
Average Distances in Square-Cell Configurations

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ABSTRACT: A square-cell configuration ("square animal") is a subgraph of the square lattice in which all inner faces are 4-cycles. We determine explicit expressions for the sum (W) of the (topological) distances between all pairs of vertices of a square-cell configuration, as well as for the related average distance \bar{W} . Such expressions are deduced for several families of symmetric square-cell configurations. For instance, if $O(n)$ stands for the octagonal square-cell configuration with n circular levels, then $W(O(n)) = (211/5)n^5 - (181/3)n^4 + (109/3)n^3 - (35/3)n^2 + (22/15)n$ and $\bar{W}(O(n)) = 2[(7n^2 - 10n + 4)(7n^2 - 10n + 3)]^{-1}W(O(n))$. © 2000 John Wiley & Sons, Inc. Int J Quant Chem 76: 611–617, 2000

Key words: square-cell configuration; square lattice; distance (in square-cell configuration); lattice animals; square animals

Introduction

The square lattice and its finite subgraphs (defined below and called square-cell configurations) are frequently encountered in statistical physics, where they are used for construction of mathematical theories—so-called lattice models—of a variety of phenomena, such as magnetization, phase transition, random walks, percolation, fractal growth, surface phenomena, and characterization

(see, for instance, [1–11] and the references cited therein). Therefore, the properties of the square lattice and the square-cell configurations have attracted considerable attention. In this work, we examine one such property, namely, the average topological distance between the vertices of a square-cell configuration. This quantity is a convenient and intuitively plausible measure of the compactness of the respective square-cell configuration and may be useful whenever random walks on it are considered (see, in particular, section 5.4 in [2]).

Let S be a square-cell configuration, and $V(S)$ its vertex set. Let $|V(S)| = N$. The distance $d(x, y|S)$ between two vertices x and y of S is equal to the smallest number of steps in which one can get

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from x to y (or vice versa). The sum of all such distances will be denoted by $W = W(S)$:

$$W(S) = \sum_{\{x,y\} \subseteq V(S)} d(x,y|S)$$

and the average (or mean) distance in S by $\overline{W} = \overline{W}(S)$:

$$\overline{W}(S) = \frac{W(S)}{\binom{N}{2}} = \frac{2W(S)}{N(N-1)}. \quad (1)$$

At this point, it is worth mentioning that W is just the same as the *Wiener index* (for a recent review, see [12, 13]), a structure-descriptor defined on molecular graphs, the first time used 50 years ago by Wiener for predicting physicochemical properties of alkanes [14]. Mathematicians have independently examined the same quantity, calling it *graph distance* [15] or *graph admittance* [16], but were not concerned with square-cell configurations. The (closely related) *average distance* of a graph has also been much studied in the mathematical literature [17–19]. To the authors' knowledge, Peter John's article [20] is the only published work dealing with the calculation of W of square-cell configurations.

Square-cell Configurations: Definition and Basic Properties

A *complete grid* (also called *mesh* [11, 21]) is the Cartesian product of two paths. It can also be described as a rectangular (sub)lattice. A *grid graph* is a subgraph of a complete grid. A *square-cell configuration* is a grid graph having the property that, when embedded in the plane, all its inner faces are 4-cycles. In this article, we concentrate on some families of symmetric and compact square-cell configurations.

Recall that the names *square animal* or *square lattice animal* [3, 11, 21, 22] and *polyomino* [23] are synonymous to what here is called as a square-cell configuration.

It has been shown in [24] that any grid graph is a median graph and thus a partial binary Hamming graph as well. For the purpose of this work, it is not necessary to specify median and Hamming graphs, and we refer to [25] for definitions and additional information.

So, square-cell configurations are partial binary Hamming graphs. For these graphs, an important relation Θ was introduced by Djoković [26] (see also [25, 27–29]). Let G be a connected graph with vertex set $V(G)$ and edge set $E(G)$. If $e = xy \in E(G)$ and

$f = uv \in E(G)$, then $e\Theta f$ holds if $d(x,u) + d(y,v) \neq d(x,v) + d(y,u)$. The relation Θ is reflexive and symmetric, yet it needs not be transitive. We denote its transitive closure by Θ^* and call the equivalence classes of Θ^* the *cuts* of G . Hence, the cuts of G are pairwise disjoint subsets of $E(G)$. Winkler [27] proved that a connected graph is a partial binary Hamming graph if and only if it is bipartite and $\Theta^* = \Theta$.

As we already mentioned, our square-cell configurations are embedded into the plane (in the natural way). From this point of view, there are two kinds of cuts: those embracing horizontal edges and those with vertical edges. We call the cuts with vertical edges C_1 -cuts, whereas those with horizontal edges will be referred to as C_2 -cuts. In Figure 1, a square-cell configuration is shown possessing five C_1 -cuts and seven C_2 -cuts. The five C_1 -cuts are indicated by parallel lines.

If G is a partial binary Hamming graph, then it is well known that the graph obtained from G by removing all edges of an arbitrary cut has exactly two connected components. With this in mind, we formulate the following proposition from [30]:

Proposition 1. Let G be a partial binary Hamming graph on N vertices and with k cuts. For $i = 1, 2, \dots, k$, let N_i be the number of vertices of G in one of the components of the graph obtained from G by removing the i 'th cut. Then,

$$W(G) = \sum_{i=1}^k N_i(N - N_i).$$

Proposition 1 provides a simple method for the calculation of the sum of distances and average distances of partial binary Hamming graphs, which is particularly suitable for the chemically very important class of hexagonal systems. This was elaborated in more detail in [31] and several explicit expressions are given in [32].

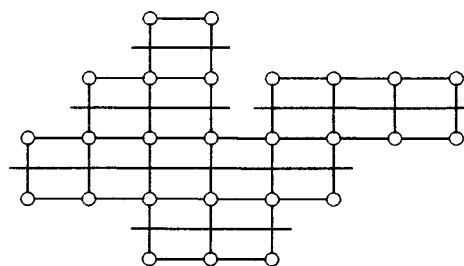


FIGURE 1. A square-cell configuration and its C_1 -cuts.

The main purpose of this article was to demonstrate that this approach is also quite simple to apply to other partial binary Hamming graphs, for instance, to square-cell configurations. We show this by computing general expressions for W for several families of these graphs. We think that for additional square-cell configurations or other partial binary Hamming graphs of interest to the readers it will not be difficult to obtain the corresponding formulas for W along the same lines.

In what follows, N will denote the number of vertices of the square-cell configuration considered. In addition, expressions of the form

$$\sum_i \left[(i(2n+2) - 1)(N - (i(2n+2) - 1)) \right]$$

will be written as

$$\sum_i \left[(i(2n+2) - 1)(N - \mathcal{F}) \right],$$

that is, \mathcal{F} will stand for the value of the "first bracket." Moreover, for a square-cell configuration S , we will use W_1 and W_2 to denote the partial sums from Proposition 1, corresponding to the C_1 -cuts and C_2 -cuts, respectively. Hence, $W(S) = W_1 + W_2$.

Rectangulars, Octagons, and Hexagons

We begin our computations with three relatively simple representatives of square-cell configurations: rectangular square-cell configurations, octagonal square-cell configurations, and hexagonal square-cell configurations.

RECTANGULARS

For $n \geq 1$ and $1 \leq k \leq n$, let $R(n, k)$ be the rectangular square-cell configuration. The definition of $R(n, k)$ should be clear from the example $R(8, 5)$ shown in Figure 2.

For $R(n, k)$, we have

$$N = (n+1)(k+1)$$

$$W_1 = \sum_{i=1}^k \left[(i(n+1))(N - \mathcal{F}) \right]$$

$$W_2 = \sum_{i=1}^n \left[(i(k+1))(N - \mathcal{F}) \right].$$

The sum of distances of $R(n, k)$ is equal to $W_1 + W_2$, and simplifying the expression, we obtain

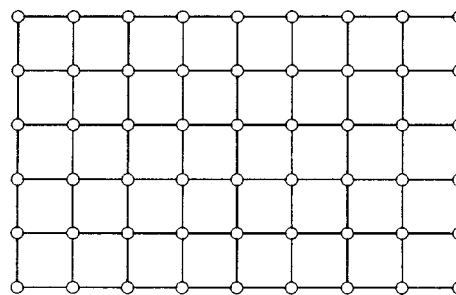


FIGURE 2. The rectangular square-cell configuration $R(8, 5)$.

Proposition 2. For any $n \geq 1$ and $1 \leq k \leq n$, we have

$$W(R(n, k)) = \frac{1}{6}(k+1)(k+n+2)(n+1)[k(n+1)+n]$$

$$\overline{W}(R(n, k)) = \frac{1}{3}(k+n+2).$$

By setting $n = r - 1$ and $k = s - 1$, where $r \geq 2$, $s \geq 2$, the above formulas reduce to

$$W(R(r-1, s-1)) = \frac{1}{6}(rs)(r+s)(rs-1) \quad (2)$$

$$\overline{W}(R(r-1, s-1)) = \frac{1}{3}(r+s).$$

These are the well-known formulas for the Wiener number of the Cartesian product of two paths on r and s vertices, respectively; cf. [33–35].

OCTAGONS

For $n \geq 2$, let $O(n)$ be the octagonal square-cell configuration. For instance, the octagonal square-cell configuration $O(3)$ is depicted in Figure 3.

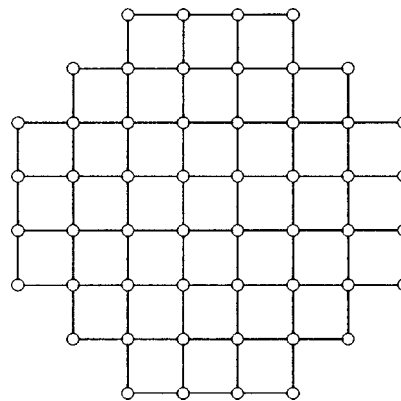


FIGURE 3. The octagonal square-cell configuration $O(3)$.

For $O(n)$, we have

$$N = 7n^2 - 4n + 1.$$

For the first n and the last n cuts of C_1 , we have

$$W'_1 = 2 \sum_{i=1}^n [(i(n+i))(N - \mathcal{F})],$$

whereas for the middle $n - 2$ cuts from C_1 ,

$$W''_1 = \sum_{i=1}^{n-2} [(2n^2 + i(3n-1))(N - \mathcal{F})].$$

Clearly, $W_1 = W'_1 + W''_1$, and, by symmetry, $W_2 = W_1$. Simplifying the expression $2(W'_1 + W''_1)$, we arrive at

Proposition 3. For any $n \geq 2$,

$$W(O(n)) = \frac{211n^5}{5} - \frac{181n^4}{3} + \frac{109n^3}{3} - \frac{35n^2}{3} + \frac{22n}{15}$$

$$\overline{W}(O(n)) = \frac{2W(O(n))}{(7n^2 - 4n + 1)(7n^2 - 4n)}.$$

HEXAGONS

For $n \geq 2$, let $H(n)$ be the hexagonal square-cell configuration. The definition of $H(n)$ should be clear from the example $H(4)$ which is shown in Figure 4.

For $H(n)$, we have $N = 4n^2$. For the first $(n - 1)$ and the last $(n - 1)$ cuts from C_1 , we have

$$W'_1 = 2 \sum_{i=1}^{n-1} [(i(i+1))(N - \mathcal{F})],$$

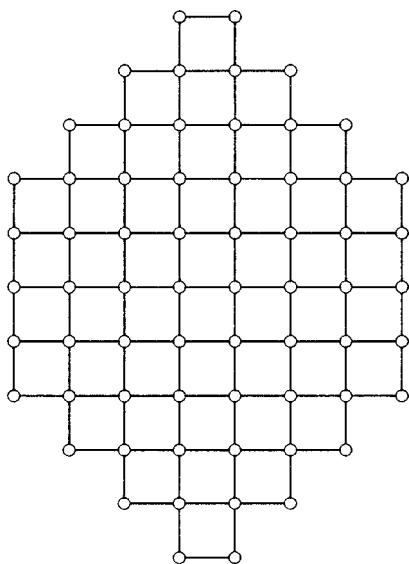


FIGURE 4. The hexagonal square-cell configuration $H(4)$.

whereas for the middle n cuts from C_1 ,

$$W''_1 = 2 \sum_{i=1}^n [(n(n-1) + i(2n))(N - \mathcal{F})].$$

Clearly, $W_1 = W'_1 + W''_1$. Now, for the first $(n - 1)$ and the last $(n - 1)$ cuts from C_2 , we have

$$W'_2 = 2 \sum_{i=1}^{n-1} [(i(n+i))(N - \mathcal{F})].$$

Since $W_2 = W'_2 + (N/2)^2$, we finally get

Proposition 4. For any $n \geq 2$,

$$W(H(n)) = \frac{158n^5}{15} - \frac{7n^3}{3} - \frac{n}{5}$$

$$\overline{W}(H(n)) = \frac{79n^3}{30} - \frac{7n}{12} - \frac{1}{20n}.$$

Rectangular Trapeziums and Trapeziums

In this section, we obtain the formulas for the average distance number of certain slightly more involved square-cell configurations: rectangular trapeziums and trapeziums. The same results can also be obtained as special cases of the bitrapeziums, which are outlined in the subsequent section. We, nevertheless, deem that it is worth considering these special cases separately, in order to demonstrate how the computations are quite simple.

In what follows, we give only expressions for $W(S)$ and $N = N(S)$ and skip the respective formula for $\overline{W}(S)$. The latter is readily obtained using Eq. (1).

RECTANGULAR TRAPEZIUMS

Let $n \geq 1$. Then, for $1 \leq k \leq n$, let $RT(n, k)$ denote the rectangular trapezium square-cell configuration. For instance, $RT(8, 6)$ is shown in Figure 5.

For $RT(n, k)$, we have

$$N = (k + 1)(n - k + 1) + \frac{k}{2}(k + 3).$$

For C_1 -cuts (from the bottom), we have

$$W_1 = \sum_{i=1}^k \left[\left(i(n+1) - \frac{1}{2}(i-1)(i-2) \right) (N - \mathcal{F}) \right].$$

Now, for the first $n - k$ cuts (from the left) from C_2 , we have

$$W'_2 = \sum_{i=1}^{n-k} [(i(k+1))(N - \mathcal{F})],$$

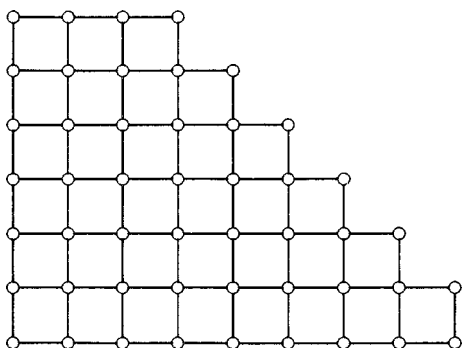


FIGURE 5. The rectangular trapezium square-cell configuration $RT(8, 6)$.

whereas for the last k cuts from C_2 ,

$$W_2'' = \sum_{i=1}^k \left[\left(\frac{i}{2}(i+3) \right) (N - \mathcal{F}) \right].$$

As $W_2 = W_2' + W_2''$, simplifying the expression $W_1 + 2(W_2' + W_2'')$, we obtain

Proposition 5. For any $n \geq 1$ and $1 \leq k \leq n$,

$$\begin{aligned} W(RT(n, k)) &= \frac{n^3(k^2 + 2k + 1)}{6} - \frac{n^2(k+1)(k^2 - 13k - 6)}{12} \\ &\quad - \frac{n(k+1)(5k^2 - 21k - 4)}{12} \\ &\quad - \frac{k(k^4 + 5k^3 + 5k^2 - 35k - 36)}{60}. \end{aligned}$$

For instance, for $k = 1$, the above formula reduces to

$$W(RT(n, 1)) = \frac{1}{3}(2n^3 + 9n^2 + 10n + 3). \quad (3)$$

Clearly, the latter formula can also be obtained from Eq. (2) by substituting $r = n + 1$ and $s = k + 1 = 2$.

Moreover, for $k = n$, the above expression for $W(RT(n, k))$ reduces to the formula for the sum of distances of rectangular-triangle square-cell configurations. Thus, if for $n \geq 1$, $T(n)$ denotes the rectangular-triangle square-cell configuration, then we have

Corollary 5.1. For any $n \geq 1$,

$$W(T(n)) = \frac{n(2n^4 + 25n^3 + 90n^2 + 95n + 28)}{30}.$$

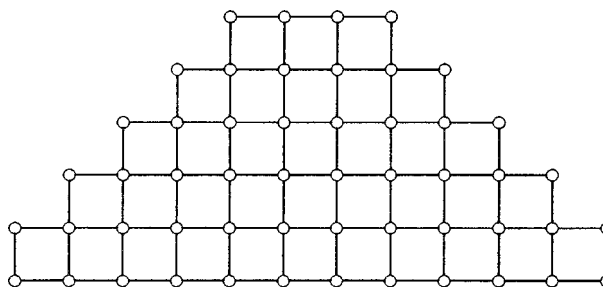


FIGURE 6. The trapezium square-cell configuration $T(11, 5)$.

TRAPEZIUMS

For $n \geq 1$ and $1 \leq k \leq \lceil n/2 \rceil$, let $T(n, k)$ stand for the trapezium square-cell configuration. The definition of $T(n, k)$ should be clear from the example $T(11, 5)$, shown in Figure 6.

For $T(n, k)$, we have

$$N = (n + 1)(k + 1) - k(k - 1)$$

$$W_1 = \sum_{i=1}^k \left[(i(n + 1) - (i - 1)(i - 2))(N - \mathcal{F}) \right]$$

$$\begin{aligned} W_2 &= 2 \sum_{i=1}^k \left[\left(\frac{i}{2}(i + 3) \right) (N - \mathcal{F}) \right] \\ &\quad + \sum_{i=1}^{n-2k} \left[\left(\frac{k}{2}(k + 3) + i(k + 1) \right) (N - \mathcal{F}) \right]. \end{aligned}$$

As $W(T(n, k)) = W_1 + W_2$, by simplifying the above expressions, we arrive at

Proposition 6. For any $n \geq 1$ and $1 \leq k \leq \lceil n/2 \rceil$,

$$\begin{aligned} W(T(n, k)) &= \frac{n^3(k^2 + 2k + 1)}{6} - \frac{n^2(2k^3 - 6k^2 - 11k - 3)}{6} \\ &\quad + \frac{n(3k^4 - 20k^3 + 19k^2 + 34k + 4)}{12} \\ &\quad - \frac{k(4k^4 - 10k^3 + 35k^2 - 35k - 24)}{30}. \end{aligned}$$

For instance, for $k = 1$, the above formula, as previously, reduces to Eq. (3).

BITRAPEZIUMS

In this section, we generalize Proposition 6 to bitrapeziums. A similar generalization is also possible for rectangular trapeziums from Proposition 5, but we leave it to the reader.

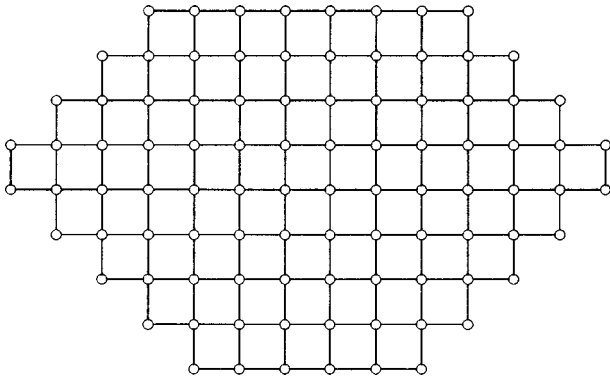


FIGURE 7. The bitrapezium square-cell configuration $BT(13, 3, 4)$.

Denote a bitrapezium system as $BT(n, k_1, k_2)$, where $0 \leq k_1 \leq \lceil n/2 \rceil - 1$ and $0 \leq k_2 \leq \lceil n/2 \rceil - 1$. For instance, $BT(13, 3, 4)$ is shown in Figure 7.

For $BT(n, k_1, k_2)$, we have

$$N = k_1(n - k_1) + k_2(n - k_2) + 2(n + 1).$$

Let N_1 and N_2 denote the number of vertices of the upper trapezium, lying above the middle cut, and the number of vertices of the lower trapezium, lying below the middle cut, respectively. Then,

$$N_1 = k_1(n - k_1) + (n + 1)$$

and

$$N_2 = k_2(n - k_2) + (n + 1).$$

Then, for the first k_1 cuts from the set C_1 , lying in the upper trapezium, we have

$$W'_1 = \sum_{i=0}^{k_1-1} \left[\left(N_1 - (i+1)(n+1) + \sum_{j=0}^i 2j \right) (n - \mathcal{F}) \right].$$

For the next k_2 cuts from the set C_1 , lying in the lower trapezium,

$$W''_1 = \sum_{i=0}^{k_2-1} \left[\left(N_2 - (i+1)(n+1) + \sum_{j=0}^i 2j \right) (n - \mathcal{F}) \right].$$

Clearly, $W_1 = W'_1 + W''_1 + N_1N_2$.

Now, for the first $k_1 + 1$ cuts from the set C_2 that are on the leftmost part of the trapezium (by the symmetry on the right most part), we have

$$W'_2 = \sum_{i=1}^{k_1+1} \left[(i(i+1))(N - \mathcal{F}) \right].$$

Without loss of generality, it may be assumed that $k_1 \leq k_2$. Then, for the next $(k_2 - k_1)$ cuts from C_2

(starting from $k_1 + 2$ to $k_2 + 1$),

$$W''_2 = \sum_{i=1}^{k_2-k_1} \left[\left((k_1 + 1)(k_1 + 2) + 2i(k_1 + 1) \frac{i}{2}(i + 1) \right) (N - \mathcal{F}) \right].$$

It remains to consider the next $n - 2(k_2 + 1)$ cuts from the set of elementary cuts C_2 . For these cuts,

$$W'''_2 = \sum_{i=1}^{n-2(k_2+1)} \left[\left((k_1 + 1)(k_1 + 2) + \frac{1}{2}(k_2 - k_1)(3k_1 + k_2 + 5) + i(k_1 + k_2 + 2) \right) (N - \mathcal{F}) \right].$$

By symmetry, $W_2 = 2W'_2 + 2W''_2 + W'''_2$. Clearly, $W(BT(n, k_1, k_2)) = W_1 + W_2$ and by simplifying we get

Proposition 7. For any $n \geq 1$ and $0 \leq k_1 \leq \lceil n/2 \rceil - 1$, and $0 \leq k_2 \leq \lceil n/2 \rceil - 1$, where $k_1 \leq k_2$, the sum of distances of $BT(n, k_1, k_2)$ is equal to

$$\begin{aligned} & n^3 \frac{(k_1 + k_2 + 2)^2}{6} \\ & - n^2 \frac{2k_1^3 - k_1(12k_2 + 17) + 2k_2^3 - 17k_2 - 18}{6} \\ & + n \frac{3k_1^4 - 4k_1^3(k_2 + 2) - k_1^2(6k_2^2 + 24k_2 + 23)}{12} \\ & - \frac{2k_1(2k_2^3 + 12k_2^2 + k_2 - 12)}{12} \\ & + n \frac{3k_2^4 - 8k_2^3 - 23k_2^2 + 24k_2 + 40}{12} \\ & - \frac{5k_1^5 + 10k_1^4 + 10k_1^3(3 - k_2^2)}{30} \\ & + \frac{5k_1^2(4k_2^3 + 12k_2^2 - k_2 - 10) - 5k_1(k_2^4 - 2k_2^2 - 1)}{30} \\ & - \frac{4k_2^5 + 10k_2^4 + 35k_2^3 + 50k_2^2 - 9k_2 - 30}{30}. \end{aligned}$$

Trapeziums can be described as $T(n, k) = BT(n, 0, k - 1)$. Hence, we can use the formula for W of bitrapezium systems obtained above, in order to obtain the expression for the trapeziums from Proposition 6:

$$\begin{aligned} & W(BT(n, 0, k - 1)) \\ & = \frac{n^3(k^2 + 2k + 1)}{6} - \frac{n^2(2k^3 - 6k^2 - 11k - 3)}{6} \end{aligned}$$

$$+ \frac{n(3k^4 - 20k^3 + 19k^2 + 34k + 4)}{12} - \frac{k(4k^4 - 10k^3 + 35k^2 - 35k - 24)}{30}.$$

Notice that due to our assumption ($k_1 \leq k_2$) we may only set $k_1 = 0$, $k_2 = k - 1$ ($k \geq 1$) in the above expression to get the desired equation for W of the trapeziums. If we also set $k_2 = 0$, then the above formula reduces to the previous Eq. (3).

In conclusion, we mention two additional special cases: If n is even, then for $k_1 = k_2 = n/2 - 1$, we obtain the formula for even symmetric bitrapeziums, that is,

Corollary 7.1. For any even $n \geq 2$,

$$W(BT(n, n/2 - 1, n/2 - 1)) = \frac{n(7n^4 + 70n^3 + 190n^2 + 80n - 92)}{120}.$$

Finally, if n is odd, we set $k_1 = k_2 = (n - 1)/2$ to obtain W of odd symmetric bitrapeziums:

Corollary 7.2. For any odd $n \geq 1$,

$$W(BT(n, (n - 1)/2, (n - 1)/2)) = \frac{(7n^5 + 70n^4 + 250n^3 + 380n^2 + 223n + 30)}{120}.$$

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