The Number of Independent Sets In Hexagonal Graphs

Zhun Deng, Jie Ding, Kathryn Heal, and Vahid Tarokh

***Abstract*—We derive the tightest known bounds on η, the growth rate of the logarithm of the number of independent sets on a hexagonal lattice. To obtain these bounds, we generalize a method proposed by Calkin and Wilf. Their original strategy cannot immediately be used to derive bounds for η, due to the difference in symmetry between square and hexagonal lattices, so we propose a modified method and an algorithm to derive rigorous bounds on η. In particular, we prove that $1.546440708536001 \leq \eta \leq 1.5513$, which improves upon the best known bounds of $1.5463 \leq \eta \leq 1.5527$ given by Nagy and Zeger. Our lower bound matches the numerical estimate of Baxter up to 9 digits after the decimal point, and our upper bound can be further improved by following our method.**

***Index Terms*—Hexagonal lattice, independent set, transfer matrix.**

I. Introduction

Given a lattice $\mathfrak{L}$ and a set of vertices R in $\mathfrak{L}$, an *independent set within region* R is a subset of R for which no two elements are neighbors (Fig. 1). Let $f_{\mathfrak{L}}(R)$ denote the number of independent sets within region R, let $|R|$ be the number of vertices in R, and let $R_1 \subset R_2 \subset \cdots$ be a sequence of finite subsets of $\mathfrak{L}$ for which $\bigcup_{k=1}^{\infty} R_k = \mathfrak{L}$. We are interested in computing

$$\eta = \lim_{k\to\infty} \frac{\log_2 f_{\mathbb{A}_2}(R_k)}{|R_k|}, \tag{1}$$

if such a limit exists, where $\mathbb{A}_2$ denotes the two dimensional hexagonal lattice. This problem, which is also referred to as the hard triangle model problem, was first proposed by Baxter [1], [2]. Baxter's work conjectured the existence of, and provided some estimates for, the above limit η.

In this paper, we evaluate a particular sequence $R_k,\ k = 1, 2, \cdots$, and derive a new approach to establish rigorous lower and upper bounds on that limit, inspired by the work of Calkin and Wilf [3]. To the best of our knowledge, the strongest known result is $1.5463 \leq \eta \leq 1.5527$ as derived by Nagy and Zeger in [4]. We provide a method to derive rigorous bounds that improve upon their result. Specifically, we prove that $1.546440708536001 \leq \eta \leq 1.5513$.

It is worth noting that the lower bound matches the numerical estimate of Baxter, which is $\eta \approx 1.546440708787561419$, up to 9 digits after the decimal point.

II. Transfer Matrix for Hexagonal Graph

A. Notations

In this paper, we denote the Fibonacci numbers by $\{F_i\}_{i=0}^{\infty}$, i.e., $F_0 = 1, F_1 = 1$, and $F_i = F_{i-1} + F_{i-2}$. For real-valued vectors $\boldsymbol{y}$ and $\boldsymbol{z}$ of the same size, $\langle \boldsymbol{y}, \boldsymbol{z}\rangle$ denotes their inner product. Let $\mathbf{1}_{k\times 1}$ denote $k \times 1$ vector of all ones, and $\mathbf{0}_{k\times j}$ denote $k \times j$ matrix of all zeros. We drop the subscripts $k \times 1$ and $k \times j$ whenever there is no ambiguity. For any real-valued matrix $\boldsymbol{A}$, let $\lambda_{\max}(\boldsymbol{A})$, $\boldsymbol{A}^{\mathrm{T}}$, and $\mathrm{Trace}(\boldsymbol{A})$ respectively denote the largest absolute value of the eigenvalues, the transpose, and the sum of all the diagonal elements of $\boldsymbol{A}$. The following inequality holds for any real-valued symmetric matrix $\boldsymbol{A}$ of size $k \times k$ and positive integer n:

$$(\lambda_{\max}(\boldsymbol{A}))^n \geq \frac{\langle \mathbf{1}_{k\times 1}, \boldsymbol{A}^n \mathbf{1}_{k\times 1}\rangle}{\langle \mathbf{1}_{k\times 1}, \mathbf{1}_{k\times 1}\rangle}. \tag{2}$$

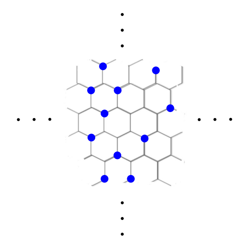


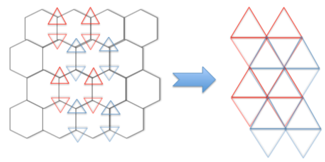
Fig. 1: Illustration of infinite hexagonal grid graph, where the objects are placed on the vertices and no two objects are neighbors

B. Transfer Matrix

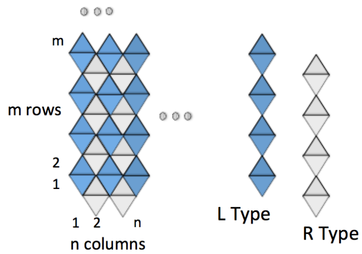
We can transform the independent set problem into an equivalent checkerboard problem by placing a triangle on each vertex, as shown in Fig. 2a. In this way, the lattice is transformed into a grid of triangles, and the number of independent sets is equal to the number of distinct arrangements of 0's and 1's on a checkerboard of triangles such that no pair of neighboring elements are both ones. Here, two triangles are said to be neighbors if they share an edge.

Let $G_{m,n}$ denote the zigzag-shaped region shown in Fig. 2b, where m is the number of points in each column and n is the number of column vectors. The columns are categorized into two different types: the columns whose first element (the bottommost triangle) lies above those of the neighboring columns is referred to as "L" type. All remaining columns are referred to as "R" type. Assume that the leftmost column of $G_{m,n}$ is "L" type. We note that an "L" type vector, say $[1, 0, 0, 0, 0, 0, 0, 1]^T$, is different from $[1, 0, 0, 0, 0, 0, 0, 1]^T$ of "R" type. It is easy to observe that an "L" type vector cannot be attached to an "L" type vector, while an "R" type vector can be attached to an "L" type vector.

Let $f(m, n)$ denote the total number of valid arrangements of 0's and 1's in $G_{m,n}$. Then for this set of regions the value



(a) Illustration of how triangles are placed on an infinite hexagonal grid graph so that the original problem is transformed into a checkerboard code problem



(b) Illustration of the set of regions ($R_k, k = 1, 2, \cdots$) considered in the paper

Fig. 2: Illustration of $G_{m,n}$ which consists of "L" type and "R" type

of (1) becomes

$$\eta = \lim_{m\to\infty, n\to\infty} f(m,n)^{\frac{1}{mn}}, \tag{3}$$

if the limit exists. We will prove the existence of this limit and provide a lower and an upper bound for η in Sections III, IV, and V.

A column vector is considered "valid" if for every pair of neighboring elements, those elements are not both one. Let a_m denote the number of valid column vectors with size m. Then, $a_m = 3^{m/2}$ for even m and $a_m = 2 \cdot 3^{(m-1)/2}$ for odd m. We denote the collection of all the "L" type and "R" type valid column vectors of size m by $\mathfrak{X}_m = \{\boldsymbol{x}_i\}_{i=1}^{2a_m}$. Without loss of generality, the "L" type vectors are assumed to be arranged before the "R" type vectors in $\mathfrak{X}_m$, i.e., $\{\boldsymbol{x}_i\}_{i=1}^{a_m}$ are "L" type. All columns of $G_{m,n}$ belong to $\mathfrak{X}_m$.

We define the transfer matrix $\boldsymbol{T}_m$ to be a $2a_m \times 2a_m$ binary matrix whose (i,j)th entry is

$$\boldsymbol{T}_m[i,j] = \begin{cases} 1 & \text{if } \boldsymbol{x}_j \text{ can be attached to } \boldsymbol{x}_i \\ & \text{(on the the right side of } \boldsymbol{x}_i\text{)} \\ 0 & \text{otherwise,} \end{cases}$$

for $1 \le i, j \le 2a_m$. We note that $\boldsymbol{T}_m$ is a symmetric matrix by construction. In the rest of the paper, the subscript "L" and "R" denotes vector of L type and R type. And the superscripts "T" are added to vectors of "L" and "R" to show they are arranged in a vertical way. Next, we provide a simple example.

Example 1. *If m=2, the valid columns are $[0,0]_L^T$, $[0,1]_L^T$, $[1,0]_L^T$, $[0,0]_R^T$, $[0,1]_R^T$, and $[1,0]_R^T$. The transfer matrix $\boldsymbol{T}_2$ is*

$$\boldsymbol{T}_2 = \begin{pmatrix} \boldsymbol{0} & \boldsymbol{A}^{(LR)} \\ \boldsymbol{A}^{(RL)} & \boldsymbol{0} \end{pmatrix}, \text{ where } \boldsymbol{A}^{(LR)} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 0 & 1 \end{pmatrix}$$

and $\boldsymbol{A}^{(RL)} = (\boldsymbol{A}^{(LR)})^T$.

Next, let $f(m,n,i)$ denote the number of valid arrangements in $G_{m,n}$ whose rightmost column is $\boldsymbol{x}_i$. Then

$$f(m,n+1,j) = \sum_{i=1}^{2a_m} f(m,n,i)\boldsymbol{T}_m[i,j]. \tag{4}$$

We define $\boldsymbol{f}_{m,n} = [f(m,n,1), f(m,n,2), \cdots, f(m,n,2a_m)]$, and rewrite (4) as

$$\boldsymbol{f}_{m,n+1} = \boldsymbol{f}_{m,n}\boldsymbol{T}_m, \text{ and } \boldsymbol{f}_{m,1} = [1,1\cdots,1,0,0,\cdots,0],$$

composed of a_m 1's. Thus,

$$f(m,n) = \boldsymbol{f}_{m,1}\boldsymbol{T}_m^{n-1}\boldsymbol{1}. \tag{5}$$

By symmetry, $f(m,n)$ remains the same if the leftmost column is "R" type instead of "L" type, i.e.,

$$f(m,n) = (\boldsymbol{1} - \boldsymbol{f}_{m,1})\boldsymbol{T}_m^{n-1}\boldsymbol{1}. \tag{6}$$

By combining (5) and (6) we obtain

$$2f(m,n) = \langle \boldsymbol{1}, \boldsymbol{T}_m^{n-1}\boldsymbol{1}\rangle. \tag{7}$$

III. The Existence of The Limit η

The existence of the double limit η can be proved using the "subadditivity" property (see [5]–[7]). For completeness, we provide a rigorous proof of the existence of η and its equivalent expression. We will use the new expression to derive the lower and upper bounds on η in the remaining two sections.

The following lemma is an immediate consequence of the Perron-Frobenius Theorem and Proposition 4.2.1 in [5].

Lemma 1. *Let $\boldsymbol{A}$ be a real-valued $r \times r$ matrix that is nonnegative and irreducible. Then $\boldsymbol{A}$ has a positive eigenvector $\boldsymbol{v} = [\boldsymbol{v}[1], \boldsymbol{v}[2], \cdots, \boldsymbol{v}[r]]^T$ with corresponding eigenvalue $\lambda_{\max}(\boldsymbol{A})$. Furthermore, for any positive integer n the following inequality holds:*

$$\frac{e}{d}(\lambda_{\max}(\boldsymbol{A}))^n \le \langle \boldsymbol{1}, \boldsymbol{A}^n\boldsymbol{1}\rangle \le \frac{rd}{e}(\lambda_{\max}(\boldsymbol{A}))^n,$$

where $e = \min\{\boldsymbol{v}[1], \boldsymbol{v}[2], \cdots, \boldsymbol{v}[r]\}$ and $d = \max\{\boldsymbol{v}[1], \boldsymbol{v}[2], \cdots, \boldsymbol{v}[r]\}$.

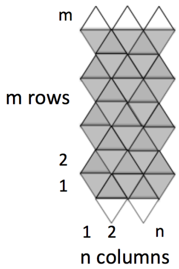
We can use Lemma 1 to prove the following lemma.

Lemma 2. *For any given positive integer m, we have*

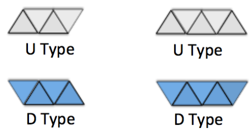
$$\begin{aligned} \lim_{n\to\infty}[f(m,n)^{\frac{1}{mn}}] &= \lim_{n\to\infty}\left[\left(\frac{1}{2}\langle \boldsymbol{1}, \boldsymbol{T}_m^{n-1}\boldsymbol{1}\rangle\right)^{\frac{1}{mn}}\right] \\ &= (\lambda_{\max}(\boldsymbol{T}_m))^{\frac{1}{m}}. \end{aligned} \tag{8}$$

Proof. The matrix $\boldsymbol{T}_m$ is irreducible because the directed graph it represents is strongly-connected. In fact, we can build a path from one vertex to any other vertex by inserting vertices that represent the all-zero vectors. Furthermore, Lemma 1 implies that there are positive constants d and e (that depend on m) for which

$$\frac{e}{d}(\lambda_{\max}(\boldsymbol{T}_m))^{n-1} \le \langle \boldsymbol{1}, \boldsymbol{T}_m^{n-1}\boldsymbol{1}\rangle \le \frac{2a_m d}{e}(\lambda_{\max}(\boldsymbol{T}_m))^{n-1}. \tag{9}$$



(a) Illustration of the shaded part of $G_{m,n}$



(b) Illustration of "D" type and "U" type ($n = 4$ on the left, and $n = 5$ on the right)

Fig. 3: Illustration of the shaded part of $G_{m,n}$, which consists of "D" type and "U" type.

Raising both sides of (9) to the power of $1/(n-1)$ and letting $n \to \infty$, we obtain

$$\lim_{n\to\infty} \left\langle \mathbf{1}, \boldsymbol{T}_m^{n-1}\mathbf{1} \right\rangle^{1/(n-1)} = \lambda_{\max}(\boldsymbol{T}_m),$$

which implies the existence of the limit in (8). □

Theorem 1. *Both of the limits* $\lim_{m\to\infty}\lim_{n\to\infty} f(m,n)^{\frac{1}{mn}}$ *and* $\lim_{m,n\to\infty} f(m,n)^{\frac{1}{mn}}$ *exist and they are equal.*

Proof. Please refer to the extended version of this paper [8]. □

IV. The Lower Bound

We consider the shaded part of $G_{m,n}$ ($n > 1$), denoted by $G_{m,n}^{\text{shaded}}$ shown in Fig. 3a. Similar to the arguments in the previous section, we recognize $G_{m,n}^{\text{shaded}}$ as a concatenation of "D" type and "U" type valid row vectors (Fig. 3b). Here, a row vector is referred to as "valid" if it has no two neighboring elements that are both ones. It is easy to observe that there are $b_n = F_{n+1}$ valid row vectors. Let $\mathfrak{W}_n = \{\boldsymbol{w}_i\}_{i=1}^{2b_n}$ denote the collection of all the "D" type and "U" type valid row vectors of size n (without loss of generality, the "D" type are arranged before the "U" type within $\mathfrak{W}_n$, i.e., $\{\boldsymbol{w}_i\}_{i=1}^{b_n}$ are of "D" type). We define the corresponding transfer matrix $\boldsymbol{Y}_n$ to be a $2b_n \times 2b_n$ binary matrix whose entry in position (i,j) is

$$\boldsymbol{Y}_n[i,j] = \begin{cases} 1 & \text{if } \boldsymbol{w}_j \text{ can be attached to } \boldsymbol{w}_i \text{ (on top of } \boldsymbol{w}_i\text{)} \\ 0 & \text{otherwise,} \end{cases}$$

for $1 \le i, j \le b_n$.

Example 2. *If* $n = 3$, *the valid rows are* $[0,0,0]_D$, $[0,0,1]_D$, $[0,1,0]_D$, $[1,0,0]_D$, $[1,0,1]_D$, $[0,0,0]_U$, $[0,0,1]_U$, $[0,1,0]_U$, $[1,0,0]_U$, $[1,0,1]_U$, *and the transfer matrix* $\boldsymbol{Y}_3$ *is*

$$\boldsymbol{Y}_3 = \begin{pmatrix} \mathbf{0} & \boldsymbol{A}^{(DU)} \\ \boldsymbol{A}^{(UD)} & \mathbf{0} \end{pmatrix},$$

where

$$\boldsymbol{A}^{(DU)} = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \end{pmatrix}$$

and

$$\boldsymbol{A}^{(UD)} = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \end{pmatrix}.$$

It is easy to observe that each column of $G_{m,n}^{\text{shaded}}$ is of size $m-1$. Similar to the derivation of (7), the number of distinct arrangements satisfying the hexagonal constraint in $G_{m,n}^{\text{shaded}}$ is $\frac{1}{2}\langle \mathbf{1}, \boldsymbol{Y}_n^{m-2}\mathbf{1}\rangle$. Furthermore, the number of points in $G_{m,n}$ but not in $G_{m,n}^{\text{shaded}}$ is $nm - n(m-1) = n$. Thus there exists a positive number $c_{m,n}$ (which depends on m, n) such that $1 \le c_{m,n} \le 2^n$ and

$$\frac{1}{2}\langle \mathbf{1}, \boldsymbol{T}_m^{n-1}\mathbf{1}\rangle = f(m,n) = c_{m,n}\frac{1}{2}\langle \mathbf{1}, \boldsymbol{Y}_n^{m-2}\mathbf{1}\rangle. \tag{10}$$

From Identity (10) and the fact that $\boldsymbol{T}_m$ is symmetric, we obtain that for any positive integer q,

$$\begin{aligned} (\lambda_{\max}(\boldsymbol{T}_m))^n &\ge \frac{\langle \boldsymbol{T}_m^q\mathbf{1}, \boldsymbol{T}_m^n\boldsymbol{T}_m^q\mathbf{1}\rangle}{\langle \boldsymbol{T}_m^q\mathbf{1}, \boldsymbol{T}_m^q\mathbf{1}\rangle} = \frac{\langle \mathbf{1}, \boldsymbol{T}_m^{n+2q}\mathbf{1}\rangle}{\langle \mathbf{1}, \boldsymbol{T}_m^{2q}\mathbf{1}\rangle} \\ &\ge \frac{c_{m,n+2q+1}}{c_{m,2q+1}}\frac{\langle \mathbf{1}, \boldsymbol{Y}_{n+2q+1}^{m-2}\mathbf{1}\rangle}{\langle \mathbf{1}, \boldsymbol{Y}_{2q+1}^{m-2}\mathbf{1}\rangle} \\ &\ge \frac{1}{2^{2q+1}}\frac{\langle \mathbf{1}, \boldsymbol{Y}_{n+2q+1}^{m-2}\mathbf{1}\rangle}{\langle \mathbf{1}, \boldsymbol{Y}_{2q+1}^{m-2}\mathbf{1}\rangle}. \end{aligned}$$

Following a similar argument to the proof of Lemma 2, for any positive integer n, $\boldsymbol{Y}_n$ is irreducible and $\lim_{m\to\infty}\langle \mathbf{1}, \boldsymbol{Y}_n^m\mathbf{1}\rangle^{1/m} = \lambda_{\max}(\boldsymbol{Y}_n)$. Thus,

$$\begin{aligned} \eta &= \lim_{m\to\infty}\left[(\lambda_{\max}(\boldsymbol{T}_m))^{\frac{1}{m}}\right] \\ &\ge \left[\lim_{m\to\infty}\left(\frac{1}{2^{2q+1}}\frac{\langle \mathbf{1}, \boldsymbol{Y}_{n+2q+1}^{m-2}\mathbf{1}\rangle}{\langle \mathbf{1}, \boldsymbol{Y}_{2q+1}^{m-2}\mathbf{1}\rangle}\right)^{\frac{1}{m}}\right]^{\frac{1}{n}} \\ &= \left(\frac{\lambda_{\max}(\boldsymbol{Y}_{n+2q+1})}{\lambda_{\max}(\boldsymbol{Y}_{2q+1})}\right)^{\frac{1}{n}}. \end{aligned} \tag{11}$$

Choosing $n = 1, q = 1$, we obtain

$$\eta \ge \frac{\lambda_{\max}(\boldsymbol{Y}_4)}{\lambda_{\max}(\boldsymbol{Y}_3)} = 1.5444\,.$$

Furthermore, using the algorithm proposed in the following subsection, we can compute $\boldsymbol{Y}_n$ for large n to arrive at even tighter lower bounds. For instance, by using $\boldsymbol{Y}_{15}$ and $\boldsymbol{Y}_{14}$, we have

$$\eta \ge \frac{\lambda_{\max}(\boldsymbol{Y}_{15})}{\lambda_{\max}(\boldsymbol{Y}_{14})} = 1.546440708536001\,. \tag{12}$$

A. Algorithm

In this section, we develop a technique that recursively constructs $\boldsymbol{Y}_n$. Let $\mathfrak{D}_n = \{\boldsymbol{d}_1^{(n)}, \cdots, \boldsymbol{d}_{F_{n+1}}^{(n)}\}$ denote the set of all valid "D" type row vectors of size n equipped with a partial binary ordering. Then the elements of $\mathfrak{D}_n$ are given by

$$\boldsymbol{d}_i^{(n)} = \begin{cases} \left[0, \boldsymbol{d}_i^{(n-1)}\right] & 1 \le i \le F_n \ , \\ \left[1, 0, \boldsymbol{d}_{i-F_n}^{(n-2)}\right] & F_n + 1 \le i \le F_{n+1} \ . \end{cases} \tag{13}$$

We define $\mathfrak{U}_n = \{\boldsymbol{u}_1^{(n)}, \cdots, \boldsymbol{u}_{F_{n+1}}^{(n)}\}$, the set of all valid "U" type row vectors of size n in an analogous manner. Let

$$\boldsymbol{Y}_n = \begin{pmatrix} \boldsymbol{0} & \boldsymbol{A}_n^{(DU)} \\ \boldsymbol{A}_n^{(UD)} & \boldsymbol{0} \end{pmatrix},$$

where

$$\boldsymbol{A}_n^{(DU)}[i,j] = \begin{cases} 1 & \text{if } \boldsymbol{u}_j^{(n)} \text{ can be attached to } \boldsymbol{d}_i^{(n)}, \\ 0 & \text{otherwise,} \end{cases}$$

$$\boldsymbol{A}_n^{(UD)}[i,j] = \begin{cases} 1 & \text{if } \boldsymbol{d}_j^{(n)} \text{ can be attached to } \boldsymbol{u}_i^{(n)}, \\ 0 & \text{otherwise,} \end{cases}$$

for $1 \le i, j \le F_{n+1}$. Let

$$\boldsymbol{P}_n^{(DU)}[i,j] = \begin{cases} 1 & \text{if } \boldsymbol{u}_j^{(n)} \text{ can be attached to } \boldsymbol{d}_i^{(n)} \\ & \text{and the leftmost element of } \boldsymbol{d}_i^{(n)} \text{ is 0,} \\ 0 & \text{otherwise,} \end{cases}$$

for $1 \le i \le F_n$, $1 \le j \le F_{n+1}$ (Fig. 4a), and let

$$\boldsymbol{P}_n^{(UD)}[i,j] = \begin{cases} 1 & \text{if } \boldsymbol{d}_j^{(n)} \text{ can be attached to } \boldsymbol{u}_i^{(n)} \\ & \text{and the leftmost element of } \boldsymbol{u}_i^{(n)} \text{ is 0,} \\ 0 & \text{otherwise,} \end{cases}$$

for $1 \le i \le F_n$, $1 \le j \le F_{n+1}$ (Fig. 4b). Let

$$\boldsymbol{Q}_n^{(DU)}[i,j] = \begin{cases} 1 & \text{if } \boldsymbol{u}_j^{(n)} \text{ can be attached to } \boldsymbol{d}_i^{(n)}, \\ & \text{and the leftmost element of } \boldsymbol{u}_j^{(n)} \text{ is 0,} \\ 0 & \text{otherwise,} \end{cases}$$

for $1 \le i \le F_{n+1}$, $1 \le j \le F_n$ (Fig. 4c), and

$$\boldsymbol{Q}_n^{(UD)}[i,j] = \begin{cases} 1 & \text{if } \boldsymbol{d}_j^{(n)} \text{ can be attached to } \boldsymbol{u}_i^{(n)}, \\ & \text{and the leftmost element of } \boldsymbol{d}_j^{(n)} \text{ is 0,} \\ 0 & \text{otherwise,} \end{cases}$$

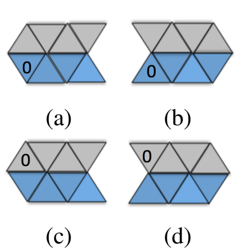


Fig. 4: Concatenation types of size four. Arrangements correspond to (a) $\boldsymbol{P}_n^{(DU)}$, (b) $\boldsymbol{P}_n^{(UD)}$, (c) $\boldsymbol{Q}_n^{(DU)}$, and (d) $\boldsymbol{Q}_n^{(UD)}$.

for $1 \le i \le F_{n+1}$, $1 \le j \le F_n$ (Fig. 4d).

By Equation (13) and the above definitions, $\boldsymbol{A}_n^{(DU)}$ and $\boldsymbol{A}_n^{(UD)}$ (for $n > 2$) can be written

$$\boldsymbol{A}_n^{(DU)} = \begin{pmatrix} \boldsymbol{A}_{n-1}^{(UD)} & \boldsymbol{Q}_{n-1}^{(UD)} \\ \boldsymbol{P}_{n-1}^{(UD)} & \boldsymbol{0} \end{pmatrix} \tag{14}$$

$$\boldsymbol{A}_n^{(UD)} = \begin{pmatrix} \boldsymbol{A}_{n-1}^{(DU)} & \boldsymbol{Q}_{n-1}^{(DU)} \\ \boldsymbol{P}_{n-1}^{(DU)} & \boldsymbol{A}_{n-2}^{(UD)} \end{pmatrix}. \tag{15}$$

Moreover, $\mathfrak{D}_{n-1} = \mathfrak{D}_{n-2} \cup \mathfrak{D}_{n-3}$ implies that

$$\boldsymbol{d}_i^{(n)} = \begin{cases} \left[0, 0, \boldsymbol{d}_i^{(n-2)}\right] & 1 \le i \le F_{n-1} \ , \\ \left[0, 1, 0, \boldsymbol{d}_{i-F_{n-1}}^{(n-3)}\right] & F_{n-1} + 1 \le i \le F_n \ , \\ \left[1, 0, \boldsymbol{d}_{i-F_n}^{(n-2)}\right] & F_n + 1 \le i \le F_{n+1} \ . \end{cases}$$

Thus, we can rewrite $\boldsymbol{P}_{n-1}^{(DU)}$, $\boldsymbol{P}_{n-1}^{(UD)}$, $\boldsymbol{Q}_{n-1}^{(DU)}$ and $\boldsymbol{Q}_{n-1}^{(UD)}$ as

$$\boldsymbol{P}_{n-1}^{(DU)} = \begin{pmatrix} \boldsymbol{A}_{n-2}^{(UD)} & \boldsymbol{Q}_{n-2}^{(UD)} \end{pmatrix}, \quad \boldsymbol{P}_{n-1}^{(UD)} = \begin{pmatrix} \boldsymbol{A}_{n-2}^{(DU)} & \boldsymbol{Q}_{n-2}^{(DU)} \end{pmatrix}, \tag{16}$$

$$\boldsymbol{Q}_{n-1}^{(DU)} = \begin{pmatrix} \boldsymbol{A}_{n-2}^{(UD)} \\ \boldsymbol{P}_{n-2}^{(UD)} \end{pmatrix}, \quad \boldsymbol{Q}_{n-1}^{(UD)} = \begin{pmatrix} \boldsymbol{A}_{n-2}^{(DU)} \\ \boldsymbol{P}_{n-2}^{(DU)} \end{pmatrix}. \tag{17}$$

Furthermore,

$$\boldsymbol{A}_2^{(DU)} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 0 \end{pmatrix}, \quad \boldsymbol{A}_2^{(UD)} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 1 \end{pmatrix},$$

$$\boldsymbol{A}_3^{(DU)} = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \end{pmatrix}, \quad \boldsymbol{A}_3^{(UD)} = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \end{pmatrix},$$

$$\boldsymbol{P}_2^{(DU)} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}, \quad \boldsymbol{P}_2^{(UD)} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 0 & 1 \end{pmatrix},$$

$$\boldsymbol{P}_3^{(DU)} = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 & 1 \end{pmatrix}, \quad \boldsymbol{P}_3^{(UD)} = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 & 1 \end{pmatrix},$$

$$\boldsymbol{Q}_2^{(DU)} = \begin{pmatrix} 1 & 1 \\ 1 & 1 \\ 1 & 1 \end{pmatrix}, \quad \boldsymbol{Q}_2^{(UD)} = \begin{pmatrix} 1 & 1 \\ 1 & 0 \\ 1 & 1 \end{pmatrix},$$

$$\boldsymbol{Q}_3^{(DU)} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 0 & 1 \end{pmatrix}, \quad \boldsymbol{Q}_3^{(UD)} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 0 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}.$$

Given the above recursion and initial values, we can recursively construct $\boldsymbol{Y}_{14}$ and $\boldsymbol{Y}_{15}$, and compute the lower bound in (12).

V. The Upper Bound

Since $\boldsymbol{T_m}$ is a real-valued symmetric matrix, the following inequality holds:

$$\lambda_{\max}(\boldsymbol{T}_m) \leq \left(\mathrm{Trace}(\boldsymbol{T}_m^{2n})\right)^{\frac{1}{2n}},$$

where

$$\mathrm{Trace}(\boldsymbol{T}_m^{2n}) = \sum_{1 \leq t_0, t_1, \cdots, t_{2n-1} \leq 2a_m} T_m[t_0, t_1]\, T_m[t_1, t_2] \cdots T_m[t_{2n-1}, t_0].$$

For each of the nonzero product terms in the above summation, $T_m[t_i, t_j]$ is equal to one. It follows that the sum is the total number of valid arrangements of column vectors $(\boldsymbol{x}_{t_0}, \boldsymbol{x}_{t_1}, \cdots, \boldsymbol{x}_{t_{2n-1}}, \boldsymbol{x}_{t_0})$ in a zigzag manner from left to right (Fig. 5).

Let $\tau(m,n)$ denote the number of such valid arrangements restricted to the shaded part (Fig. 3a). Similar to (10), there exists a positive number $\hat{c}_{m,n}$ (which depends on m, n) such that $1 \leq \hat{c}_{m,n} \leq 2^{2n+1}$ and $\mathrm{Trace}(\boldsymbol{T}_m^{2n}) = \hat{c}_{m,n}\tau(m,n)$. We define the "D2" and "U2" type vectors to be respectively the row vectors of "D" and "U" types in which no two neighboring elements are both ones and in which the first entry is equal to the last entry. Next, we calculate $\tau(m,n)$ by recognizing the shaded part as a concatenation of "D2" type and "U2" type row vectors of size $2n+1$. We define the corresponding transfer matrix $\boldsymbol{B}_n$ in an analogous manner to $\boldsymbol{Y}_n$. Clearly, the size of $\boldsymbol{B}_n$ is $2(F_{2n-2} + F_{2n}) \times 2(F_{2n-2} + F_{2n})$ $(n > 1)$. Using a calculation similar to that of Identity (4), we obtain $\tau(m,n) = \frac{1}{2}\langle \mathbf{1}, \boldsymbol{B}_n^{m-2}\mathbf{1}\rangle$. We thus have the following result.

Lemma 3. *For any positive integer n, the following inequality holds:*

$$\eta = \lim_{m\to\infty}\left[(\lambda_{\max}(\boldsymbol{T}_m))^{\frac{1}{m}}\right] \leq \left[\limsup_{m\to\infty}\left(\mathrm{Trace}(\boldsymbol{T}_m^{2n})^{\frac{1}{2n}}\right)^{\frac{1}{m}}\right]$$
$$= \left[\limsup_{m\to\infty}\left(\frac{\hat{c}_{m,n}}{2}\langle \mathbf{1}, \boldsymbol{B}_n^{m-2}\mathbf{1}\rangle\right)^{\frac{1}{m}}\right]^{\frac{1}{2n}} = (\lambda_{max}(\boldsymbol{B}_n))^{\frac{1}{2n}}.$$

The proof is similar to that of Lemma 2.

Example 3. *If n=2, the "D2" and "U2" type row vectors are* $[0,0,0,0,0]_D$, $[0,0,0,1,0]_D$, $[0,0,1,0,0]_D$, $[0,1,0,0,0]_D$, $[0,1,0,1,0]_D$, $[1,0,0,0,1]_D$, $[1,0,1,0,1]_D$ $[0,0,0,0,0]_U$, $[0,0,0,1,0]_U$, $[0,0,1,0,0]_U$, $[0,1,0,0,0]_U$, $[0,1,0,1,0]_U$, $[1,0,0,0,1]_U$, $[1,0,1,0,1]_U$. *The transfer matrix $\boldsymbol{B}_2$ is*

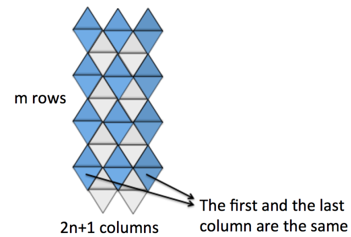


Fig. 5: Illustration of how $\boldsymbol{B}_n$ is constructed

$$\boldsymbol{B}_2 = \begin{pmatrix} \mathbf{0} & \boldsymbol{A}^{(DU2)} \\ \boldsymbol{A}^{(UD2)} & \mathbf{0} \end{pmatrix},$$

where

$$\boldsymbol{A}^{(DU2)} = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 1 & 1 & 0 & 0 \end{pmatrix}$$

and

$$\boldsymbol{A}^{(UD2)} = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 & 0 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix}.$$

The corresponding upper bound is $\eta \leq 1.5513$. Better bounds can be obtained via more strategic choices of matrix; this will be left to interested readers.

Thus, we obtain $1.546440708536001 \leq \eta \leq 1.5513$.

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