Part II

Spanning Trees with Applications to the Embedding of Polytopes on Small Integer Grids

Chapter 5

On the Maximum Number of Spanning Trees of a Planar Graph

5.1 Introduction

Let $G = (V, E)$ be a planar graph with $n = |V|$ vertices, and let $T(G)$ be the number of spanning trees of G.

We study lower and upper bounds for the maximum number of spanning trees of a planar graph. If we add edges to a planar graph, the number of spanning trees grows. Hence, we deal with triangulated planar graphs, since they are the graphs containing a largest number of spanning trees.

We also study upper bounds for the specific cases of graphs with no triangular faces, and graphs with neither triangular nor quadrangular faces. Note that any planar graph must contain at least a pentagonal face, because the dual graph is also planar and hence it has a vertex of degree 5.

In Section 5.2 we present a new method based on transfer matrices for computing the asymptotic number of spanning trees of some recursively constructible families of graphs, from which we obtain lower bounds. We prove the following theorem.

Theorem. 1. *The maximum number of spanning trees over the set $\mathcal{G}_n$ of all planar graphs with n vertices is bounded by*

$$\lim_{n\to\infty}\left(\max_{G\in\mathcal{G}_n} T(G)\right)^{\frac{1}{n}} \geq 5.029545\ldots$$

2. *If we consider the set $\mathcal{G}_n^4$ of all planar graphs of smallest face cycle 4, then the maximum number of spanning trees is bounded by*

$$\lim_{n\to\infty}\left(\max_{G\in\mathcal{G}_n^4} T(G)\right)^{\frac{1}{n}} \geq 3.209912\ldots$$

Part 1 and Part 2 of this theorem correspond to Theorems 5.4 and 5.6 respectively.

In Section 5.3, upper bounds for the number of spanning trees of planar triangulated graphs, and planar graphs with smallest face cycle 4 and 5 are studied. Several techniques are discussed, and the obtained results compared. For graphs without triangles, the best results are obtained using a probabilistic method and Suen's inequality. The following theorem summarizes the obtained results.

Theorem. *Given a planar graph G,*

1. $T(G) \leq 5.\bar{3}^n$;
2. *If G is a 3-connected graph with smallest face cycle at least 4, then*
$$T(G) < \left[\exp\left(\ln 4 - \frac{1}{8}\right)\right]^n < 3.529988^n;$$
3. *If G is a 3-connected graph with smallest face cycle 5, then*
$$T(G) < \left[\exp\left(\frac{2}{3}\ln 3 + \frac{1}{3}\ln 4 - \frac{4}{27}\right)\right]^n < 2.847263^n.$$

Here $5.\bar{3}$ denotes the periodic number $5.333333\ldots$.

Part 1 is proved in Theorem 5.7. Other attempts for triangulated graphs using Suen's inequality are shown in Section 5.3.3. For Parts 2 and 3 we refer to the corresponding Theorems 5.10 and 5.11, in Section 5.3.3.

In Section 5.4 we relate the number of spanning trees with the number of spanning forests with three and four trees, each rooted at one pinned vertex, obtaining upper bounds for the number of such forests of a graph. This is in relation with Chapter 6, where we use the obtained bounds on the number of spanning forests for bounding the size of the integer grid in which a 3-polytope can be embedded.

For our application to embed 3-polytopes in small integer grids we only use the upper bounds on the number of spanning trees. The obtained lower bounds on the number of spanning trees are not used, but they give us an idea of how tight the upper bounds are.

5.2 Lower Bounds for T

For obtaining lower bounds we compute the asymptotic number of spanning trees of some families of graphs with many edges that have a regular structure. It turns out that one of these families has the largest known number of spanning trees.

For this computation we develop a transfer-matrix method that works for families of graphs with a regular construction, known as *recursively constructible families of graphs*. These families are presented in Section 5.2.1. The transfer-matrix approach is described in Section 5.2.2. With this method we enumerate the number of spanning trees for some families of planar lattice graphs with small width.

The problem is that we are restricted by the dimension of the transfer matrices, which becomes too large when we increase the width. Hence we follow a different strategy: we use the bound given by Shrock and Wu [49]. In that paper, values for the number of spanning trees of different infinite lattices are given. Their families have periodic conditions on the boundaries and hence they are not planar graphs. We show, using algebraic properties of the transfer matrices, that their asymptotic values for the number of spanning trees remain the same if we change some boundary conditions, and hence the lower bounds given in [49] are also valid for planar graphs. This is described in Section 5.2.5.

5.2.1 Recursively Constructible Families of Graphs

We say that a sequence of graphs $\{G_k\}_{k\geq 0}$ is a *recursively constructible family of graphs* if it can can be built in a regular way from a given initial graph, by means of a repeated fixed sequence of elementary operations involving addition of vertices and edges, and deletion of edges.

The idea of recursively constructible family of graphs appeared in a joint work with Marc Noy [43]. The formal definition of this concept is a little bit complicated and it can be found in Appendix B. In particular, the definition implies that the same number of edges has to be added in every step.

For example, consider the family $\{L_k\}_{k\geq 0}$ of ladder graphs with diagonals, where L_k consists of k attached squares with diagonals. See Figure 5.1. The initial graph of the family, L_0, consists of only one edge, the first graph L_1 consists of one square with diagonal, the second graph L_2 consists of two squares with diagonals, and so on. We construct L_{k+1} from L_k by adding two new vertices and a fixed set consisting of four new adjacencies. Starting from the initial graph L_0 and repeating this adding operation, we obtain $L_1, L_2, L_3, \ldots$. So we construct in this recursive way the whole family $\{L_k\}_{k\geq 0}$.

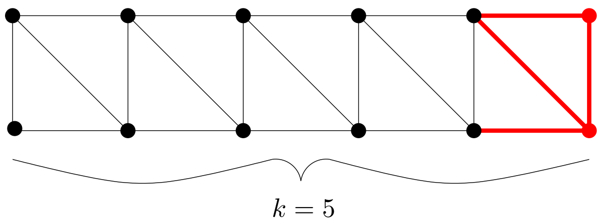

Figure 5.1: L_5, five attached squares with diagonals. It is obtained adding to L_4 two new vertices and the set of thick edges.

Other families with a regular construction are grids $\{G_{W\times k}\}_{k\geq 0}$ of squares with diagonals, with fixed width W and growing length k. For obtaining the grid $G_{W\times(k+1)}$ from the grid $G_{W\times k}$ we add W new vertices and a fixed set of adjacencies. See Figure 5.2 for an example with $W = 4$.

Also prisms $\{P_{W\times k}\}_{k\geq 0}$ of squares with diagonals are recursively constructible. For obtaining the prism $P_{W\times(k+1)}$ from the prism $P_{W\times k}$ we first delete the edges connecting column 1 and column k, and second we add a new column of vertices $k+1$ adjacent to columns 1 and k by means of a fixed set of edges. See Figure 5.3.

The family $\{K_k\}_{k\geq 0}$ of complete graphs is an example which is not a recursively constructible family, since at each step we must add on edge more than in the previous step, hence we are not adding a fixed set of edges.

A more General Framework: the Tutte Polynomial

The number of spanning trees is a very special case of the Tutte polynomial. Although we do not need it for understanding what is going on in this chapter, we write a few words about the Tutte polynomial since we started to work with recursively constructible families of graphs and the transfer-matrix method within this more general framework.

The Tutte polynomial of a graph $G = (V, E)$ is defined as

$$TP(G; x, y) = \sum_{A \subseteq E} (x-1)^{r(E)-r(A)}(y-1)^{|A|-r(A)},$$

where, for every subset $A \subseteq E$, its rank $r(A)$ is $|V|$ minus the number of components of the spanning subgraph (V, A). Usually the Tutte polynomial is denoted by $T(G; x, y)$ in the literature, but we denote it here by $TP(G; x, y)$ to avoid confusions with $T(G)$, the number of spanning trees.

The Tutte polynomial contains much information on the graph G; we refer to [12, 55] for background information. For example, by setting $y = 0$ we obtain essentially the chromatic polynomial of G, and by setting $x = 0$ we obtain essentially the flow polynomial of G. Also, special evaluations of the Tutte polynomial give the number of spanning forests, the number of acyclic orientations, the number of spanning connected subgraphs, or the number of totally cyclic orientations in G. In particular, $TP(G; 1, 1)$ is equal to $T(G)$, the number of spanning trees in G.

We can associate the Tutte polynomial to a given a recursively constructible family of graphs $\{G_k\}_{k\geq 0}$, obtaining a sequence of polynomials $\{TP(G_k; x, y)\}_{k\geq 0}$. It follows that the regularity on the graphs is translated in polynomial terms into a recurrence relation. Hence, we go from a combinatorial object like a family of graphs to an algebraic object like the recurrence relation satisfied by a family of polynomials.

Biggs, Damerell and Sands [9] call a family $\{G_k\}_{k\geq 0}$ of graphs *recursive* if their Tutte polynomials satisfy a homogeneous linear recurrence relation with polynomial coefficients, that is,

$$TP(G_{k+r}; x, y) + p_1(x, y)\, TP(G_{k+r-1}; x, y) + \cdots + p_r(x, y)\, TP(G_k; x, y) = 0,$$

where the $p_i(x, y)$ are polynomials with integral coefficients independent of k, $1 \leq i \leq r$. This

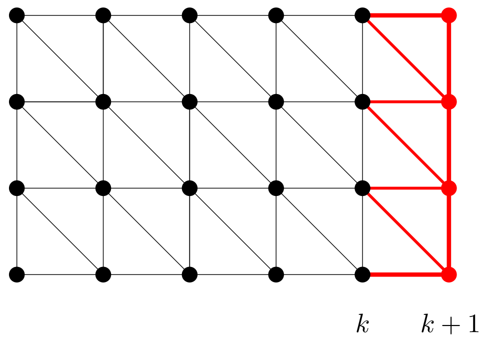

Figure 5.2: The family $\{G_{4\times k}\}_{k\geq 0}$. The set of thick edges are added in the step from $G_{4\times k}$ to $G_{4\times(k+1)}$.

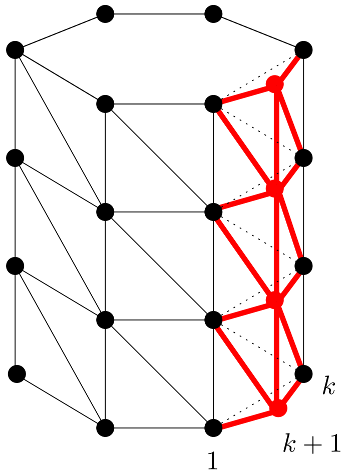

Figure 5.3: The family $\{P_{4\times k}\}_{k\geq 0}$. Dotted edges are the set of deleted adjacencies, and thick edges the set of added adjacencies in the step from $P_{4\times k}$ to $P_{4\times(k+1)}$.

condition is equivalent to the fact that the ordinary generating function

$$\sum_{k\geq 0} TP(G_k; x, y)\, z^k$$

is a rational function in x, y and z. They show, using the contraction-deletion rule, that several families of graphs, like cycles, ladders and wheels, are recursive. All these families have in common the fact that they can be constructed from an initial graph by the repeated application of a fixed graph operation.

In a joint work with Marc Noy [43] we proved the following theorem:

Theorem 5.1. *Every recursively constructible family of graphs is recursive.*

The proof is based on a transfer-matrix method, and it is an extension of the one introduced in [13] for computing the Tutte polynomial of a square lattice. The corresponding linear recurrence can be found explicitly, although the computations usually involve very large matrices. An important novelty in our approach is that we can also delete edges, an operation that corresponds algebraically to multiply by the inverse of a certain transfer matrix. The deletion of edges allows us to include in this framework families with cyclic boundary conditions, like toroidal lattices.

Theorem 5.1 is also true for all special evaluations of the Tutte polynomial, in particular for the number of spanning trees:

Corollary 5.1. *If a family of graphs $\{G_k\}_{k\geq 0}$ is recursively constructible, then their number of spanning trees satisfy a homogeneous linear recurrence relation with integral coefficients, that is,*

$$T(G_{k+r}) + \alpha_1 T(G_{k+r-1}) + \cdots + \alpha_r T(G_k) = 0.$$

Proof. By setting $\alpha_i = p_i(1, 1)$, for $1 \leq i \leq r$, the corollary follows. □

For example, the previously defined family $\{L_k\}_{k\geq 0}$ of ladders with diagonals satisfies

$$T(L_{k+2}) - 7\,T(L_{k+1}) + T(L_k) = 0\,, \tag{5.1}$$

as we show later.

5.2.2 Enumerating T via Transfer Matrices

We apply the transfer-matrix method to compute directly the number of spanning trees, without going over the Tutte polynomial, which would be computationally much more complicated. The approach is based on the storage in a transfer matrix Λ of the contributions to the number of spanning trees of the new edge subsets appearing in the step from G_k to G_{k+1}.

The transfer-matrix method is described more generally in Chapter 7, where it is used to analyze the growth in the number of polyominoes on a twisted cylinder as the number of cells increases.

An Example: the Family of Ladders with Diagonals

We explain the argument here in the case of the family $\{L_k\}_{k\geq 0}$ of ladder graphs with diagonals. The graph L_k is viewed as the union of L_{k-1} and a graph M consisting of a square with diagonals with the edge of the first column deleted.

A *partial spanning tree* is the part of the spanning tree which is already constructed, lying at the left of the last added column of vertices. A partial spanning tree is not necessarily connected, but it must be possible to connect it in the future. Note that in the case of ladders with diagonals, a partial spanning tree is either a spanning tree or a spanning forest with two trees.

In general, each connected component of a partial spanning tree must contain at least one vertex of the last added column or the first one. In the particular case of the family $\{L_k\}_{k\geq 0}$, the spanning tree or each of the two trees constituting the partial spanning tree must contain at least one vertex of the last added column.

Every spanning tree T_k of L_k is obtained from a partial spanning tree T_{k-1} of L_{k-1} and a subset of edges δ of $E(M)$. If we want to use this fact in a recursive scheme, for every partial spanning tree T_{k-1} of L_{k-1} and every subset δ of edges of M we must be able to know if the obtained subset of edges $T_k = T_{k-1} \cup \delta$ is a partial spanning tree of L_k or not, without knowledge of the whole T_{k-1}, but from the information about the connected components given by the last added column of T_{k-1} and T_k.

Given T_{k-1}, a partial spanning tree of L_{k-1}, we label the two vertices in the $(n-1)$th column according to the connected component of T_{k-1} to which they belong. The components are labelled sequentially as they appear. In this way we get a *state* $s(T_{k-1}) = (s_1, s_2)$, where the s_i are the labels of the components. For our family we have two possible states, (A, A) and (A, B), which correspond respectively to the cases when the two vertices 1 and 2 of the $(n-1)$th column belong to the same component or to different components. See the example of Figure 5.4. Note that the connected components induce a partition on the set of vertices, hence the states (A, A) and (A, B) correspond to the two possible partitions of $\{1, 2\}$: the partitions $\{1, 2\}$ and $\{1\} \cup \{2\}$ respectively.

Then, from the knowledge of the state $s = s(T_{k-1})$ and the new added edge subset δ, we can deduce if T_k is a partial spanning tree or not: it cannot contain cycles and each connected component must contain a new added vertex to guarantee that it can be connected later, i. e., δ cannot isolate any component of T_{k-1} from the two rightmost vertices.

Definition 5.1. *Let s be a state of a partial spanning tree T_{k-1} of the ladder L_{k-1}, and a subset δ of $E(M)$. If the subgraph $T_{k-1} \cup \delta$ of L_k obtained by adding the edge-set δ to T_{k-1} is a partial spanning tree T_k, we call the state of T_k* successor state *of s, and we denote it by $succ_\delta(s)$.*

We have an example in Figure 5.4.

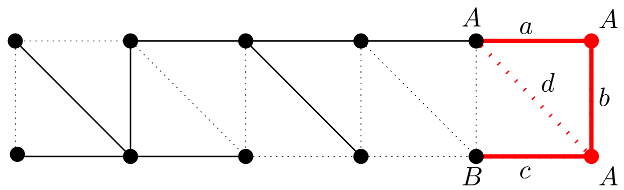

Figure 5.4: In this example, $s = (A, B)$ in L_4. We add δ, consisting of the edges $\{a, b, c\}$ (drawn in thick lines). Since the two new vertices belong to the same connected component, $succ_\delta(s) = (A, A)$.

Definition 5.2. *Given a recursively constructible family of graphs, we say that a state s is a* valid state *if it is reachable from some initial state, and from s we can reach the final state $(A, A \ldots, A)$ (otherwise we could not obtain a spanning tree, which is connected at the end), by repeating a finite number of times the computation of the successor state.*

Note that if the family of graphs is connected, then it has a non-empty set of valid states.

For every possible state s of L_{k-1}, we consider all $2^{|E(M)|}$ edge subsets δ of $E(M)$, and for each δ, if the result is a partial spanning tree, we compute its corresponding successor state $succ_\delta(s)$, otherwise we throw the combination of s and δ away. This happens when, after the addition of δ, a cycle appears or some components are isolated forever, that is, there is no valid successor state. Note that all successor states that can be obtained in this way are valid states. Actually, the valid states are precisely the states given by a partial spanning tree. In order to illustrate the procedure we show in Table 5.1 the update of the states.

Next we define a transfer matrix Λ as follows. The rows and columns are indexed by the states (A, A) and (A, B). The rows correspond to the initial states, and columns correspond to the successor states. Since we have two possible states, Λ is a 2 by 2 matrix. We accumulate the contributions to the number of spanning trees of each possible edge subset δ in the matrix Λ. The matrix Λ is set initially to 0. For every state s and for every δ, if $succ_\delta(s)$ is a valid state, we increase by one unit the entry $\Lambda[s, succ_\delta(s)]$. We obtain

$$\Lambda = \begin{pmatrix} 5 & 3 \\ 3 & 2 \end{pmatrix}.$$

Denote by $\mathbf{t}_k$ the vector storing the number of partial spanning trees in the graph L_k. The matrix Λ is used to get from $\mathbf{t}_k$ to $\mathbf{t}_{k+1}$ in this form:

$$\mathbf{t}_{k+1} = \Lambda \cdot \mathbf{t}_k. \tag{5.2}$$

δ	$succ_\delta(A,A)$	$succ_\delta(A,B)$
$\emptyset$	–	–
$\{a\}$	(A,B)	–
$\{b\}$	–	–
$\{c\}$	(A,B)	–
$\{d\}$	(A,B)	–
$\{a,b\}$	(A,A)	–
$\{a,c\}$	(A,A)	(A,B)
$\{a,d\}$	(A,A)	–
$\{b,c\}$	(A,A)	–
$\{b,d\}$	(A,A)	–
$\{c,d\}$	–	(A,B)
$\{a,b,c\}$	–	(A,A)
$\{a,b,d\}$	–	–
$\{a,c,d\}$	–	(A,A)
$\{b,c,d\}$	–	(A,A)
$\{a,b,c,d\}$	–	–

Table 5.1: Update of the states for the family $\{L_k\}_{k\geq 0}$. a and c are the two horizontal edges of M, b is the vertical edge and d is the diagonal edge (see Figure 5.4). There are $2^4 = 16$ possible edge subsets δ. The sign $-$ means that there is no successor state.

If we write down (5.2) in explicit from, we get

$$\begin{aligned} t_{k+1}^{(A,A)} &= 5\,t_k^{(A,A)} + 3\,t_k^{(A,B)} \\ t_{k+1}^{(A,B)} &= 3\,t_k^{(A,A)} + 2\,t_k^{(A,B)} \end{aligned}$$

where t_k^s is the component of $\mathbf{t}_k$ denoting the number of partial spanning trees in L_k with the vertices of the last column in state s.

Finally, we iterate (5.2), obtaining the number of spanning trees of the family of ladders with diagonals as

$$T(L_k) = (1\ 1)\cdot\Lambda^k\cdot\begin{pmatrix}1\\0\end{pmatrix}.$$

The vector $(1\ 1)$ corresponds to the contributions of the states (A,A) and (A,B) to the number of spanning trees of the initial graph of the family, L_0, which is just an edge. There are two possible edge subsets in L_0: the empty set or the edge itself. The first one leads to the state (A,B) and the second one leads to the state (A,A). The multiplication by Λ^k iterates the system (5.2). The vector $(\,1\ 0\,)^t$ at the end, ignores all disconnected forests and adds up all connected partial spanning trees, which are those ending in state (A,A).

Using this formula, the reader can check that $T(L_0)=1,\ T(L_1)=8,\ T(L_2)=55,\ T(L_3)=377,\ \ldots$, and the recurrence (5.1) can be proved.

The General Case

The method in this example can be extended to any recursively constructible family of graphs $\{G_k\}_{k\geq 0}$. In general, for any given recursively constructible family of graphs $\{G_k\}_{k\geq 0}$ we have

$$T(G_k) = \mathbf{X}_0 \cdot \Lambda^k \cdot \mathbf{u}, \tag{5.3}$$

where Λ is the transfer matrix of the family, the vector $\mathbf{X}_0$ stores the contributions to the number of spanning trees of the initial graph of the family, G_0, and $\mathbf{u}$ is the vector $(1\ 0\ 0 \dots 0)^t$ with a 1 in the component corresponding to the connected state and zero everywhere else.

The transfer matrix Λ has rows and columns corresponding to the valid states. Hence, Λ is a square matrix of dimension the number of valid states.

We can also obtain the recurrence relation for $T(G_k)$ from the denominator of the generating function $\sum_{k\geq 0} T(G_k)z^k$, which is a rational function due to Corollary 5.1:

$$\begin{aligned}\sum_{k\geq 0} T(G_k)z^k &= \sum_{k\geq 0} \left(\mathbf{X}_0 \cdot \Lambda^k \cdot \mathbf{u}\right) z^k \\ &= \mathbf{X}_0 \cdot \sum_{k\geq 0} (\Lambda z)^k \cdot \mathbf{u} \\ &= \mathbf{X}_0 \cdot (I - \Lambda z)^{-1} \cdot \mathbf{u}\,.\end{aligned}$$

The denominator of $(I - \Lambda z)^{-1}$, i. e., the determinant of $I - \Lambda z$, gives the recurrence relation.

5.2.3 The Asymptotic Behavior of $T(G_k)$

We show that $T(G_k)$ behaves asymptotically as $\rho(\Lambda)^k$, where $\rho(\Lambda)$ is the spectral radius of Λ, that is, the largest absolute value of all eigenvalues of the matrix Λ. This is summarized in the following theorem.

Theorem 5.2. *Let $\{G_k\}_{k\geq 0}$ be any connected recursively constructible family of graphs. Then,*

$$\lim_{k\to\infty} (T(G_k))^{1/k} = \rho(\Lambda)\,.$$

To prove Theorem 5.2 we use the Perron-Frobenius Theorem, stated in Section 0.5. We show that our transfer matrix Λ satisfies the conditions of the Perron-Frobenius Theorem. It is clear that Λ is a nonnegative matrix, since it is initially set to 0 and for every pair of states $(s, succ_\delta(s))$, the corresponding entry $\Lambda[s, succ_\delta(s)]$ is increased in one unit. Let us prove the other conditions.

Lemma 5.1. *For any recursively constructible family of connected graphs, the transfer matrix Λ is irreducible.*

Proof. We prove that the underlying graph of Λ is *strongly connected*. This is equivalent to prove that from any valid state s_i we can reach any other valid state s_j after a finite number of steps $G_k \to G_{k+1}$.

This is true since, by the definition 5.2, all valid states are reachable, and from every state we can reach the state $(A, A, \dots, A)$ and vice versa. (Remember that for any connected family of graphs, there is a non-empty set of valid states). □

Lemma 5.2. *For any recursively constructible family of connected graphs, the transfer matrix Λ has at least one nonzero diagonal entry.*

Proof. Let M be the new graph added in the step $G_{k-1} \to G_k$. We show that there is an edge subset δ of $E(M)$ such that if $s = (A, A, \ldots, A)$, then $succ_\delta(s) = (A, A, \ldots, A)$.

Any acyclic graph can be extended to a spanning tree. Hence, if we have a spanning tree in G_{k-1}, it can be extended it to a spanning tree in G_k by adding an edge subset δ. The added edges of δ, are incident to at least one new vertex of G_k (we cannot add an edge between two old vertices, otherwise we would have a cycle). Hence, $\delta \subseteq E(M)$.

Thus the first entry of the diagonal of Λ, which is the number of edge subsets of M that lead from the initial state $(A, A, \ldots, A)$ to the successor state $(A, A, \ldots, A)$, is at least one. □

The next corollary follows from Lemma 5.1 and Lemma 5.2.

Corollary 5.2. *The transfer matrix Λ is primitive.*

Hence the conditions of Perron-Frobenius Theorem are satisfied. Now we can prove Theorem 5.2.

Proof of Theorem 5.2. From (5.3), Corollary 5.2 and the Perron-Frobenius Theorem, we have

$$\begin{aligned}\lim_{k\to\infty} \frac{T(G_k)}{\rho(\Lambda)^k} &= \lim_{k\to\infty} \frac{\mathbf{X}_0 \cdot \Lambda^k \cdot \mathbf{u}}{\rho(\Lambda)^k} \\ &= \mathbf{X}_0 \cdot \left(\lim_{k\to\infty} \frac{\Lambda^k}{\rho(\Lambda)^k} \right) \cdot \mathbf{u} \\ &= \mathbf{X}_0 \cdot L \cdot \mathbf{u}\,,\end{aligned}$$

where $L = zv^t$, $\Lambda z = \rho(\Lambda)z$, $\Lambda^t v = \rho(\Lambda)v$, $z > 0$, $v > 0$ and $z^t v = 1$.

Note that $\mathbf{X}_0$ and $L > 0$, thus the real number $\theta = \mathbf{X}_0 \cdot L \cdot \mathbf{u}$ is positive and we obtain

$$\lim_{k\to\infty} \frac{T(G_k)}{\rho(\Lambda)^k} = \theta > 0\,.$$

Then

$$\lim_{k\to\infty} T(G_k)^{1/k} = \lim_{k\to\infty} \theta^{1/k} \rho(\Lambda)^{k/k} = \rho(\Lambda)\,.$$

□

Thanks to Theorem 5.2 we have, for example, that the family of ladders with diagonals described in Section 5.2.2 satisfies

$$\lim_{k\to\infty} T(L_k)^{1/k} = \rho\left(\begin{pmatrix} 5 & 3 \\ 3 & 2 \end{pmatrix}\right) = \frac{7}{2} + \frac{3}{2}\sqrt{5}$$

and, since at each step we add two new vertices, we have $n = 2k$, where n denotes the number of vertices of the graph. Hence we can write

$$\lim_{k\to\infty} T(L_k)^{1/2k} = \sqrt{\frac{7}{2} + \frac{3}{2}\sqrt{5}} = 2.618033\ldots$$

In general, given a family of graphs $\{G_k\}_{k\geq 0}$ with $n = n(k)$ vertices, we denote by $T^\infty(G_\infty)$ the limit $\lim_{k\to\infty} T(G_k)^{1/n(k)}$. With this notation we write

$$T^\infty(L_\infty) = 2.618033\ldots$$

5.2.4 Results

We have implemented Maple routines for computing the transfer matrices of several families of planar graphs with many triangles which we expected to have large number of spanning trees.

For the family $\{G'_{W\times k}\}_{k\geq 0}$ of grids of squares with diagonals of width W and growing k with an extra vertex adjacent to the top vertices and the bottom vertices (see Figure 5.5), we have obtained the following values

$$T^{\infty}(G'_{2\times\infty}) = 4.390256\ldots$$
$$T^{\infty}(G'_{3\times\infty}) = 4.608977\ldots$$
$$T^{\infty}(G'_{4\times\infty}) = 4.718901\ldots$$
$$T^{\infty}(G'_{5\times\infty}) = 4.784489\ldots$$
$$T^{\infty}(G'_{6\times\infty}) = 4.827803\ldots$$

The states encode $W+1$ vertices: the W vertices in the kth column and one extra vertex. Using that the graph is planar, that two encoded vertices of the right boundary can only be connected by a path lying on the left, and that the extra vertex is adjacent to the top and bottom boundaries of the grid, we deduce that the number of valid states is the number of non-crossing partitions of a set of $W+1$ elements.

The number of non-crossing partitions of a set of r elements is precisely the rth Catalan number [29, 51]. Hence, $G'_{W\times\infty}$ uses as many states as the $(W+1)$st Catalan number . The sequence of the first Catalan numbers is $(1, 2, 5, 14, 42, 132, 429, 1430, \ldots)$. Thus, for the family $\{G'_{6\times k}\}_{k\geq 0}$ we have already 429 states.

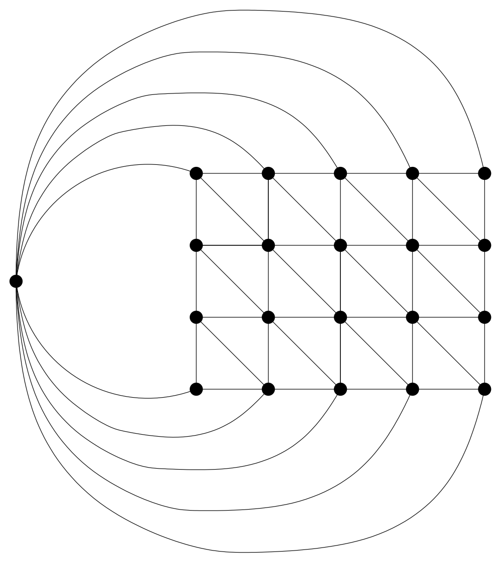

Figure 5.5: The graph $G'_{4\times 5}$ of the family $\{G'_{4\times k}\}_{k\geq 0}$.

For the family $\{P'_{W\times k}\}_{k\geq 0}$ of prism grids of squares with diagonals of width W and growing k with two extra vertices, one adjacent to all top vertices and the other adjacent to all bottom vertices (see Figure 5.6), the obtained result is

$$T^{\infty}(P'_{2\times\infty}) = 4.390256\ldots$$

We only have computed the transfer matrix for $W = 2$. We need to codify $2W+2$ vertices (two columns of W vertices each, for the cyclic boundary condition, and the two extra vertices). The number of valid states for this family is the number of non-crossing partitions of a set of $2W + 2$ elements. For the family $\{P'_{2\times k}\}_{k\geq 0}$, we have already 132 valid states, the number of non-crossing partitions of a set of 6 elements.

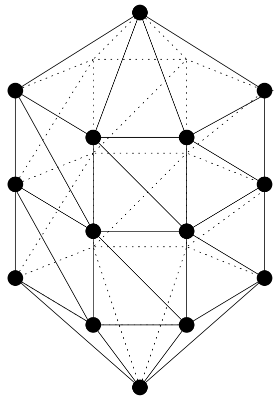

Figure 5.6: A graph of the family $\{P'_{3\times k}\}_{k\geq 0}$.

We have obtained the best results with the family of cylinder grids $\{C_{W\times k}\}_{k\geq 0}$ of squares with diagonals, wrapping around from the top vertices to the bottom vertices, with fixed width W and growing k. This family can be seen as a triangular cylindrical lattice. See Figure 5.7. The results are

$$\begin{aligned} T^{\infty}(C_{3\times\infty}) &= 4.546149\ldots \\ T^{\infty}(C_{4\times\infty}) &= 4.752157\ldots \\ T^{\infty}(C_{5\times\infty}) &= 4.850303\ldots \\ T^{\infty}(C_{6\times\infty}) &= 4.904405\ldots \end{aligned} \tag{5.4}$$

The states encode W vertices. By planarity, and since the encoded vertices can only be connected by a path lying on the left, there are as many valid states as non-crossing partitions of a set of W elements, that is the Wth Catalan number. For example, for the family $\{C_{6\times k}\}_{k\geq 0}$ we have 132 states.

So the best obtained lower bound with this method is 4.904405..., given by the family $\{C_{6\times k}\}_{k\geq 0}$.

We could not compute the asymptotic behavior of the number of spanning trees for families with larger width due to the huge number of states.

The dimension of the transfer matrix equals the number of valid states. In general, for any recursively constructible family of graphs of any kind, the number of states is the number of partitions of a set of r elements, where r is the number of vertices that we codify. The sequence of the first numbers of set partitions is $(1, 2, 5, 15, 52, 203, 877, 4140, \ldots)$. These numbers, also

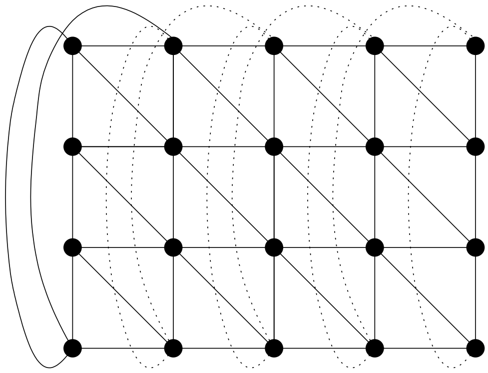

Figure 5.7: The graph $C_{4\times 5}$ of the family $\{C_{4\times k}\}_{k\geq 0}$.

known as Bell numbers $B(r)$, grow very fast with r. It follows from [11, page 9 (6.2.7)], that their asymptotic growth is

$$B(r) \approx \left(\frac{r}{e\log r}\right)^r.$$

(This is an underestimate.) The Bell numbers grow more than exponentially but less than $r!$.

We are dealing with connected planar graphs. As we have seen, in our case not all set partitions are valid states; the valid states are then a subset of all set partitions. In the case of planar graphs, the number of valid states is reduced to the number of non-crossing partitions of a set of r elements, that is the r-th Catalan number. The problem is that the Catalan numbers still grow very fast: their asymptotic growth is essentially 4^n.

Hence the above method is not computationally feasible for high values of r, as the required space to store the transfer matrix grows exponentially. For example, for families where 10 vertices are codified ($r = 10$) the transfer matrix is a 16796 by 16796 matrix. Even for small values of r, the computation requires already a lot of space.

5.2.5 Removing Periodic Boundary Conditions to Obtain a Bound for Planar Graphs

In [49], Shrock and Wu consider the problem of enumerating spanning trees on graphs and lattices, obtaining bounds on the number of spanning trees, and inequalities relating the numbers of spanning trees of different sorts of infinite lattice families of graphs. They present a general formulation for the enumeration of spanning trees on lattices in $d \geq 2$ dimensions, which is applied to the hypercubic, body-centered cubic, face-centered cubic, and specific lattices of dimension 2 including the triangular lattice, the so-called kagomé, the diced, 4-8-8 (bathroom-tile) lattices, the Union Jack, and 3-12-12 lattices. They obtain closed-form expressions for the number of spanning trees for these lattices of finite sizes.

Let $\hat{C}_{W\times k}$ be the graph obtained from $C_{W\times k}$ by connecting the last column to the first column in the same way as all other adjacent columns in $C_{W\times k}$ are connected. See Figure 5.8. Shrock and Wu refer to this graphs as triangular grid graphs with *periodic boundary conditions*. As the other families studied in [49] (all with periodic conditions on the boundaries), they can be embedded on the torus, but they are not planar graphs.

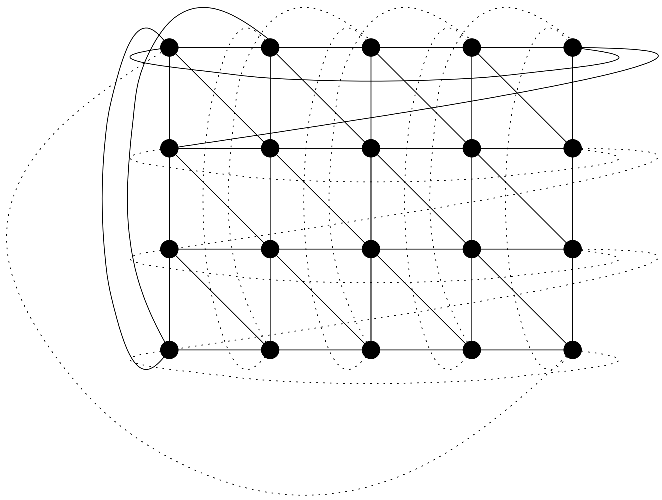

Figure 5.8: The graph $\hat{C}_{4\times 5}$ of the family $\{\hat{C}_{4\times k}\}_{k\geq 0}$.

The graphs $\hat{C}_{W\times k}$ are more regular and symmetric than the graphs $C_{W\times k}$, in which the boundary vertices are distinguished from the remaining vertices. Therefore, an explicit formula for the number of spanning trees in $\hat{C}_{W\times k}$ can be derived by spectral methods, and the limit for $k\to\infty$ can be calculated analytically:

$$T^\infty(\hat{C}_{W\times\infty}) = \exp\left(\frac{1}{W}\sum_{k=0}^{W-1}\ln\left(3-\cos\omega_k+((1-\cos\omega_k)(7-\cos\omega_k))^{1/2}\right)\right),$$

where $\omega_k = 2\pi k/W$. This summation can be explicitly carried out for a given W. Their results coincide with our results in (5.4) for $T^\infty(C_{W\times\infty})$, for all the computed values of the width W. We prove below in Theorem 5.3 that this is true in general.

For $W\to\infty$, Wu [57] shows that

$$\begin{aligned}\lim_{W\to\infty}(T^\infty(\hat{C}_{W\times\infty})) &= \exp\left(\frac{3\sqrt{3}}{\pi}\left(1-\frac{1}{5^2}+\frac{1}{7^2}-\frac{1}{11^2}+\frac{1}{13^2}-\cdots\right)\right) \qquad (5.5)\\ &= 5.029545\ldots\end{aligned}$$

(see also [49, (2.18) and (2.19)]). The triangular lattice $\hat{C}_{W\times\infty}$ is the family for which Shrock and Wu obtain a largest result.

It turns out that the spectral radius of the transfer matrices of both families $\{C_{W\times\infty}\}_{k\geq 0}$ and $\{\hat{C}_{W\times\infty}\}_{k\geq 0}$ is the same. We can prove the following theorem:

Theorem 5.3.

$$T^\infty(C_{W\times\infty}) = T^\infty(\hat{C}_{W\times\infty})$$

Proof. We prove this by comparing the transfer-matrix method on the family $\{\hat{C}_{W\times k}\}_{k\geq 0}$ with the family $\{C_{W\times k}\}_{k\geq 0}$.

To calculate $T^\infty(\hat{C}_{W\times\infty})$ by the transfer-matrix method, we build $\hat{C}_{W\times k}$ by first building up $C_{W\times k}$ recursively in the usual way, and adding a subset $\hat{\delta}$ of the edges between the last and first column at the end.

We now also have to consider partial spanning trees of $C_{W\times k}$ whose components are not necessarily connected to the right boundary. The condition on partial spanning trees is that each component contains at least one vertex of the leftmost *or* the rightmost column. In addition to the partition of the right boundary vertices into components, a state must also remember the components to which the left boundary vertices belong. A state $\hat{s}$ is thus a vector of $2W$ numbers $\hat{s} = (s_0, s)$, encoding the components among the W vertices of the leftmost column (in the vector s_0) and the W vertices in the rightmost column (in the vector s). We use again the convention of assigning labels to components in the order in which they first appear.

Let $\hat{\Lambda}$ denote the transfer matrix for this larger set of states Σ. We have

$$T(\hat{C}_{W\times k}) = \hat{\mathbf{X}}_0 \cdot \hat{\Lambda}^k \cdot \hat{\mathbf{u}}\,.$$

The initial vector $\hat{\mathbf{X}}_0$ has a 1 for each state $\hat{s} = (s_0, s)$ that corresponds to a subset of edges of the graph $C_{W\times 0}$ (a cycle of length W), and 0 otherwise. (These states have $s_0 = s$.) The vector $\hat{\mathbf{u}}$ encodes the possible ways of combining the connected components of each state $\hat{s} = (s_0, s)$ into a single tree by adding a subset $\hat{\delta}$ of "wrap-around" edges between the left and the right boundary.

Let us now relate $\hat{\Lambda}$ to the transfer matrix Λ for the original recursion for computing $T(C_{W\times k})$. We will establish the lemma by showing $\rho(\hat{\Lambda}) = \rho(\Lambda)$.

For this purpose, we decompose the set of states Σ in

$$\Sigma = \Sigma_0 \cup \Sigma_1 \cup \cdots \cup \Sigma_d \cup \cdots \cup \Sigma_W,$$

according to the number d of components of $\hat{s} = (s_0, s)$ which are disconnected from the right boundary. This is the number of different indices in s_0 that do not occur in s. Accordingly, we write $\hat{\Lambda}$ in block form as

$$\hat{\Lambda} = \begin{pmatrix} B_{00} & B_{01} & B_{02} & \dots & B_{0W} \\ & B_{11} & B_{12} & \dots & B_{1W} \\ & & B_{22} & \dots & B_{2W} \\ & & & \ddots & \vdots \\ 0 & & & & B_{WW} \end{pmatrix},$$

where each block B_{ij} contains the contributions to the number of spanning trees from a state of Σ_i to a successor state of Σ_j. This matrix is block upper triangular: a component which is isolated from the right boundary will remain isolated when edges are added on the right, thus the number d of isolated components cannot decrease.

It follows that

$$\rho(\hat{\Lambda}) = \max\{\, \rho(B_{00})\,,\, \rho(B_{11})\,,\, \dots\,,\, \rho(B_{WW})\,\}. \tag{5.6}$$

For analyzing B_{dd} let us further divide the states $\hat{s} = (s_0, s)$ in

$$\Sigma_d = \Sigma_d^0 \cup \Sigma_d^1 \cup \cdots \cup \Sigma_d^e \cup \cdots \cup \Sigma_d^W,$$

according to the number of components of s_0 which are connected to the right boundary. This is the number of indices of s_0 that also occur in s. (We must have $1 \le d+e \le W$, but for ease of notation we ignore this constraint).

Accordingly, we can write

$$B_{dd} = \begin{pmatrix} A^d_{00} & & & 0 \\ A^d_{10} & A^d_{11} & & \\ \vdots & & \ddots & \\ A^d_{W0} & A^d_{W1} & \dots & A^d_{WW} \end{pmatrix}$$

in block lower-triangular form: different components in s_0 can become connected, but no new connected components can appear. Thus

$$\rho(B_{dd}) = \max\{\, \rho(A^d_{00})\,,\, \rho(A^d_{11})\,,\, \dots\,,\, \rho(A^d_{WW})\,\}. \tag{5.7}$$

Let us now look at the successor of a state $\hat{s} = (s_0, s) \in \Sigma^e_d$ when a set δ of edges is added on the right. We are mostly interested in successor states in the same class Σ^e_d because these are the states which determine $\rho(A^d_{ee})$ and eventually $\rho(\hat{\Lambda})$.

Let $C_{W\times k} \to C_{W\times(k+1)}$ be the original recursion for $C_{W\times k}$.

First, there are the edge sets δ which can be legally added to the state s in the step $C_{W\times k} \to C_{W\times(k+1)}$. In addition, there are edge sets δ which leave some components disconnected from the right. However, these transitions increase d and contribute to some matrix $B_{dd'}$ with $d' > d$. Thus we only need to consider transitions δ that lead from s to a legal successor $succ_\delta(s)$ in the original recursion $C_{W\times k} \to C_{W\times(k+1)}$, and which are encoded in the transfer matrix Λ.

For each δ, we have

$$\widehat{succ}_\delta((s_0, s)) = (s'_0, succ_\delta(s)),$$

where s'_0 reflects the changes in labels when going from s to $succ_\delta(s)$: any labels of s that were relabeled in $succ_\delta(s)$ because some components were united (and higher labels were consequently shifted down) must be similarly relabeled in s_0, yielding s'_0. If any such relabeling took place in s'_0, however, it means that some components in s_0 were united. (Recall that the components appearing in s_0 have the smallest labels.) Such successor states belong to $\Sigma^{e'}_d$ with $e' < e$ and do not contribute anything to A^d_{ee}.

The only edge sets that contribute to the diagonal blocks A^d_{ee} are therefore the sets δ which leave s_0 intact and are legal in the original recursion $C_{W\times k} \to C_{W\times(k+1)}$:

$$\widehat{succ}_\delta((s_0, s)) = (s_0, succ_\delta(s))$$

If we group the states $(s_0, s) \in \Sigma^e_d$ according to s_0, and order the states with the same s_0 according to s as they appear in Λ, we can write

$$A^d_{ee} = \begin{pmatrix} D^{(1)}_{d,e} & & & 0 \\ & D^{(2)}_{d,e} & & \\ & & \ddots & \\ 0 & & & D^{(t)}_{d,e} \end{pmatrix}$$

where $s^{(1)}_0, s^{(2)}_0, \dots, s^{(t)}_0$ are the different values of the vector s_0. All transitions δ encoded in one of these blocks $D^{(t)}_{d,e}$ are also legal transitions for the original recursion $C_{W\times k} \to C_{W\times(k+1)}$.

Therefore, since each block encodes only part of the legal transitions δ, we have

$$D^{(t)}_{d,e} \leq \Lambda$$

Thus,

$$\rho(A^d_{ee}) = \max\{\, \rho(D^{(1)}_{d,e}) \,,\, \ldots \,,\, \rho(D^{(t)}_{d,e}) \,\} \leq \rho(\Lambda),$$

which yields, with (5.6) and (5.7)

$$\rho(\hat{\Lambda}) \leq \rho(\Lambda).$$

To obtain the converse inequality, consider the states $\hat{s} = (s_0, s)$ in Σ^1_0. All vertices in the left column belong to a single component which is connected to the right boundary, and $s_0 = (A, A, \ldots, A)$. The edge sets which lead to a successor state in the same class Σ^1_0 are precisely the ones which lead to a legal successor state in the original step $C_{W\times k} \to C_{W\times(k+1)}$. Thus we have

$$A^0_{11} = \Lambda$$

and hence, by (5.6) and (5.7),

$$\rho(\hat{\Lambda}) \geq \rho(A^0_{11}) = \rho(\Lambda).$$

We have proved that the family $\{C_{W\times k}\}_{k\geq 0}$ has the same spectral radius with or without periodic conditions on the vertical boundaries, and the theorem follows. □

Corollary 5.3. *The number of spanning trees of the family of cylindrical triangular lattices is given by*

$$\lim_{W\to\infty} (T^{\infty}(C_{W\times\infty})) = 5.029545\ldots$$

Hence we conclude with the following result.

Theorem 5.4. *The maximum number of spanning trees over the set $\mathcal{G}_n$ of all planar graphs with n vertices is bounded by*

$$\lim_{n\to\infty} \left(\max_{G\in\mathcal{G}_n} T(G) \right)^{\frac{1}{n}} \geq 5.029545\ldots$$

(*The exact expression is given in* (5.5).)

Proof. We use the known result which says that if a function $f : \mathbb{N} \to \mathbb{R}$ is supermultiplicative, that is, $f(n+m) \geq f(n) \cdot f(m)$ and exponentially bounded, that is, there exist a $K \in \mathbb{R}$ such that $f(n) \leq K^n$, then the limit $\lim_{n\to\infty} f(n)^{1/n}$ exists [34].

Our function $f(n) = \max_{G\in\mathcal{G}_n} T(G)$ is supermultiplicative, since given a graph A with n vertices and a graph B with m vertices, the number of spanning trees satisfies

$$T(A \cup B \cup e) = T(A) \cdot T(B)\,,$$

for any edge e adjacent to a vertex of A and a vertex of B.

The function $f(n) = \max_{G\in\mathcal{G}_n} T(G)$ is also exponentially bounded: in Section 5.3 we give upper bounds for the number of spanning trees. Theorem 5.7 gives the upper bound

$$T(G) \leq 5.\bar{3}^n,$$

where $5.\bar{3}$ denotes the periodic number $5.333333\ldots$.

Hence, the limit

$$\lim_{n\to\infty}\left(\max_{G\in\mathcal{G}_n} T(G)\right)^{\frac{1}{n}}$$

exists, and by Corollary 5.3 we have the result. □

5.2.6 Square Grids

For lower bounding the maximum number of spanning trees of a planar graph with smallest face cycle 4, we use arguments analogous to the triangulated case.

Let $\{Q_{W\times k}\}_{k\geq 0}$ be the family of square cylinder grid graphs, wrapping around from the top vertices to the bottom vertices, with fixed width W and growing length k. Shrock and Wu [49] obtained the number of spanning trees for the family $\{\hat{Q}_{W\times k}\}_{k\geq 0}$, where the graph $\hat{Q}_{W\times k}$ is obtained from $Q_{W\times k}$ by connecting the last column to the first column in the same way as all other adjacent columns in $Q_{W\times k}$ are connected. We call this graphs square grid graphs with periodic boundary conditions. See Figure 5.9.

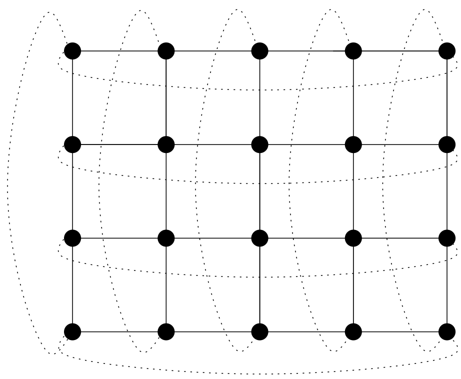

Figure 5.9: The square grid 4×5 with periodic boundary conditions.

In [49] is given the following limit for $T(\hat{Q}_{W\times k})$:

$$T^{\infty}(\hat{Q}_{W\times\infty}) = \exp\left(\frac{1}{W}\sum_{k=0}^{W-1}\ln\left(2-\cos\omega_k+\left((2-\cos\omega_k)^2-1\right)^{1/2}\right)\right),$$

where $\omega_k = 2\pi k/W$.

For W arbitrarily large, we have [57]

$$\begin{aligned}\lim_{W\to\infty}(T^{\infty}(\hat{Q}_{W\times\infty})) &= \exp\left(\frac{4}{\pi}\left(1-\frac{1}{3^2}+\frac{1}{5^2}-\frac{1}{7^2}+\frac{1}{9^2}-\cdots\right)\right) \\ &= 3.209912\ldots\end{aligned} \tag{5.8}$$

(see also [49, (2.17)]).

As for triangular grid graphs, the spectral radius of the transfer matrices of both families $\{Q_{W\times\infty}\}_{k\geq 0}$ and $\{\hat{Q}_{W\times\infty}\}_{k\geq 0}$ is the same. We have

Theorem 5.5.

$$T^{\infty}(Q_{W\times\infty}) = T^{\infty}(\hat{Q}_{W\times\infty})$$

The proof is analogous to the proof of Theorem 5.5.

Corollary 5.4. *The number of spanning trees of the family of square cylinder grid graphs is given by*

$$\lim_{W\to\infty}(T^{\infty}(Q_{W\times\infty})) = 3.209912\ldots$$

We conclude with the following result.

Theorem 5.6. *The maximum number of spanning trees over the set $\mathcal{G}_n^4$ of all planar graphs of smallest face cycle 4 with n vertices is bounded by*

$$\lim_{n\to\infty}\left(\max_{G\in\mathcal{G}_n^4} T(G)\right)^{\frac{1}{n}} \geq 3.209912\ldots$$

(*The exact expression is given in* (5.8).)

The proof is analogous to the proof of Theorem 5.4, using Corollary 5.4.

5.3 Upper Bounds for T

Let $G = (V, E)$ be a planar graph with $n = |V|$ vertices, m edges, and f faces. First we recall a known result that we use several times.

Lemma 5.3. *A planar graph G and its dual G^* have the same number of spanning trees.*

The best obtained bound that we have found for general planar graphs is given by the following theorem.

Theorem 5.7. *If G is a planar graph, then*

$$T(G) \leq \left(\frac{16}{3}\right)^n = 5.\bar{3}^n$$

We denote by $5.\bar{3}$ the periodic number $5.333333\ldots$.

Proof. If we add edges to a graph, the number of spanning trees grows. We add edges to G while maintaining its planarity, until we obtain a triangulated planar graph G_T which satisfies $T(G) \leq T(G_T)$.

Since G_T is triangulated, its dual graph G_T^* is 3-regular. We apply to G_T^* the upper bound for κ-regular graphs with $\kappa \geq 3$, due to McKay [39], Chung and Yau [15]:

$$T(G_T^*) \leq \left(\frac{2\ln n^*}{n^*\kappa\ln\kappa}\right)(c_\kappa)^{n^*},$$

where n^* is the number of vertices of the dual graph G_T^*, and

$$c_\kappa = \frac{(\kappa-1)^{\kappa-1}}{(\kappa^2-2\kappa)^{\frac{\kappa}{2}-1}}$$

is the leading term.

For $\kappa = 3$, we have $c_3 = 4\sqrt{3}/3$. The graph G_T^* has $2n-4$ vertices (which correspond to the faces of G_T), therefore we obtain the upper bound

$$T(G_T^*) \leq c_3^{2n-4} \leq \left(\frac{16}{3}\right)^n = 5.\bar{3}^n$$

This bound is also valid for $T(G)$, since $T(G) \leq T(G_T) = T(G_T^*)$ (the last equality holds by Lemma 5.3). □

Recall that the lower bound that we have for the maximum number of spanning trees of a planar graph is $5.029545^n \ldots$, given in Theorem 5.4.

A next step would be to try to improve this bound by using the planarity of G^*, which is not considered in the proofs in [15, 39], but this seems difficult.

A *face cycle* in a graph G is a cycle with edges in the boundary of a face of G. We say that a graph has *smallest face cycle k* if its shortest face cycle has length k. A graph with smallest face cycle 4 is a graph without triangles but at least one quadrilateral face. A graph with smallest face cycle 5 has neither triangular nor quadrilateral faces, but at least a pentagonal face. Note that a 3-connected planar graph must contain always a triangle, a quadrilateral face or a pentagonal face, because the dual graph is also planar and hence its average degree is less than 6, thus the dual graph has minimum degree at most 5.

We have tried several different techniques for bounding $T(G)$, obtaining new bounds for the cases of planar graphs with smallest face cycle 4 and 5. The applied techniques and results are discussed in the sections below. Although the obtained bounds for general planar graphs are not better than the one given in Theorem 5.7, we would also like to give an overview of the results using these alternative methods.

5.3.1 The Outgoing Edge Approach for Upper Bounding T

For every vertex $v \in V$, let $d_v = d(v)$ denote the degree of v. We can easily show the following lemma:

Lemma 5.4. *The number of spanning trees is bounded by the product of vertex degrees:*

$$T(G) \leq \prod_{v \in V \setminus \{r\}} d_v, \tag{5.9}$$

for an arbitrary vertex r.

Proof. Choose a vertex r to be the root. Consider the directed graph obtained by replacing every edge by two directed arcs, one in each direction, except for the root, which has only ingoing edges.

We can obtain all spanning trees just selecting one outgoing edge to each vertex different than the root. We denote by $\mathcal{R}$ such a selection. See Figure 5.10. Within the selection $\mathcal{R}$, cycles can appear, but the process is injective, i. e., we do not obtain twice the same spanning tree. This is because a spanning tree obtained in this way has a directed path from each leaf to the root, and this is the only possible orientation.

Hence

$$T(G) \leq \prod_{v \in V \setminus \{r\}} d_v,$$

since d_v is the number of possibilities of selecting one outgoing edge to each vertex different from the root. □

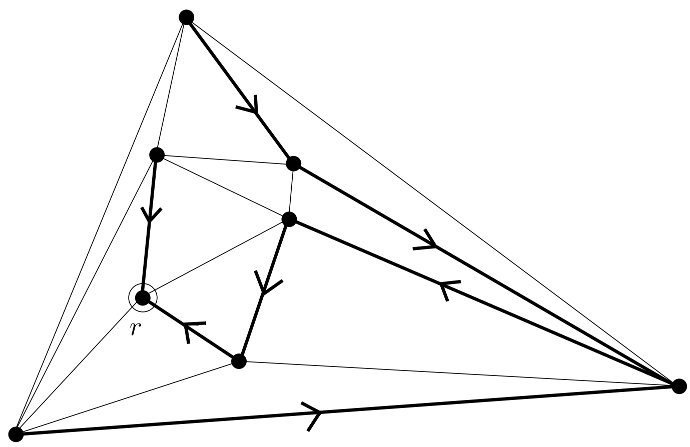

Figure 5.10: A planar graph with a selected root r and a selection of outgoing edges that forms a spanning tree.

This gives an upper bound of 6^n for planar graphs, because

$$T(G) \leq \prod_{v \in V \setminus \{r\}} d_v \leq \prod_{v \in V} d_v \leq \left(\frac{\sum_{v \in V} d_v}{n} \right)^n < 6^n. \tag{5.10}$$

The second inequality holds by the arithmetic-geometric means inequality. The last inequality holds since the average degree of a planar graph is less than 6.

The bound (5.10) is a quite relaxed bound. The error comes from counting selections of outgoing edges that contain cycles, since they do not constitute any spanning tree. Hence, one can try to improve the bound by excluding cyclic selections, and this is what we do in the following sections.

5.3.2 Removing Sets of Independent Edges

In this section, the bounds are obtained quite easily but they are improved by later sections. Therefore, some details are only sketched, as for example the details about linear programming towards the end of the section.

Consider the 2-cycles formed by both directed arcs along the same edge. Since in $\mathcal{R}$ we select at most one outgoing edge per vertex, we can only find several 2-cycles in $\mathcal{R}$ if they are along independent edges. As a first attempt, we can improve the bound (5.10) a little by considering matchings on G and applying the following lemma.

Lemma 5.5. *Suppose* $(x_1, y_1), (x_2, y_2), \ldots, (x_{|M|}, y_{|M|})$ *are the edges of a matching* M *of the graph* G*, and* $z_1, \ldots, z_u$ *are the unmatched vertices* ($u > 0$)*. Then*

$$T(G) \leq \prod_{k=1}^{|M|} (d(x_k)d(y_k) - 1) \prod_{i=1}^{u-1} d(z_i).$$

Proof. The error on the bound given in Lemma 5.4 comes from counting selections that contain cycles. For forming a tree, we must exclude cycles. In particular, we can exclude 2-cycles by considering a matching M, and excluding the possibility that, for an edge (x_k, y_k) in M, both directed arcs along the edge form a 2-cycle. Then we can substitute, in the product of Lemma 5.4, $d(x_k)d(y_k)$ by $d(x_k)d(y_k) - 1$. We can do this for each $k = 1 \ldots |M|$, since given two edges of the matching (x_{k_1}, y_{k_1}) and (x_{k_2}, y_{k_2}), the existence of a 2-cycle between x_{k_1} and y_{k_1} is independent of the existence of a 2-cycle between x_{k_2} and y_{k_2}.

Since the root has no outgoing edge, it cannot be contained in any cycle. In particular, it cannot be contained in any 2-cycle, hence we count it as one of the unmatched vertices. The product of degrees over the unmatched vertices has only $u-1$ factors because in (5.9) the root is excluded. ☐

For applying the bound given by Lemma 5.5, we look at the size of a maximum matching $M_{\max}$ in our graph. Let $\delta(G)$ the minimum degree of G. In [42], Nishizeki and Baybars establish the following lower bounds for the size of the maximum matchings:

Theorem 5.8. *Let G be a planar 3-connected graph with n vertices. We have*

- $|M_{\max}| \geq \left\lceil \frac{n+4}{3} \right\rceil$
- *If $\delta(G) \geq 4$, then $|M_{\max}| \geq \left\lceil \frac{3n+8}{7} \right\rceil$*
- *If $\delta(G) = 5$, then $|M_{\max}| \geq \left\lceil \frac{9n+20}{19} \right\rceil$*

In the same paper it is also proved that a 4-connected planar graph is Hamiltonian, and hence it has a perfect matching, that is, a matching of $\left\lfloor \frac{n}{2} \right\rfloor$ vertices.

For our application, we assume the graph G to be 3-connected, since we want to lift it to a polytope.

Proposition 5.1. *If G is a planar 3-connected graph with n vertices, then*

$$T(G) < 5.943922^n.$$

Proof. By Lemma 5.5 we have

$$T(G) \leq \prod_{k=1}^{|M_{\max}|} (d(x_k)d(y_k) - 1) \prod_{i=1}^{n-2|M_{\max}|} d(z_i). \tag{5.11}$$

We want to maximize the expression (5.11) above under the constraint

$$\sum_{v \in V} d(v) \leq 6n - 12\,,$$

given by the Handshaking Lemma and the fact that a planar graph has at most $3n-6$ edges. We claim that, under the weaker constraint

$$\sum_{v \in V} d(v) \leq 6n\,,$$

(5.11) is maximized by

$$(6 \cdot 6 - 1)^{|M_{\max}|}\, 6^{n-2|M_{\max}|}.$$

This can be seen using an exchanging argument: We want to show that the amount (5.11) only grows when each pair of degrees $d(v_1)$ and $d(v_2)$ such that $d(v_1) - d(v_2) \geq 2$ is exchanged by $d(v_1) - 1$ and $d(v_2) + 1$ respectively. To prove this, we have to distinguish several cases, depending on the position where $d(v_1)$ and $d(v_2)$ occur in the product (5.11). For two vertices x_k and y_k matched to each other, such that $d(x_k) - d(y_k) \geq 2$, it is easy to see that

$$d(x_k)d(y_k) - 1 \leq (d(x_k) - 1)\,(d(y_k) + 1) - 1.$$

It two vertices z_i and z_j are both unmatched, satisfying $d(z_i) - d(z_j) \geq 2$, we have

$$d(z_i)d(z_j) \leq (d(z_i) - 1)\,(d(z_j) + 1)\,.$$

For two vertices x_k and x_l both matched but not to each other, such that $d(x_k) - d(x_l) \geq 2$, we have

$$(d(x_k)d(y_k) - 1)\,(d(x_l)d(y_l) - 1) \leq ((d(x_k) - 1)\,d(y_k) - 1)\,((d(x_l) + 1)\,d(y_l) - 1)\,.$$

Similarly, for a vertex x_k matched and a vertex z_i unmatched, such that $d(x_k) - d(z_i) \geq 2$, we have

$$(d(x_k)d(y_k) - 1)\,d(z_i) \leq ((d(x_k) - 1)\,d(y_k) - 1)\,(d(z_i) + 1)\,.$$

Finally, for a vertex x_k matched and a vertex z_i unmatched, such that $d(z_i) - d(x_k) \geq 2$, we have

$$(d(x_k)d(y_k) - 1)\,d(z_i) \leq ((d(x_k) + 1)\,d(y_k) - 1)\,(d(z_i) - 1)\,.$$

Within this exchange, the constraint $\sum_{v \in V} d(v) \leq 6n$ is maintained since the sum of degrees remains the same. At the end, the degrees have at most two different values that differ only in one unit. Since the average degree is at most 6, we have

$$\begin{aligned} T(G) &\leq \prod_{k=1}^{|M_{\max}|} (d(x_k)d(y_k) - 1) \prod_{i=1}^{n-2|M_{\max}|} d(z_i) \\ &\leq (6 \cdot 6 - 1)^{|M_{\max}|}\, 6^{n-2|M_{\max}|} \\ &\leq \left(35^{\frac{1}{3}}\, 6^{\frac{1}{3}}\right)^n \\ &< 5.943922^n. \end{aligned}$$

For the third inequality we have used that $\delta(G) \geq 3$ because G is 3-connected, and, by Theorem 5.8, G has a maximum matching $M_{\max}$ of size at least $\lceil \frac{n+4}{3} \rceil$. □

In graphs with smallest face cycle 4, each face is bounded by 4 or more edges, hence $2f \leq m$, and by Euler's formula, we have $m \leq 2n - 4$. Then, the average degree is given by

$$\frac{\sum_{v \in V} d_v}{n} = \frac{2\,m}{n} \leq \frac{2(2n-4)}{n} < 4$$

and from (5.10) we obtain $T(G) < 4^n$.

If the smallest face cycle is 5, each face is bounded by 5 or more edges, hence $5f \leq 2m$, and by Euler's Formula, we have $m \leq 5/3n - 10/3$. Then, the average degree is

$$\frac{\sum_{v \in V} d_v}{n} = \frac{2\,m}{n} \leq \frac{2(5/3n - 10/3)}{n} < 3.\bar{3}$$

and from (5.10) we have $T(G) < 3.\bar{3}^n$.

We have also improved these two upper bounds by removing maximum matchings, not on G, but on the dual graph G^*, because it gives better bounds. The dual graph G^* is also 3-connected, and by Lemma 5.3 it satisfies $T(G) = T(G^*)$.

If G has smallest face cycle at least 4, then $\delta(G^*) \geq 4$ and, by Theorem 5.8, G^* has a maximum matching of size at least $\left\lceil \frac{3f+8}{7} \right\rceil$. In case G has smallest face cycle 5, then $\delta(G^*) = 5$ and G^* has a maximum matching of size at least $\left\lceil \frac{9f+20}{19} \right\rceil$.

These two special cases are not so simple as the general case, where we know that the largest number of spanning trees is given by triangulated graphs. For graphs with smallest face cycle 4 or 5, the largest number of spanning trees could be given by a graph with faces of different length, hence the vertices of the dual graph may have different degrees. We have modelled the situation by a linear program, whose variables are the number of matched edges between vertices of given degrees, and the number of unmatched vertices of given degrees. As linear constraints we have taken the size of a maximum matching, the Handshaking Lemma, the bounds on the number of vertices of G^*, and the fact that the sum of number of matched and unmatched vertices equals the number of vertices of G^*.

The obtained results are, if G has smallest face cycle 4,

$$T(G) \leq \left((4 \cdot 4 - 1)^{\frac{3}{7}} 4^{\frac{1}{7}}\right)^f < 3.890879^n.$$

In case G has smallest face cycle 5,

$$T(G) \leq \left((5 \cdot 5 - 1)^{\frac{9}{19}} 5^{\frac{1}{19}}\right)^f < 2.886566^n.$$

We have not tried to improve the bounds on the minimum size of a maximum matching of G^* for our concrete cases, since the mentioned results are not too far from the best bound we could obtain by this method in the optimal case: if we would have a perfect matching, by resetting the constraints, the solution of the linear problem would be $T(G) < 3.872984$ for graphs with smallest face cycle 4, and $T(G) < 2.884410$ for graphs with smallest face cycle 5. We obtain stronger bounds in the next section with a different technique.

One could improve the bound of Lemma 5.5 by excluding larger cycles, like 3-cycles, 4-cycles, etc. For example, any independent triangle $x_1x_2x_3$ would contribute to the product of Lemma 5.4 with a factor of

$$d(x_1)d(x_2)d(x_3) - 2 - d(x_1) - d(x_2) - d(x_3)$$

instead of $d(x_1)d(x_2)d(x_3)$. We subtract 2 from $d(x_1)d(x_2)d(x_3)$ since it corresponds to both directed 3-cycles along the triangle, and we subtract $d(x_i)$ since it corresponds to the case when we have a 2-cycle between x_j and x_k and the outgoing edge of x_i can be any edge, $i, j, k = 1, 2, 3$.

5.3.3 A Probabilistic Model. Suen's Inequality

As an application, in Chapter 6 we lift the graph G to a polytope. Therefore we assume the graph G to be 3-connected.

Consider the selection of edges $\mathcal{R}$ described in the proof of Lemma 5.4: choose a root vertex r, and treat G as a directed graph where every edge has two possible directions, with the exception that the root has only ingoing edges. We view at this selection as a random selection, obtained with the random process consisting in selecting at random one outgoing edge to each vertex different than r. Within this process, we obtain all spanning trees exactly once.

Such a random selection of outgoing edges forms a tree if and only if it does not contain a cycle. Hence we can write

$$\begin{aligned} T(G) &= \prod_{v \in V \setminus \{r\}} d_v \cdot \text{Prob}\,(\text{a random selection } \mathcal{R} \text{ of outgoing edges forms a tree}) \\ &= \prod_{v \in V \setminus \{r\}} d_v \cdot \text{Prob}\,(\text{a random selection } \mathcal{R} \text{ of outgoing edges does not form a cycle}), \end{aligned} \tag{5.12}$$

where the random selection of outgoing edges is for all vertices except for the root. The goal is then to exclude cyclic selections. Given a random selection $\mathcal{R}$, the existence of different cycles in $\mathcal{R}$ are not independent events but also not very dependent.

We improve the results of Section 5.3.2 by using Suen's inequality. Suen's inequality uses the concept of a dependency graph. Let $\{X_i\}_{i \in \mathcal{I}}$ be a family of random variables, defined on a common probability space. A *dependency graph* for $\{X_i\}$ is a graph L with vertex set $\mathcal{I}$ such that if A and B are two disjoint subsets of $\mathcal{I}$ with no edge in L between a vertex of A and a vertex of B, then the families $\{X_i\}_{i \in A}$ and $\{X_i\}_{i \in B}$ are mutually independent. In particular, two variables X_i and X_j are independent unless there is an edge in L between i and j. If there exists such an edge, we write $i \sim j$. Suen's inequality is useful in cases in which there exists a sparse dependency graph. The expected value of a random variable X is denoted by $\mathbb{E}X$. The following theorem is a special case of Suen's inequality [31]:

Theorem 5.9. *Let I_i, $i \in \mathcal{I}$, be a finite family of Bernoulli random variables with success probability p_i, having a dependency graph L. Let $X = \sum_i I_i$ and $\lambda = \mathbb{E}X = \sum_i p_i$. Moreover, let $\Delta = \frac{1}{2} \sum_i \sum_{j: i \sim j} \mathbb{E}(I_i I_j)$ and $\zeta = \max_i \sum_{k \sim i} p_k$. Then*

$$\text{Prob}\,(X = 0) \leq \exp\,(-\lambda + \Delta e^{2\zeta}).$$

Let $\mathcal{R}$ be a random selection of outgoing edges for all vertices except for the root r. Let $\mathcal{D}$ denote the set of all directed cycles in the graph obtained from G by replacing every edge by two directed arcs except for the root, which has only ingoing edges. Note that a cycle of $\mathcal{D}$ cannot contain the root r. In other words, $\mathcal{D}$ is the set of all directed cycles c that could appear in $\mathcal{R}$.

In our model, the indicator variables I_c correspond to the existence of the directed cycle c, for all $c \in \mathcal{D}$. I_c is 1 if the cycle c appears in $\mathcal{R}$, 0 otherwise. A directed cycle $c \in \mathcal{D}$ appears in $\mathcal{R}$ when all its arcs are present in $\mathcal{R}$, and the presence in $\mathcal{R}$ of the different arcs of c are independent events. An arc from a vertex v to the successor vertex on a particular directed cycle is present in $\mathcal{R}$ with probability $1/d_v$. Hence, if c is a directed cycle of G not containing the root, I_c is a Bernoulli variable taking the value 1 with probability $p_c = \left(\prod_{v \in c} d_v\right)^{-1}$. The random variable $X = \sum_{c \in \mathcal{D}} I_c$ counts the number of directed cycles in $\mathcal{R}$, and $\text{Prob}\,(X = 0)$ measures the probability that no cycle exists in $\mathcal{R}$, i. e., that $\mathcal{R}$ forms a spanning tree. We want an upper bound for $\text{Prob}\,(X = 0)$.

The vertices of the dependency graph are all directed cycles c in $\mathcal{D}$. Note that two directed cycles c_i and c_j in $\mathcal{R}$ never share a vertex, because every vertex different from the root has exactly one outgoing edge in $\mathcal{R}$. Hence, in the dependency graph, we connect two directed cycles c_i and c_j by an edge ($c_i \sim c_j$) if they share some vertex: if c_i and c_j share at least one vertex, the existence of c_i and the existence of c_j in $\mathcal{R}$ are incompatible events, so they are dependent events; conversely, if $c_i \sim c_j$, then they are non-disjoint cycles.

Thus, $i \sim j$ implies that $\mathbb{E}(I_i I_j) = 0$, which means that $\Delta = 0$ in Theorem 5.9. Therefore we have

$$\operatorname{Prob}(X = 0) \leq \exp(-\lambda_{\mathcal{R}}), \tag{5.13}$$

where $\lambda_{\mathcal{R}}$ is the sum of probabilities p_c for all directed cycles c that can appear in $\mathcal{R}$, that is

$$\begin{aligned} \lambda_{\mathcal{R}} = \sum_{c \in \mathcal{D}} p_c &= \sum_{c \in \mathcal{D}} \frac{1}{\prod_{v \in c} d_v} \\ &= \sum_{(i,j) \in \mathcal{C}_2} \frac{1}{d_i d_j} + \sum_{(i,j,k) \in \mathcal{C}_3} \frac{2}{d_i d_j d_k} + \sum_{(i,j,k,l) \in \mathcal{C}_4} \frac{2}{d_i d_j d_k d_l} + \dots \end{aligned} \tag{5.14}$$

where $\mathcal{C}_l$ denotes the set of all undirected cycles of length l in G, not containing the root. We have a 2 in the numerators for the cycles of length at least 3 since every cycle must be counted twice, one in each orientation (remember we consider directed cycles).

Our task is to obtain lower bounds for $\lambda_{\mathcal{R}}$, but the value of $\lambda_{\mathcal{R}}$ depends on the graph G.

From (5.12) and (5.13) we have

$$T(G) \leq \prod_{v \in V \setminus \{r\}} d_v \exp(-\lambda_{\mathcal{R}}).$$

We reduce the sum (5.14) to be finite by cutting it at a given length l, that is, considering only short cycles. Let $\lambda_{\mathcal{R}}^{(l)}$ denote this finite sum. Obviously we still have a bound for $T(G)$:

$$T(G) \leq \prod_{v \in V \setminus \{r\}} d_v \exp(-\lambda_{\mathcal{R}}^{(l)}). \tag{5.15}$$

To make it simpler we consider a slightly different model, where every vertex has an outgoing edge, including the root. Let $\mathcal{R}'$ such a random selection of outgoing edges. Note that in this model a cycle always appears in $\mathcal{R}'$. $\lambda_{\mathcal{R}'}$ is the sum of probabilities for all directed cycles that can appear in $\mathcal{R}'$, that is

$$\lambda_{\mathcal{R}'} = \sum_{(i,j) \in E} \frac{1}{d_i d_j} + \sum_{(i,j,k) \in \mathcal{C}'_3} \frac{2}{d_i d_j d_k} + \sum_{(i,j,k,l) \in \mathcal{C}'_4} \frac{2}{d_i d_j d_k d_l} + \dots$$

In the expression above, $\mathcal{C}'_l$ denotes the set of all undirected cycles of length l in G (also those including the root). Note that

$$\mathcal{C}'_l = \mathcal{C}_l \cup \{c \in \mathcal{C}'_l : r \in c\}.$$

As before, denote by $\lambda_{\mathcal{R}'}^{(l)}$ the finite sum obtained from cutting $\lambda_{\mathcal{R}'}$ at a given length l.

Considering 2-Cycles. Consider the amount

$$\prod_{v \in V} d_v \exp\left(-\lambda_{\mathcal{R}'}^{(2)}\right). \tag{5.16}$$

Let Z_2 be the logarithm of (5.16), that is

$$Z_2 := \sum_{v \in V} \ln d_v - \sum_{(i,j)\in E} \frac{1}{d_i d_j}\,.$$

The random process where every vertex has an outgoing edge is simpler to analyze than the original one where the root is only allowed to have ingoing edges. The following lemma and corollary show that actually we can work with the selection $\mathcal{R}'$ for upper bounding $T(G)$.

Lemma 5.6. *Let* $Z_2 = \sum_{v\in V} \ln d_v - \sum_{(i,j)\in E} \frac{1}{d_i d_j}$*, and let* r *be an arbitrarily chosen root vertex. Then*

$$T(G) \le \exp\left(Z_2 + K_2\right),$$

where

$$K_2 := -\ln d_r + \sum_{(r,i)\in E} \frac{1}{d_r d_i}$$

is a correction term.

Proof. We have

$$\sum_{(i,j)\in \mathcal{C}_2} \frac{1}{d_i d_j} = \sum_{(i,j)\in E} \frac{1}{d_i d_j} - \sum_{(r,i)\in E} \frac{1}{d_r d_i} \tag{5.17}$$

Hence, from (5.15) and (5.17) we have

$$\begin{aligned} T(G) &\le \exp\left(\sum_{v\in V\setminus\{r\}} \ln d_v - \lambda_{\mathcal{R}}^{(2)}\right) = \exp\left(\sum_{v\in V\setminus\{r\}} \ln d_v - \sum_{(i,j)\in \mathcal{C}_2} \frac{1}{d_i d_j}\right) \\ &= \exp\left(\sum_{v\in V\setminus\{r\}} \ln d_v - \sum_{(i,j)\in E} \frac{1}{d_i d_j} + \sum_{(r,i)\in E} \frac{1}{d_r d_i}\right) \\ &= \exp\left(Z_2 - \ln d_r + \sum_{(r,i)\in E} \frac{1}{d_r d_i}\right). \end{aligned}$$

and the lemma is proven. ☐

Corollary 5.5.

$$T(G) < \exp\left(Z_2\right).$$

Proof. Since $\delta(G)$ is at least 3 because G is 3-connected, and there are d_r edges of the form (r,i), we have

$$\sum_{(r,i)\in E} \frac{1}{d_r d_i} = \frac{1}{d_r} \sum_{(r,i)\in E} \frac{1}{d_i} \le \frac{1}{d_r} \cdot d_r \cdot \frac{1}{3} = \frac{1}{3}\,. \tag{5.18}$$

Also we have $d_r \ge 3$, hence

$$K_2 = -\ln d_r + \sum_{(r,i)\in E} \frac{1}{d_r d_i} \le -\ln 3 + \frac{1}{3} < 0\,,$$

and the corollary follows. ☐

Considering 3-Cycles.

Lemma 5.7. *Let*

$$Z_3 := \sum_{v\in V} \ln d_v - \sum_{(i,j)\in E} \frac{1}{d_i d_j} - \sum_{(i,j,k)\in \mathcal{C}_3'} \frac{2}{d_i d_j d_k},$$

and let r *be an arbitrarily chosen root vertex. Then*

$$T(G) \leq \exp\left(Z_3 + K_3\right),$$

where

$$K_3 := -\ln d_r + \sum_{(r,i)\in E} \frac{1}{d_r d_i} + \sum_{(r,i,j)\in \mathcal{C}_3'} \frac{2}{d_r d_i d_j}$$

is a correction term.

Proof. We have

$$\sum_{(i,j,k)\in \mathcal{C}_3} \frac{1}{d_i d_j d_k} = \sum_{(i,j,k)\in \mathcal{C}_3'} \frac{1}{d_i d_j d_k} - \sum_{(r,i,j)\in \mathcal{C}_3'} \frac{1}{d_r d_i d_j} \tag{5.19}$$

From (5.15), (5.17) and (5.19) we have

$$\begin{aligned}
T(G) \leq \exp\left(\sum_{v\in V\setminus\{r\}} \ln d_v - \lambda_{\mathcal{R}}^{(3)}\right) &= \exp\left(\sum_{v\in V\setminus\{r\}} \ln d_v - \sum_{(i,j)\in \mathcal{C}_2} \frac{1}{d_i d_j} - \sum_{(i,j,k)\in \mathcal{C}_3} \frac{2}{d_i d_j d_k}\right) \\
&= \exp\left(\sum_{v\in V\setminus\{r\}} \ln d_v - \sum_{(i,j)\in E} \frac{1}{d_i d_j} + \sum_{(r,i)\in E} \frac{1}{d_r d_i} - \sum_{(i,j,k)\in \mathcal{C}_3'} \frac{2}{d_i d_j d_k} + \sum_{(r,i,j)\in \mathcal{C}_3'} \frac{2}{d_r d_i d_j}\right) \\
&= \exp\left(Z_3 - \ln d_r + \sum_{(r,i)\in E} \frac{1}{d_r d_i} + \sum_{(r,i,j)\in \mathcal{C}_3'} \frac{2}{d_r d_i d_j}\right).
\end{aligned}$$

□

Corollary 5.6.

$$T(G) < \exp\left(Z_3\right).$$

Proof. Let N be the subgraph of G spanned by the vertices adjacent to r. The subset of $\mathcal{C}_3'$ of 3-cycles containing the root has the same cardinality as the set of edges of N, which is at most $3d_r - 6 < 3d_r$, since N is a planar graph with d_r vertices. Then we have

$$\sum_{(r,i,j)\in \mathcal{C}_3'} \frac{2}{d_r d_i d_j} = \frac{2}{d_r} \sum_{(r,i,j)\in \mathcal{C}_3'} \frac{1}{d_i d_j} < \frac{2}{d_r} \cdot 3d_r \cdot \frac{1}{9} = \frac{2}{3}$$

We used that $\delta(G)$ is at least 3 since G is 3-connected. Also we have $d_r \geq 3$, and (5.18) is satisfied, hence

$$K_3 = -\ln d_r + \sum_{(r,i)\in E} \frac{1}{d_r d_i} + \sum_{(r,i,j)\in \mathcal{C}_3'} \frac{2}{d_r d_i d_j} < -\ln 3 + \frac{1}{3} + \frac{2}{3} < 0,$$

and the corollary follows. □

Considering Larger Cycles. For larger cycles, the correction term K is derived from a similar lemma:

Lemma 5.8. *Let*

$$Z_l := \sum_{v \in V} \ln d_v - \sum_{(i,j) \in E} \frac{1}{d_i d_j} - \sum_{(i,j,k) \in \mathcal{C}'_3} \frac{2}{d_i d_j d_k} - \cdots - \sum_{C \in \mathcal{C}'_l} \frac{2}{\prod_{i \in C} d_i},$$

and let r be an arbitrarily chosen root vertex. Then

$$T(G) \leq \exp\left(Z_l + K_l\right),$$

where

$$K_l := -\ln d_r + \sum_{(r,i) \in E} \frac{1}{d_r d_i} + \sum_{(r,i,j) \in \mathcal{C}'_3} \frac{2}{d_r d_i d_j} + \cdots + \sum_{C \in \mathcal{C}'_l : r \in C} \frac{2}{\prod_{i \in C} d_i}$$

is a correction term.

The proof is analogous to Lemma 5.6 and Lemma 5.7.

A. The Outgoing Edge Method with Suen's Inequality for 3-Connected Planar Graphs

Considering 2-Cycles. Our goal is to maximize Z_2. Let f_{ij}, with $i \leq j$, be the number of edges connecting a vertex of degree i and a vertex of degree j. We want to write

$$Z_2 = \sum_{v \in V} \ln d_v - \sum_{(i,j) \in E} \frac{1}{d_i d_j}$$

as a linear function in the variables f_{ij}, and to maximize this linear function under some constraints.

The degree of a vertex is at least 3 because the graph G is 3-connected and at most $n-1$. We have $3 \leq i, j \leq n$. (For simplicity, we write a relaxed program: we write n instead of $n-1$ and we solve the system for more variables, which will be zero in the solution).

Then, $2f_{ii} + \sum_{j=i+1}^{n} f_{ij}$ equals the total number of edges incident to vertices of degree i, and hence

$$2f_{ii} + \sum_{\substack{j=3 \\ j \neq i}}^{n} f_{ij} = i\, n_i, \qquad i = 3 \ldots n,$$

where n_i denotes the number of vertices of G of degree i. Therefore

$$n = \sum_{i=3}^{n} n_i = \sum_{i=3}^{n} \frac{2f_{ii} + \sum_{\substack{j=3 \\ j \neq i}}^{n} f_{ij}}{i} = \sum_{3 \leq i \leq j \leq n} f_{ij} \left(\frac{1}{i} + \frac{1}{j}\right). \tag{5.20}$$

In a planar graph, each face is bounded by at least 3 edges. Thus, the total number of edge-face pairs is at least $3f$, that is, $3f \leq 2m$, and by Euler's formula, the number of edges is at most $3n-6$. Therefore

$$\sum_{3 \leq i \leq j \leq n} f_{ij} \leq 3n - 6. \tag{5.21}$$

We can rewrite Z_2 as a linear function in terms of f_{ij} as

$$\begin{aligned}
Z_2 &= \sum_{v \in V} \ln d_v - \sum_{\{v_1,v_2\} \in E} \frac{1}{d_1 d_2} \\
&= \sum_{i=3}^{n} \ln(i)\, n_i - \sum_{3 \le i \le j \le n} f_{ij}\, \frac{1}{ij} \\
&= \sum_{i=3}^{n} \ln i\, \frac{2f_{ii} + \sum_{\substack{j=3 \\ j \ne i}}^{n} f_{ij}}{i} - \sum_{3 \le i \le j \le n} f_{ij}\, \frac{1}{ij} \\
&= \sum_{3 \le i \le j \le n} f_{ij} \left(\frac{\ln i}{i} + \frac{\ln j}{j} - \frac{1}{ij} \right). \qquad (5.22)
\end{aligned}$$

From (5.20), (5.21), (5.22) and the fact that the numbers f_{ij} are non-negative, we write the following linear program:

$$\begin{aligned}
\text{maximize} \quad & Z_2 = \sum_{3 \le i \le j \le n} f_{ij} \left(\frac{\ln i}{i} + \frac{\ln j}{j} - \frac{1}{ij} \right) \\
\text{subject to} \quad & \sum_{3 \le i \le j \le n} f_{ij} \left(\frac{1}{i} + \frac{1}{j} \right) = n \\
& \sum_{3 \le i \le j \le n} f_{ij} \le 3n - 6 \\
& f_{ij} \ge 0, \quad \text{for } i, j = 3 \dots n,\ i \le j
\end{aligned} \qquad (P_2)$$

For uniformity we replace (5.21) by a weaker constraint

$$\sum_{3 \le i \le j \le n} f_{ij} \le 3n\,, \qquad (5.23)$$

obtaining a new linear program:

$$\begin{aligned}
\text{maximize} \quad & Z_2 = \sum_{3 \le i \le j \le n} f_{ij} \left(\frac{\ln i}{i} + \frac{\ln j}{j} - \frac{1}{ij} \right) \\
\text{subject to} \quad & \sum_{3 \le i \le j \le n} f_{ij} \left(\frac{1}{i} + \frac{1}{j} \right) = n \\
& \sum_{3 \le i \le j \le n} f_{ij} \le 3n \\
& f_{ij} \ge 0, \quad \text{for } i, j = 3 \dots n,\ i \le j
\end{aligned} \qquad (P_2')$$

Let Z_2^* be the optimum value which maximizes the objective function Z_2 under the constraints given in (P_2').

We solved this linear program using the commercial linear programming solver CPLEX with AMPL as a modeling interface. AMPL is a modeling language for large-scale optimization and mathematical programming problems [27].

For several values of the parameter n up to 5000, we obtained $Z_2^* = 1.708427$, which means $\exp(Z_2^*/n) = 5.520267$ (these values are rounded up). The optimum Z_2^* is achieved when

$$f_{66} = 3n \text{ and } f_{ij} = 0, \text{ for all } ij \neq 66.$$

This is true not only for the values of n checked empirically, but for any n, as it is stated in the following lemma.

Lemma 5.9. *The linear program (P_2') has the optimum value*

$$Z_2^* = \left(\ln 6 - \frac{1}{12}\right) n\,.$$

Proof. The solution $\{f_{66} = 3n,\ f_{ij} = 0 \text{ for all } ij \neq 66\}$ given above is feasible for the modified program (P_2') because it satisfies the constraints. This solution yields precisely the value of the objective function

$$3n\left(\frac{\ln 6}{6} + \frac{\ln 6}{6} - \frac{1}{36}\right) = \left(\ln 6 - \frac{1}{12}\right) n\,.$$

To see that this is the optimum solution, we form a linear combination of the constraints (5.20) and (5.23), with positive factors λ_1 and λ_2:

$$\lambda_1\left(\sum_{3\le i\le j\le n} f_{ij}\left(\frac{1}{i}+\frac{1}{j}\right) - n\right) + \lambda_2\left(\sum_{3\le i\le j\le n} f_{ij} - 3n\right) \le 0\,,$$

where λ_1 and λ_2 are obtained as the optimal dual variables associated to these constraints. This implies

$$\sum_{3\le i\le j\le n} f_{ij}\left(\lambda_1\left(\frac{1}{i}+\frac{1}{j}\right) + \lambda_2\right) \le n\,(\lambda_1 + 3\lambda_2)\,. \tag{5.24}$$

For proving that the objective function in (P_2') is upper bounded by $n\,(\lambda_1 + 3\lambda_2)$, we must prove that the coefficient of f_{ij} in the objective function is upper bounded by the coefficient of f_{ij} on the left side of (5.24). This is, we must prove

$$\frac{\ln i}{i} + \frac{\ln j}{j} - \frac{1}{ij} \le \lambda_1\left(\frac{1}{i}+\frac{1}{j}\right) + \lambda_2, \qquad 3 \le i \le j \le n,$$

or, equivalently, that the function

$$g(i,j) = \frac{\ln i - \lambda_1}{i} + \frac{\ln j - \lambda_1}{j} - \frac{1}{ij} - \lambda_2$$

is negative or zero, for all integers i, j such that $3 \le i \le j \le n$.

Let $\lambda_1 = 0.53$, and let $\lambda_2 \approx 0.392808$ be determined by the equation $g(6,6) = 0$. The equation $g(6,6) = 0$ is obtained by complementary slackness, since $f_{66} \neq 0$ in the (proposed) optimal solution.

For the rest of the values $ij \neq 66$, we prove $g(i,j) < 0$. For the values $i, j \ge 6$, we show that $g(i,j)$ is a monotone decreasing function for growing i and j, by proving that the partial derivatives $\partial g(i,j)/\partial i$ and $\partial g(i,j)/\partial j$ are negative. We have

$$\frac{\partial g(i,j)}{\partial i} = \frac{1}{i^2} - \frac{\ln i - \lambda_1}{i^2} + \frac{1}{i^2 j}\,.$$

Since $i > 0$, $\partial g(i,j)/\partial i < 0$ if and only if $1 - \ln i + \lambda_1 + \frac{1}{j} < 0$, which is true for any $i, j \geq 6$. Analogously, we can prove that $\partial g(i,j)/\partial j < 0$. Hence, for $i, j \geq 6$ we have $g(i,j) < 0$.

For i between 3 and 5, we fix i and look for the smallest integer value of j for which the function is monotone decreasing in j, or equivalently, the smallest integer value of j for which the partial derivative $\partial g(i,j)/\partial j$ is negative. For $i = 3$, $g(i,j)$ is monotone decreasing for $j \geq 7$. For $i = 4$ and $i = 5$, $g(i,j)$ is monotone decreasing for $j \geq 6$. For the remaining values of i, j, that is, for ij equal to 33, 34, 35, 36, 37, 44, 45, 46, 55, 56, the inequality $g(i,j) < 0$ can be checked directly. This implies that $g(3,j)$ is negative for $j > 7$, and that $g(4,j)$, $g(5,j)$ are negative for $j > 6$.

This proves that the objective function is upper bounded by $Z_2^* = n(\lambda_1 + 3\lambda_2)$, and, substituting the given values of λ_1 and λ_2, we have $\lambda_1 + 3\lambda_2 = \ln 6 - 1/12$. □

Since the constraints of the linear program (P_2') are weaker than the constraints of the original program (P_2), the optimum value given by Lemma 5.9 is an upper bound for the optimum value of (P_2):

Corollary 5.7. *The optimum value of the linear program (P_2) is upper bounded by*

$$Z_2^* = \left(\ln 6 - \frac{1}{12}\right) n \,.$$

Hence we conclude with the following proposition.

Proposition 5.2. *For any 3-connected planar graph G, the Outgoing Edge approach gives an upper bound of*

$$T(G) < 5.520267^n.$$

Proof. By Corollary 5.5 and Corollary 5.7, we have

$$T(G) < \left[\exp\left(\frac{Z_2^*}{n}\right)\right]^n = \left[\exp\left(\ln 6 - \frac{1}{12}\right)\right]^n < 5.520267^n.$$

□

Remark 5.1. *There is no planar graph with $f_{66} = 3n$. However, such a graph can be embedded on the torus. In fact, the situation where all vertices have degree 6 holds for the triangular grid $\{\hat{C}_{W\times k}\}_{k\geq 0}$ with periodic boundary conditions considered in Section 5.2.5, for which we obtained the maximum number of spanning trees. It has been shown in Theorem 5.3 that the difference between graphs embedded on the torus and planar graphs does not make a difference in the asymptotic growth factor for the number of spanning trees, at least for recursively constructible families of graphs.*

We did further numerical experiments. The obtained results are not proved but they are only established empirically.

Empirical Results: Considering 3-Faces. We consider now 2-cycles and 3-faces. Let $\mathcal{F}_3$ be the set of 3-face cycles of G. The number of 3-cycles of a graph is at least the number of 3-face cycles since $\mathcal{F}_3 \subset \mathcal{C}_3'$, hence we obtain a more relaxed upper bound.

Let f_{ijk}, with $i \leq j \leq k$, be the number of 3-faces constituted by a vertex of degree i, a vertex of degree j and a vertex of degree k. Here we have $3 \leq i \leq j \leq k \leq n$.

Let Z_{F3} be the upper bound of Z_3 in terms of 3-faces:

$$\begin{aligned} Z_3 &\le \sum_{v\in V} \ln d_v - \sum_{(i,j)\in E} \frac{1}{d_i d_j} - \sum_{(i,j,k)\in \mathcal{F}_3} \frac{2}{d_i d_j d_k} \\ &= Z_{F3} \end{aligned}$$

We want to write Z_{F3} as a linear function in the variables f_{ij} and f_{ijk}, and to maximize this linear function under some constraints. The term of Z_{F3} corresponding to 3-faces can be rewritten as a linear function of f_{ijk} as

$$\sum_{3\le i\le j\le k\le n} f_{ijk}\,\frac{2}{ijk}\,, \tag{5.25}$$

and, from (5.22) and (5.25), we have

$$Z_{F3} = \sum_{3\le i\le j\le n} f_{ij}\left(\frac{\ln i}{i} + \frac{\ln j}{j} - \frac{1}{ij}\right) - \sum_{3\le i\le j\le k\le n} f_{ijk}\,\frac{2}{ijk}\,. \tag{5.26}$$

We establish a condition linking triangles and edges. If f_{ijk} is the number of triangular faces, this condition is that f_{ijk} contributes 1/2 to f_{ij}, 1/2 to f_{ik}, and 1/2 to f_{jk}. This must be corrected for $i = j$ and $j = k$, and we obtain

$$2f_{ij} = \sum_{k=1}^{i-1} f_{kij} + \sum_{k=i}^{j} f_{ikj} + \sum_{k=j+1}^{n} f_{ijk} \; + f_{iij} + f_{ijj}\,, \qquad 3 \le i \le j \le n. \tag{5.27}$$

Note that if $i < j$ we are counting f_{iij} and f_{ijj} twice each, and once the f_{kij}, f_{ikj} or f_{ijk} with $k \ne i, j$; and in case $i = j$, we are counting three times f_{iii} and once the f_{kii} or f_{iik} with $k \ne i$.

From (5.20), (5.21), (5.26), (5.27) and the non-negativity of the numbers f_{ijk}, we have the following linear program:

$$\begin{aligned}
\text{maximize}\quad & Z_{F3} = \sum_{3\le i\le j\le n} f_{ij}\left(\frac{\ln i}{i} + \frac{\ln j}{j} - \frac{1}{ij}\right) - \sum_{3\le i\le j\le k\le n} f_{ijk}\,\frac{2}{ijk} \\
\text{subject to}\quad & \sum_{3\le i\le j\le n} f_{ij}\left(\frac{1}{i} + \frac{1}{j}\right) = n \\
& \sum_{3\le i\le j\le n} f_{ij} = 3n-6 \\
& 2f_{ij} = \sum_{k=1}^{i-1} f_{kij} + \sum_{k=i}^{j} f_{ikj} + \sum_{k=j+1}^{n} f_{ijk} \; + f_{iij} + f_{ijj}, \quad \text{for } i,j = 3\ldots n,\ i\le j \\
& f_{ij},\ f_{ijk} \ge 0, \quad \text{for } i,j,k = 3\ldots n,\ i\le j\le k
\end{aligned} \tag{P_3}$$

As before, for uniformity we replace (5.21) by the weaker constraint (5.23), that is

$$\sum_{3\le i\le j\le n} f_{ij} \le 3n\,,$$

obtaining a new linear program (P_3').

Let Z^*_{F3} be the optimum value which maximizes the objective function Z_{F3} under the constraints given in (P_3'). Solving (P_3') with AMPL for values of the parameter n up to 300, we obtain

$$Z^*_{F3} = \left(\ln 6 - \frac{11}{108}\right) n \,. \tag{5.28}$$

With AMPL, and writing $3n$ instead of $3n-6$, the optimum is achieved when

$$f_{66} = 3n,\ f_{ij} = 0 \ \text{ for all } ij \neq 66,\ f_{666} = 2n, \ \text{ and } f_{ijk} = 0 \text{ for all } ijk \neq 666,$$

which corresponds to the case where all edges have degree 6. This means that, if this result were true for every n, the optimum would be achieved when G is almost a graph of the family of triangular grid graphs with periodic boundary conditions. See the discussion in Remark 5.1. This is consistent with the hypothesis that the family of triangular grid graphs with periodic boundary conditions yields the largest number of spanning trees. Note that in this family all 3-cycles are 3-faces.

Since the constraints of the linear program (P_3') are weaker than the constraints of the original program (P_3), the optimum value given by (5.28) is an upper bound for the optimum value of (P_3). By Corollary 5.6, we have

$$T(G) < \left[\exp\left(\frac{Z^*_{F3}}{n}\right)\right]^n = \left[\exp\left(\ln 6 - \frac{11}{108}\right)\right]^n < 5.418981^n \tag{5.29}$$

The bound (5.29) is still far from the upper bound given by Theorem 5.7.

Considering Larger Cycles. For $l > 4$ it is very tricky to write the linear constraints that relate the number of l-cycles constituted by vertices of given degrees with the number of edges.

However, we think that it is not worth to continue working in this direction: Everything seems to indicate that the graphs that are similar to the 6-regular family $\{\hat{C}_{W\times k}\}_{k\geq 0}$ give the maximum number of spanning trees over all planar graphs. In the remainder of this section we explore heuristically the bounds that Suen's inequality would give, under the hypothesis that the triangular grid is the optimal graph. In line with Remark 5.1, we consider the 6-regular triangular grid that is embedded on the torus.

Consider a graph of this family with n vertices, and let us compute $|C_l|$, the number of cycles of length l, for some more values of l. $|C_2|$ and $|C_3|$ equal respectively to the number of edges and faces. The 4-cycles are the boundary of pairs of adjacent triangles. Hence there are as many 4-cycles as edges, that is, $|C_4| = 3n$. The 5-cycles are the boundary of triplets of adjacent triangles meeting at a vertex (see Figure 5.11). For each vertex there are 6 of these triplets, one for each possible orientation, thus $|C_5| = 6n$. The 6-cycles are hexagons (there are n hexagons, one centered at each vertex), or boundaries of groups of four triangles distributed as illustrated in Figure 5.12. Hence one can see that $|C_6| = n + 6n + 6n + 2n$. The 7-cycles are boundaries of groups of five or seven triangles distributed as illustrated in Figure 5.13. Hence, $|C_7| = 6n + 6n + 6n + 24n$.

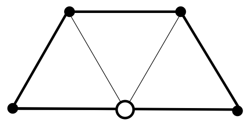

Figure 5.11: 5-cycle as the boundary of triplets of adjacent triangles meeting at the white vertex. For each vertex, there are 6 different such 5-cycles, one for each possible orientation.

Summarizing, we have

$$\begin{aligned} |C_2| &= f_{66} = 3n \\ |C_3| &= f_{666} = 2n \\ |C_4| &= 3n \\ |C_5| &= 6n \\ |C_6| &= 15n \\ |C_7| &= 42n \end{aligned}$$

If we plug these values into Lemma 5.8, we obtain

$$T(G) \leq 6^n \exp\left(-\frac{3n}{6^2} - 2\left(\frac{2n}{6^3} + \frac{3n}{6^4} + \frac{6n}{6^5} + \frac{15n}{6^6} + \frac{42n}{6^7}\right) + K_7\right) < K \cdot 5.380556^n.$$

where $K = \exp(K_7)$ is a correction term.

We could not obtain a better bound than this if we would write down a linear program which considers l-cycles up to $l = 7$, and it is still quite far from the bound of $5.\bar{3}^n$ given in Theorem 5.7. Also, for larger l, the improvement is every time much smaller.

B. Suen's Inequality for 3-Connected Graphs with Smallest Face Cycle at Least 4

Let G be a 3-connected planar graph with smallest face cycle at least 4.

Considering 2-Cycles. If we only consider 2-cycles, we can write a linear program (P_2^4) analogous to (P_2), with the difference that now the graph has at most $2n - 4$ edges. Hence, instead of (5.21), we have the constraint

$$\sum_{3 \leq i \leq j \leq n} f_{ij} \leq 2n - 4. \tag{5.30}$$

For uniformity we replace (5.30) by a weaker constraint

$$\sum_{3 \leq i \leq j \leq n} f_{ij} \leq 2n\,, \tag{5.31}$$

obtaining a new linear program $(P_2^{4'})$.

For values of n up to 1000, we obtain with AMPL a rounded up value of $\exp(Z_2^{4^*}/n) = 3.529988$, where $Z_2^{4^*}$ is the optimum value of the linear program $(P_2^{4'})$. The optimum value $Z_2^{4^*}$ is achieved when

$$f_{44} = 2n, \quad \text{and } f_{ij} = 0 \quad \text{for all } ij \neq 44.$$

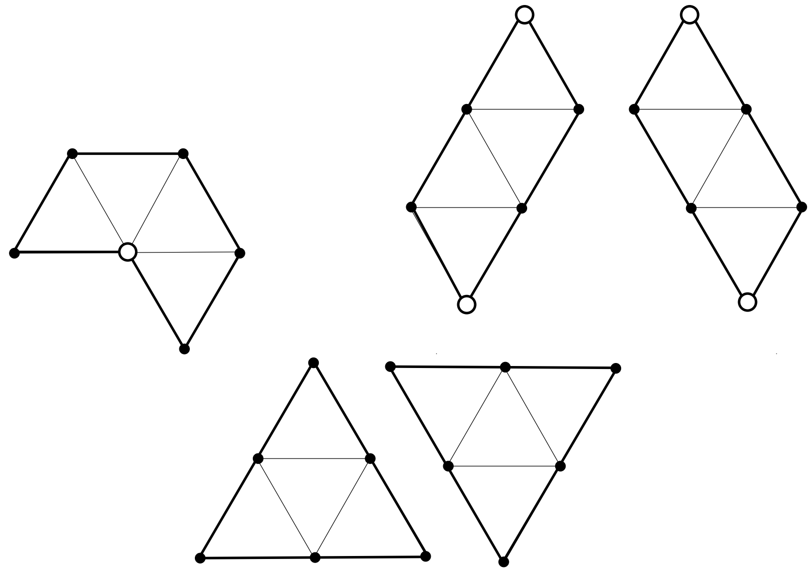

Figure 5.12: 6-cycles as the boundary of four triangles. Top left: The four triangles meet at the white vertex. For each vertex, there are 6 different such 6-cycles, one for each possible orientation. Top right: Four aligned triangles. For each vertex v, there are 12 possible such 6-cycles with extreme vertex v (2 for each triangle incident to v), but in total each 6-cycle is counted twice since it has two extreme vertices. (Extreme vertices are drawn white in the figure.) Hence the graph has $12n/2 = 6n$ 6-cycles of this kind. Bottom: The four triangles form a big equilateral triangle, and its boundary is the 6-cycle. Since each triangle of the graph is the central triangle of exactly one of this big triangles, there are in total $2n$ cycles of this kind (as many as triangles).

We formally prove this for every n.

Lemma 5.10. *The linear program* $(P_2^{4'})$ *has the optimum value*

$$Z_2^{4^*} = \left(\ln 4 - \frac{1}{8}\right) n\,.$$

Proof. The proof is analogous to the proof of Lemma 5.9.

The solution $\{f_{44} = 2n,\ f_{ij} = 0 \ \text{ for all } ij \neq 44\}$ given above is feasible for the modified program $(P_2^{4'})$ because it satisfies the constraints. This solution yields precisely the value of the objective function

$$2n\left(\frac{\ln 4}{4} + \frac{\ln 4}{4} - \frac{1}{16}\right) = \left(\ln 4 - \frac{1}{8}\right) n\,.$$

To see that this is the optimum solution we form a linear combination of the constraints (5.20) and (5.31), with factors λ_1 and λ_2:

$$\lambda_1\left(\sum_{3\le i\le j\le n} f_{ij}\left(\frac{1}{i}+\frac{1}{j}\right) - n\right) + \lambda_2\left(\sum_{3\le i\le j\le n} f_{ij} - 2n\right) \le 0\,,$$

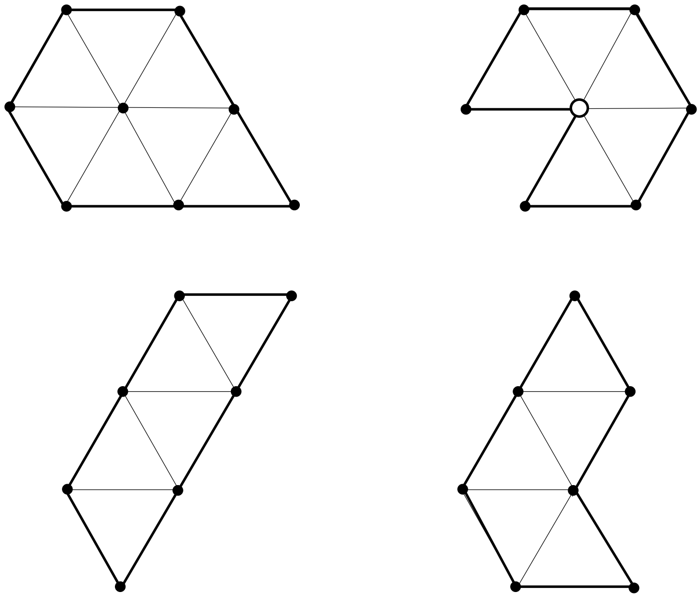

Figure 5.13: Top left: 7-cycles as the boundary of seven triangles, obtained by adding one triangle adjacent to one of the six sides of an hexagon. There are 6 ways to get it, and n hexagons, hence the number of such 7-cycles is $6n$. Top right: 7-cycles as the boundary of five triangles meeting at a vertex, drawn white. For each vertex, there are 6 possible such 7-cycles, one for each orientation. Bottom: 7-cycles as the boundary of five triangles, obtained from the group of four triangles in Figure 5.12 (top right), by adding one triangle adjacent to one of the six sides. We must take into account that if the triangle is added at the end as in the third picture, then it is counted twice in total. We have $6n$ and $4 \cdot 6n$ 7-cycles distributed as in the bottom first and second picture respectively.

where λ_1 and λ_2 are obtained as the optimal dual variables associated to these constraints.

As in Lemma 5.9 we must show that the function

$$g(i,j) = \frac{\ln i - \lambda_1}{i} + \frac{\ln j - \lambda_1}{j} - \frac{1}{ij} - \lambda_2$$

is negative or zero, for all integers i, j such that $3 \leq i \leq j \leq n$.

Since $f_{44} \neq 0$ in the (proposed) optimal solution, we obtain by complementary slackness the equation $g(4,4) = 0$. By taking $\lambda_1 = 0$ and $\lambda_2 \approx 0.630647$ determined by the equation $g(4,4) = 0$, we can prove that $g(i,j)$ is negative everywhere, except $g(4,4) = 0$. □

Since the constraints of the linear program $(P_2^{4\prime})$ are weaker than the constraints of the original program (P_2^4), we have:

Corollary 5.8. *The optimum value of the linear program (P_2^4) is upper bounded by Z_2^{4*}.*

Theorem 5.10. *For a 3-connected planar graph G with smallest face cycle at least 4, the*

Outgoing Edge approach gives an upper bound of

$$T(G) < \left[\exp\left(\ln 4 - \frac{1}{8}\right)\right]^n < 3.529988^n.$$

Proof. By Corollary 5.5 and Corollary 5.8, we have

$$T(G) < \left[\exp\left(\frac{Z_2^{4*}}{n}\right)\right]^n,$$

and substituting the value of $Z_2^{4^*}$ given in Lemma 5.10 we have the result. □

There is no planar graph with no triangles and $f_{44} = 2n$, but such a graph can be embedded on the torus. The situation where all vertices have degree 4 holds for the square grid with periodic boundary conditions considered in Section 5.2.6.

Recall that, by Theorem 5.6, the lower bound on the maximum number of spanning trees for graphs with smallest face cycle 4 is $3.209912^n \ldots$.

We carried out further more numerical experiments. The obtained results are not proved but they are only established empirically.

Empirical Results: Considering 4-Faces and 5-Faces. We can assume that G has only 4-faces and 5-faces: add edges to the original graph, keeping the smallest face cycle being 4. We can only add chords to the faces while not creating triangles. This can be done if we correctly add chords to the faces with at least 6 sides. For example, we can add a chord to a 6-face creating two 4-faces. If we keep on adding chords till we cannot continue, we get at the end a graph where all faces have length 4 or 5. When we add edges, the number of spanning trees grows, which is fine since we are searching upper bounds.

We consider now 2-cycles, 4-faces and 5-faces. Let $\mathcal{F}_4$ and $\mathcal{F}_5$ be the set of 4-face cycles and 5-face cycles of G respectively. Since the number of 4-face cycles (5-face cycles) of a graph is at least the number of 4-faces (5-faces), we obtain a more relaxed upper bound.

Let f_{ijkl} and f_{ijklm} be respectively the number of 4-faces and 5-faces constituted by vertices of degrees given by the indices $ijkl$ and $ijklm$ ($3 \leq i, j, k, l, m \leq n$). The indices $ijkl$ and $ijklm$ are always ordered according to their lexicographically minimum cyclic permutation. We write $\{ijkl\} \in \mathcal{F}_4$ and $\{ijklm\} \in \mathcal{F}_5$ when $ijkl$ or $ijklm$ constitute a 4-face cycle or a 5-face cycle with the indicated degrees, and the indices are correctly ordered.

We want to establish a condition linking edges and 4-faces and 5-faces, similar to the one for edges and triangles established in (5.27). If we only had 4-faces, we would have

$$\begin{aligned} 2f_{ij} &= \sum_{k,l} \left(f_{ijkl} + f_{kijl} + f_{klij} + f_{iklj} + f_{kjil} + f_{klji}\right), \qquad \text{if } i < j \\ 2f_{ii} &= \sum_{k,l} \left(f_{ijkl} + f_{kijl} + f_{klij} + f_{iklj}\right). \end{aligned}$$

In this equation, if $i < j$ we are counting 2 times f_{iijj}, f_{iiij}, f_{ijjj}, f_{ijik} and f_{ijkj}, where $k \neq i, j$, 4 times f_{ijij}, and once all other variables. If $i = j$ we are counting 4 times f_{iiii}, 2 times f_{iiik}, and once all other variables, which have the form f_{iikl}, with $k, l \neq i$. With this linking equation we are balancing how many times we count every edge with respect to its two incident faces. Actually these faces could be quadrilaterals or pentagons. Hence, the linking condition is indeed

$$
\begin{aligned}
2f_{ij} &= \sum_{k,l} \left(f_{ijkl} + f_{kijl} + f_{klij} + f_{iklj} + f_{kjil} + f_{klji}\right) \\
&\quad + \sum_{k,l,m} \left(f_{ijklm} + f_{kijlm} + f_{klijm} + f_{klmij} + f_{iklmj} + f_{kjilm} + f_{kljim} + f_{klmji}\right); \\
2f_{ii} &= \sum_{k,l} \left(f_{ijkl} + f_{kijl} + f_{klij} + f_{iklj}\right) \\
&\quad + \sum_{k,l,m} \left(f_{ijklm} + f_{kijlm} + f_{klijm} + f_{klmij} + f_{iklmj}\right). \qquad (5.32)
\end{aligned}
$$

The following constraint, corresponding to Euler's formula, is also needed.

$$\sum_{3\le i\le j\le n} f_{ij} - \sum_{\{i,j,k,l\}\in\mathcal{F}_4} f_{ijkl} - \sum_{\{i,j,k,l,m\}\in\mathcal{F}_5} f_{ijklm} = n-2\,. \qquad (5.33)$$

From (5.20), (5.32), (5.33), we write the following linear program:

$$
\begin{aligned}
\text{maximize}\quad & Z_5^4 = \sum_{3\le i\le j\le n} f_{ij}\left(\frac{\ln i}{i} + \frac{\ln j}{j} - \frac{1}{ij}\right) - \sum_{\{i,j,k,l\}\in\mathcal{F}_4} \frac{f_{ijkl}}{ijkl} - \sum_{\{i,j,k,l,m\}\in\mathcal{F}_5} \frac{f_{ijklm}}{ijklm} \\
\text{subject to}\quad & \sum_{3\le i\le j\le n} f_{ij}\left(\frac{1}{i} + \frac{1}{j}\right) = n \\
& \sum_{3\le i\le j\le n} f_{ij} - \sum_{\{i,j,k,l\}\in\mathcal{F}_4} f_{ijkl} - \sum_{\{i,j,k,l,m\}\in\mathcal{F}_5} f_{ijklm} \le n \\
& \text{and}\quad (5.32)
\end{aligned}
\qquad (P_{45}^4)
$$

Note that the constraint (5.30) can be omitted since it is implied by the others.

Let ${Z_5^4}^*$ is the optimum value that maximizes the objective function Z_5^4 under the constraints given in (P_{45}^4). We solved this linear program with AMPL for several values of n up to 25, obtaining

$$\exp({Z_5^4}^*/n) = 3.502518^n.$$

(The result is rounded up.) Hence, by Lemma 5.8, we would obtain a bound of

$$T(G) \le K \cdot 3.502518^n. \qquad (5.34)$$

where $K = \exp(K_5)$ is a correction term.

This is what would come out, but this result is only established empirically. We have not formally proved that the result (5.34) is true for any value of n. It could be a little bit complicated since there are many non-zero dual variables. But the difference between the bound (5.34) and the bound in Theorem 5.10 is very small.

For the checked values of n, the optimum is achieved when almost all vertices have degree 4, and almost all faces are quadrilaterals. We conjecture then that the family of square grid graphs with periodic boundary conditions described in Section 5.2.6 gives the maximum number of spanning trees for planar graphs without triangles. Note that in this family all 4-cycles are 4-faces.

Considering Larger Cycles. For $l > 6$ it is tricky to write down the linear program constraints relating the number of l-cycles constituted by vertices of given degrees with the number of edges.

However, as in the general case, we think that it is not worth to continue working in this direction: Everything seems to indicate that the graphs that are similar to the 4-regular family of square grid graphs with periodic boundary conditions described in Section 5.2.6 give the maximum number of spanning trees over all planar graphs. In the remainder of this section, we explore heuristically the bounds that Suen's inequality would give, under the hypothesis that the square grid is the optimal graph. We consider the 4-regular square grid embedded on the torus.

Consider the 4-regular family of square grid graphs with periodic boundary conditions which we think that gives the maximum number of spanning trees for planar graphs without triangles. This family has $2n$ edges, no 3-cycles, and n faces, which are the 4-cycles. The 6-cycles are the boundary of two adjacent squares. This means that there are as many 6-cycles as edges, that is, $|C_6| = 2n$. The 8-cycles are the boundary of three squares, as in Figure 5.14, or the boundary of a big square formed by 4 faces (there are n of such big squares, one centered at each vertex). Hence $|C_8| = 6n + n = 7n$. The 10-cycles are boundaries of groups of four or five squares distributed as illustrated in Figure 5.15. Hence $|C_{10}| = 8n + 18n = 26n$. There are no cycles of odd length.

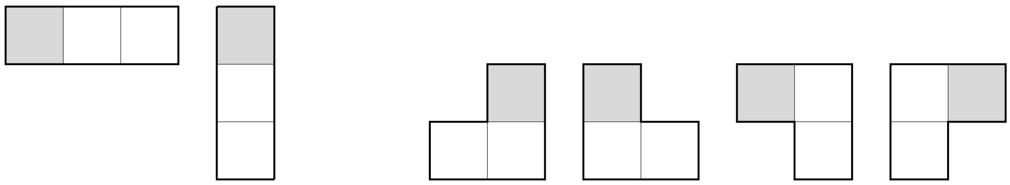

Figure 5.14: 8-cycles as the boundary of three squares. For each square Q, there are 6 of these 8-cycles with Q in the shadowed position. (We do not count twice the same 8-cycle.)

If we plug this values into Lemma 5.8 we obtain

$$\begin{aligned} T(G) &\leq 4^n \exp\left(-\frac{|C_2|}{4^2} - 2\left(\frac{|C_4|}{6^4} + \frac{|C_6|}{6^6} + \frac{|C_8|}{6^8} + \frac{|C_{10}|}{6^{10}}\right) + K_{11}\right) \\ &= 4^n \exp\left(-\frac{2n}{4^2} - 2\left(\frac{n}{6^4} + \frac{2n}{6^6} + \frac{7n}{6^8} + \frac{26n}{6^{10}}\right) + K_{11}\right) \\ &< K \cdot 3.498178^n. \end{aligned}$$

where $K = \exp(K_{11})$ is a correction term.

We could not obtain a better bound than this if we could write a linear program which considers l-cycles up to $l = 11$. Also, for larger l, the improvement is every time much smaller.

C. Suen's Inequality for 3-Connected Graphs with Smallest Face Cycle 5

Let G be a 3-connected planar graph with smallest face cycle 5.

Considering 2-Cycles. If we only consider 2-cycles we can write a linear program (P_2^5) analogous to (P_2). The difference is that now the graph has at most $5/3n - 10/3$ edges. Hence

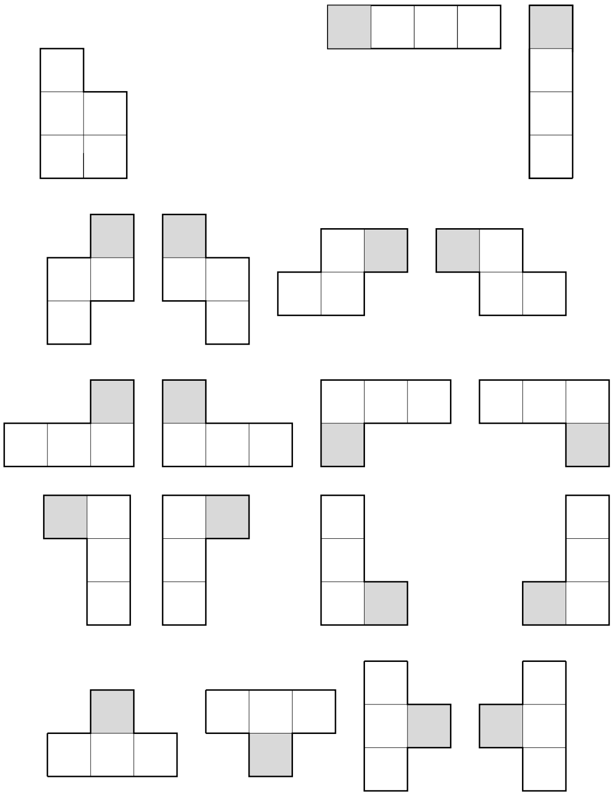

Figure 5.15: Top left: 10-cycles as the boundary of 5 squares, one square attached to the side of a big square. There are 8 ways to attach it, and n such big squares, hence $8n$ such 10-cycles. The rest: 10-cycles as the boundary of four squares. For each square Q, there are 18 such 10-cycles with Q in the shadowed position, and they are counted once.

the constraint (5.21) is substituted by

$$\sum_{3\le i\le j\le n} f_{ij} \le \frac{5}{3}n - \frac{10}{3}\,. \tag{5.35}$$

Let $(P_2^5)'$ be the linear program obtained by replacing (5.35) by the weaker constraint

$$\sum_{3\le i\le j\le n} f_{ij} \le \frac{5}{3}n\,. \tag{5.36}$$

Let $Z_2^{5^*}$ be the optimum value of the linear program $(P_2^5)'$. For several values of the parameter n up to 1000, we obtain with AMPL a rounded up value of $\exp(Z_2^{5^*}/n) = 2.847263$. The optimum value $Z_2^{5^*}$ of the objective function is achieved when

$$f_{33} = n/3,\ f_{34} = 4n/3,\ \text{ and } f_{ij} = 0 \ \text{ for all } ij \ne 33 \text{ or } ij \ne 34.$$

This corresponds to the case where all vertices have degree 3 or 4, $n/3$ of the edges are between vertices of degree 3, and $4n/3$ of the edges are between a vertex of degree 3 and a vertex of degree 4. We formally prove it for every n.

Lemma 5.11. *The linear program* $(P_2^5)'$ *has the optimum value*

$$Z_2^{5^*} = \left(\frac{2}{3}\ln 3 + \frac{1}{3}\ln 4 - \frac{4}{27}\right) n\,.$$

Proof. The proof is analogous to the proof of Lemma 5.9.

The solution $\{f_{33} = n/3,\ f_{34} = 4n/3,\ f_{ij} = 0 \text{ for all } ij \neq 33 \text{ or } ij \neq 34\}$ given above is feasible for $(P_2^5)'$ because it satisfies the constraints. This solution yields the value of the objective function

$$\frac{n}{3}\left(\frac{\ln 3}{3} + \frac{\ln 3}{3} - \frac{1}{9}\right) + \frac{4n}{3}\left(\frac{\ln 3}{3} + \frac{\ln 4}{4} - \frac{1}{12}\right) = \left(\frac{2}{3}\ln 3 + \frac{1}{3}\ln 4 - \frac{4}{27}\right) n\,.$$

To see that this is the optimum solution, we form a linear combination of the constraints (5.20) and (5.36), with factors λ_1 and λ_2:

$$\lambda_1\left(\sum_{3\le i\le j\le n} f_{ij}\left(\frac{1}{i} + \frac{1}{j}\right) - n\right) + \lambda_2\left(\sum_{3\le i\le j\le n} f_{ij} - \frac{5}{3}n\right) \le 0\,,$$

where λ_1 and λ_2 are obtained as the optimal dual variables associated to these constraints.

As in Lemma 5.9 we must show that the function

$$g(i,j) = \frac{\ln i - \lambda_1}{i} + \frac{\ln j - \lambda_1}{j} - \frac{1}{ij} - \lambda_2$$

is negative or zero, for all integers i, j such that $3 \le i \le j \le n$.

We obtain by complementary slackness the equations $g(3,4) = 0$ and $g(4,4) = 0$, since $f_{34}, f_{44} \neq 0$ in the (proposed) optimal solution. Solving the system of equations $\{g(3,4) = 0,\ g(4,4) = 0\}$ we obtain $\lambda_1 \approx -0.014433$ and $\lambda_2 \approx 0.630864$. For this values of λ_1 and λ_2, we can prove that $g(i,j)$ is negative everywhere, except $g(3,4) = 0$ and $g(4,4) = 0$. □

Since the constraints of the linear program $(P_2^5)'$ are weaker than the constraints of the original program (P_2^5), we have:

Corollary 5.9. *The optimum value of the linear program* (P_2^5) *is upper bounded by* $Z_2^{5^*}$.

Theorem 5.11. *For a 3-connected planar graph G with smallest face cycle 5, the Outgoing Edge approach gives an upper bound of*

$$T(G) < \left[\exp\left(\frac{2}{3}\ln 3 + \frac{1}{3}\ln 4 - \frac{4}{27}\right)\right]^n < 2.847263^n.$$

Proof. By Corollary 5.5 and Corollary 5.9, we have

$$T(G) < \left[\exp\left(\frac{Z_2^{5^*}}{n}\right)\right]^n,$$

and substituting the value of $Z_2^{5^*}$ given in Lemma 5.11 we have the result. □

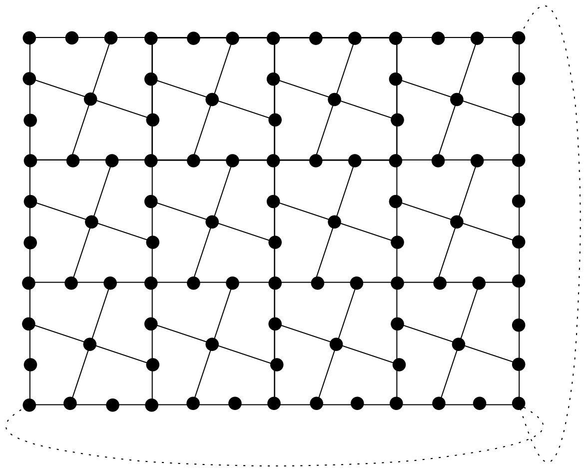

Figure 5.16: Grid where all faces are pentagons, satisfying $f_{33} = n/3$, $f_{34} = 4n/3$, and $f_{ij} = 0$ for all $ij \neq 33$ or $ij \neq 34$. The grid has periodic boundary conditions: the top vertices are identified with the bottom boundary vertices, and the left boundary vertices are identified with the right boundary vertices.

There is no planar graph with smallest face cycle 5 and $f_{33} = n/3$, $f_{34} = 4n/3$, and $f_{ij} = 0$ for all $ij \neq 33$ or $ij \neq 34$, since, as we said above, a planar graph with smallest face cycle 5 has at most $5/3n - 10/3$ edges. However, such a graph can be embedded on the torus. The situation holds for the grid with periodic conditions illustrated in Figure 5.16.

We can assume that G has only 5-faces, 6-faces and 7-faces: If we add edges to the graph, the number of spanning trees grows. Similarly as in the previous section, we add chords while keeping the smallest face cycle being 5, till we cannot continue, and we obtain a graph where all faces have length 5, 6 or 7.

It is too tricky to write a linear program which considers the deletion of 5-faces, 6-faces and 7-faces, and we do not expect that this brings a significant improvement.

5.4 Upper Bounds for the Number of Forests

For embedding 3-polytopes in small integer grids in Chapter 6, we need to upper bound the number of spanning forests of a planar graph with three and four trees, each rooted at one chosen vertex. The number of spanning forests with three trees is used for embedding 3-polytopes with at least one triangular face. The number of spanning forest with four trees is used for embedding 3-polytopes with no triangular face but a quadrilateral face.

We bound the number of spanning forests in terms of the number of spanning trees, and we use the upper bounds for spanning trees given in Section 5.3.

Lemma 5.12. *Let G be a planar graph with three selected vertices v_1, v_2, v_3. Let $F^3(G)$ be the set of spanning forests of G with three trees, each one rooted at one chosen vertex v_1, v_2, v_3. Then,*

$$\frac{T(G)}{4n^2} \leq |F^3(G)| \leq (n-1)^2\, T(G).$$

Proof. Let T be a spanning tree of G and let v_1, v_2, v_3 be three chosen vertices. We obtain from T a spanning forest with three trees, each one rooted at one chosen vertex, by removing two edges that disconnect v_1, v_2, v_3. We can disconnect v_1 from v_2 by removing any of the edges of the path from v_1 to v_2. This can be done in at most $n-1$ ways. The vertex v_3 is still connected to either v_1 or v_2, by a path of at most $n-1$ edges. By removing one of these edges, we obtain the desired spanning forest. Hence, a spanning forest can be obtained from T in at most $(n-1)^2$ ways, so $|F^3(G)| \leq (n-1)^2\, T(G)$.

This bound is not very tight, but it is also not too relaxed: $|F^3(G)|$ is at least $T(G)/4n^2$. To see this, let F be a spanning forest with three trees F_1, F_2, F_3, each rooted at one chosen vertex. From F we can obtain a spanning tree by adding two edges a and b; a connects F^1 with F^2 or F^3, and b connects the remaining component with the component containing a. The graph G has at most $3n-6$ edges because it is planar, and the spanning forest F has $n-3$ edges. Hence a and b can be chosen within a set of $3n-6-(n-3) = 2n-3$ remaining edges. Thus we can obtain a spanning tree in at most $4n^2$ ways, and this proves the lower bound of the theorem. □

A tight example for the upper bound on $|F^3(G)|$ given in Lemma 5.12 is illustrated in Figure 5.17, where the three paths from the unique degree-3 vertex to the chosen vertices v_1, v_2, v_3 have length $(n-1)/3$. This graph has one spanning tree and $1/3(n-1)^2$ spanning forests with three trees, each one rooted at one chosen vertex. Hence, in this example, $|F^3(G)| = 1/3\,(n-1)^2\,T(G)$.

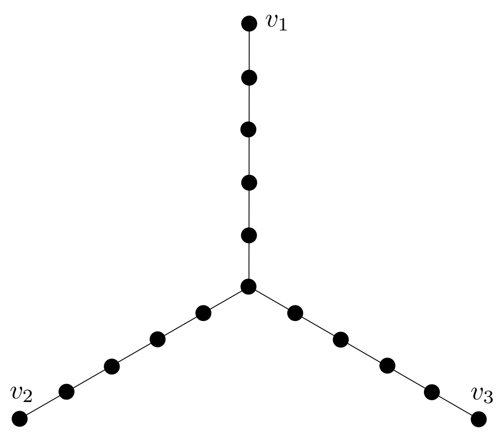

Figure 5.17: Example with $|F^3(G)| = 1/3\,(n-1)^2\,T(G)$. The three paths from the unique degree-3 vertex to the chosen vertices v_1, v_2, v_3 have length $(n-1)/3$, where n is the number of vertices of the graph.

A tight example for the lower bound on $|F^3(G)|$ in Lemma 5.12 is illustrate in Figure 5.18, where, given a spanning forest with three trees, each one rooted at one chosen vertex v_1, v_2, v_3, we can obtain a spanning tree in n^2 ways (up to a constant factor).

Consider now the case when G is a graph with no triangular face, but at least one quadrilateral face, and consider the number of spanning forests with four trees.

Lemma 5.13. *Let G be a planar graph with smallest face cycle at least 4. Let $|F^4(G)|$ be the set of spanning forests of G with four trees, each one rooted at one chosen vertex v_1, v_2, v_3, v_4.*

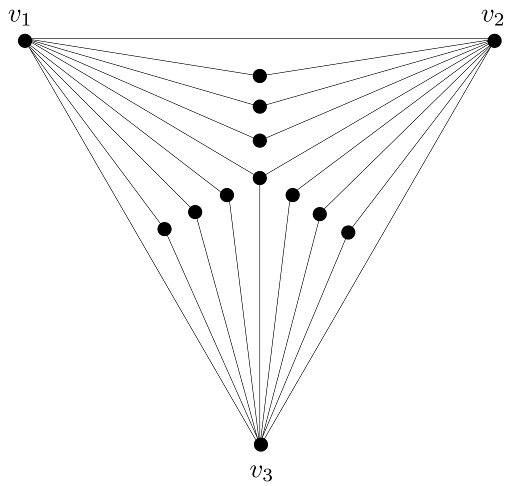

Figure 5.18: Example with $T(G) \approx n^2|F^3(G)|$.

Then,

$$\frac{T(G)}{n^3} \leq |F^4(G)| \leq (n-1)^3\, T(G).$$

Proof. Let T be a spanning tree of G and let v_1, v_2, v_3, v_4 be four chosen vertices. Analogously as in Theorem 5.12, we obtain from T a spanning forest with four components, each one rooted at one chosen vertex, by removing three edges that disconnect the chosen vertices. Each chosen vertex v_i can be disconnected from another chosen edge v_j by removing an edge of the path from v_i to v_j, and this can be done in at most $n-1$ ways. We must do this three times for disconnecting the four chosen vertices from each other. Hence, a spanning forest is obtained from T in at most $(n-1)^3$ ways, so $|F^4(G)| \leq (n-1)^3\, T(G)$.

To see that the bound is not too relaxed, we lower bound $|F^4(G)|$ in terms of $T(G)$. Let F be a spanning forest with four components F_1, F_2, F_3, F_4, each one rooted at one chosen vertex. From F we can obtain a spanning tree by adding three edges a, b and c connecting the four components. The graph G has at most $2n-4$ edges since each face is bounded by at least 4 edges, and the spanning forest F has $n-4$ edges. Hence a, b and c can be chosen within a set of $2n-4-(n-4) = n$ edges. Thus we can obtain a spanning tree in at most n^3 ways, and this proves the lower bound for $|F^4(G)|$. ∎