} \qquad w_{13} w_{14} w_1 w_6 = w_{14} w_{16} w_5 w_{14} \qquad w_{13} w_{14} w_2 w_8 = w_{14} w_{16} w_6 w_{16}$$

$$w_{13} w_{14} w_4 w_8 = w_{14} w_{16} w_8 w_{16} \qquad w_{15} w_{13} w_9 w_1 = w_{16} w_{15} w_{13} w_9 \qquad w_{15} w_{13} w_{11} w_1 = w_{16} w_{15} w_{15} w_9$$

$$w_{15} w_{13} w_{12} w_3 = w_{16} w_{15} w_{16} w_{11} \qquad w_{15} w_{13} w_{12} w_4 = w_{16} w_{15} w_{16} w_{12} \qquad w_{15} w_{14} w_9 w_5 = w_{16} w_{16} w_{13} w_{13}$$

$$w_{15} w_{14} w_9 w_6 = w_{16} w_{16} w_{13} w_{14} \qquad w_{15} w_{14} w_{11} w_5 = w_{16} w_{16} w_{15} w_{13} \qquad w_{15} w_{14} w_{11} w_6 = w_{16} w_{16} w_{15} w_{14}$$

Similarly, all Type 2 constraints are as follows.

$$-w_3w_2w_9w_5 = w_4w_4w_{13}w_{13} \qquad -w_3w_2w_9w_6 = w_4w_4w_{13}w_{14} \qquad -w_3w_2w_{11}w_5 = w_4w_4w_{15}w_{13}$$

$$-w_3w_2w_{11}w_6 = w_4w_4w_{15}w_{14} \qquad -w_3w_6w_9w_5 = w_4w_8w_{13}w_{13} \qquad -w_3w_6w_9w_6 = w_4w_8w_{13}w_{14}$$

$$-w_3w_6w_{11}w_5 = w_4w_8w_{15}w_{13} \qquad -w_3w_6w_{11}w_6 = w_4w_8w_{15}w_{14} \qquad -w_5w_9w_2w_3 = w_6w_{11}w_6w_{11}$$

$$-w_5w_9w_2w_4 = w_6w_{11}w_6w_{12} \qquad -w_5w_9w_4w_3 = w_6w_{11}w_8w_{11} \qquad -w_5w_9w_4w_4 = w_6w_{11}w_8w_{12}$$

$$-w_5w_{13}w_2w_3 = w_6w_{15}w_6w_{11} \qquad -w_5w_{13}w_2w_4 = w_6w_{15}w_6w_{12} \qquad -w_5w_{13}w_4w_3 = w_6w_{15}w_8w_{11}$$

$$-w_5w_{13}w_4w_4 = w_6w_{15}w_8w_{12} \qquad -w_{11}w_2w_9w_5 = w_{12}w_4w_{13}w_{13} \qquad -w_{11}w_2w_9w_6 = w_{12}w_4w_{13}w_{14}$$

$$-w_{11}w_2w_{11}w_5 = w_{12}w_4w_{15}w_{13} \qquad -w_{11}w_2w_{11}w_6 = w_{12}w_4w_{15}w_{14} \qquad -w_{11}w_6w_9w_5 = w_{12}w_8w_{13}w_{13}$$

$$-w_{11}w_6w_9w_6 = w_{12}w_8w_{13}w_{14} \qquad -w_{11}w_6w_{11}w_5 = w_{12}w_8w_{15}w_{13} \qquad -w_{11}w_6w_{11}w_6 = w_{12}w_8w_{15}w_{14}$$

$$-w_{13}w_9w_2w_3 = w_{14}w_{11}w_6w_{11} \qquad -w_{13}w_9w_2w_4 = w_{14}w_{11}w_6w_{12} \qquad -w_{13}w_9w_4w_3 = w_{14}w_{11}w_8w_{11}$$

$$-w_{13}w_9w_4w_4 = w_{14}w_{11}w_8w_{12} \qquad -w_{13}w_{13}w_2w_3 = w_{14}w_{15}w_6w_{11} \qquad -w_{13}w_{13}w_2w_4 = w_{14}w_{15}w_6w_{12}$$

$$-w_{13}w_{13}w_4w_3 = w_{14}w_{15}w_8w_{11} \qquad -w_{13}w_{13}w_4w_4 = w_{14}w_{15}w_8w_{12}$$

Solving all Type 1 and Type 2 constraints gives the following solution set.

$$
\begin{aligned}
[w_1, ..., w_{16}] &= [7, -1, -1, -1, -1, -1, 0, -1, 1, 0, -1, -1, -1, -1, 1, 7] \\
&= [7, -1, -1, -1, -1, 1, 0, 1, 1, 0, 1, 1, -1, 1, -1, 7] \\
&= [7, -1, -1, -1, 1, -1, 0, -1, -1, 0, -1, -1, -1, 1, -1, 7] \\
&= [7, -1, -1, -1, 1, 1, 0, 1, -1, 0, 1, 1, -1, -1, 1, 7] \\
&= [7, -1, -1, 1, -1, -1, 0, 1, 1, 0, -1, 1, 1, 1, -1, 7] \\
&= [7, -1, -1, 1, -1, 1, 0, -1, 1, 0, 1, -1, 1, -1, 1, 7] \\
&= [7, -1, -1, 1, 1, -1, 0, 1, -1, 0, -1, 1, 1, -1, 1, 7] \\
&= [7, -1, -1, 1, 1, 1, 0, -1, -1, 0, 1, -1, 1, 1, -1, 7] \\
&= [7, -1, 1, -1, -1, -1, 0, -1, -1, 0, -1, 1, -1, -1, -1, 7] \\
&= [7, -1, 1, -1, -1, 1, 0, 1, -1, 0, 1, -1, -1, 1, 1, 7] \\
&= [7, -1, 1, -1, 1, -1, 0, -1, 1, 0, -1, 1, -1, 1, 1, 7] \\
&= [7, -1, 1, -1, 1, 1, 0, 1, 1, 0, 1, -1, -1, -1, -1, 7] \\
&= [7, -1, 1, 1, -1, -1, 0, 1, -1, 0, -1, -1, 1, 1, 1, 7] \\
&= [7, -1, 1, 1, -1, 1, 0, -1, -1, 0, 1, 1, 1, -1, -1, 7] \\
&= [7, -1, 1, 1, 1, -1, 0, 1, 1, 0, -1, -1, 1, -1, -1, 7] \\
&= [7, -1, 1, 1, 1, 1, 0, -1, 1, 0, 1, 1, 1, 1, 7] \\
&= [7, 1, -1, -1, -1, -1, 0, 1, -1, 0, -1, -1, -1, -1, -1, 7] \\
&= [7, 1, -1, -1, -1, 1, 0, -1, -1, 0, 1, 1, -1, 1, 1, 7] \\
&= [7, 1, -1, -1, 1, -1, 0, 1, 1, 0, -1, -1, -1, 1, 1, 7] \\
&= [7, 1, -1, -1, 1, 1, 0, -1, 1, 0, 1, 1, -1, -1, -1, 7] \\
&= [7, 1, -1, 1, -1, -1, 0, -1, -1, 0, -1, 1, 1, 1, 1, 7] \\
&= [7, 1, -1, 1, -1, 1, 0, 1, -1, 0, 1, -1, 1, -1, -1, 7] \\
&= [7, 1, -1, 1, 1, -1, 0, -1, 1, 0, -1, 1, 1, -1, -1, 7] \\
&= [7, 1, -1, 1, 1, 1, 0, 1, 1, 0, 1, -1, 1, 1, 7] \\
&= [7, 1, 1, -1, -1, -1, 0, 1, 1, 0, -1, 1, -1, -1, 1, 7] \\
&= [7, 1, 1, -1, -1, 1, 0, -1, 1, 0, 1, -1, 1, 1, -1, 7] \\
&= [7, 1, 1, -1, 1, -1, 0, 1, -1, 0, -1, 1, -1, 1, -1, 7] \\
&= [7, 1, 1, -1, 1, 1, 0, -1, -1, 0, 1, -1, -1, -1, 1, 7] \\
&= [7, 1, 1, 1, -1, -1, 0, -1, 1, 0, -1, -1, 1, 1, -1, 7] \\
&= [7, 1, 1, 1, -1, 1, 0, 1, 1, 0, 1, 1, 1, -1, 1, 7] \\
&= [7, 1, 1, 1, 1, -1, 0, -1, -1, 0, -1, -1, 1, -1, 1, 7] \\
&= [7, 1, 1, 1, 1, 1, 0, 1, -1, 0, 1, 1, 1, 1, -1, 7]
\end{aligned}
$$

Any of these assignments are sufficient for calculating $t_{n,m}$.

References

References

[HO18]   Kyungpyo Hong and Seungsang Oh. "Bounds on Multiple Self-avoiding Polygons".
         In: *Canadian Mathematical Bulletin* 61.3 (Sept. 2018), pp. 518–530. ISSN: 1496-
         4287. DOI: 10.4153/cmb-2017-072-x. URL: http://dx.doi.org/10.4153/CMB-
         2017-072-x.

[OEI]   OEIS Foundation Inc. *The On-Line Encyclopedia of Integer Sequences.* Published
         electronically at http://oeis.org.