# Statistics of Maximal Independent Sets in Grid-like Graphs

Iowa State University, Summer 2024 REU

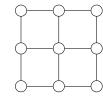
Cole Swain Levi Axelrod Luke Hawranick Nathan Bickel

January 1, 2025

### What are Independent sets?

#### Definition

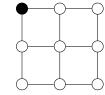
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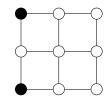
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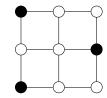
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# **Maximal Independent Sets**

#### **Definition**

A maximal independent set (MIS) I in a graph G is an independent set that is not a proper subset of an independent set.



#### **Goals**

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Let G be a graph. We define

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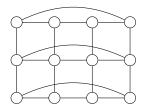
$$MIS(G) := \{ M \subseteq V(G) : M \text{ is a maximal independent set.} \}$$

We are interested in determining statistics of MIS's such as:

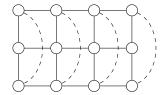
- Enumerating MIS's
- Describing symmetries
- Enumerating non-isomorphic MIS's
- Finding the average size of MIS's

# **Grid-like Graphs**

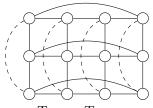
The four graphs are drawn below for m = 3 and n = 4:



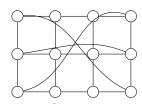
Fat Cylinder:  $FC_{m \times n}$ 



Thin Cylinder:  $TC_{m \times n}$ 



Torus:  $T_{m \times n}$ 



Möbius Strip:  $M_{m \times n}$ 

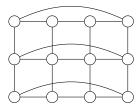
#### **Local and Global Structure**

Our grid graphs are Cartesian products of paths and cycles.

#### Definition

Let G be an  $m \times n$  grid-like graph. The **local structure** is the subgraph induced by a vertical slice of the graph, and the **global structure** is the subgraph induced horizontally.

For example, the fat cylinder has local path structure and global cyclic structure:



Fat Cylinder:  $FC_{m \times n}$ 

#### **States**

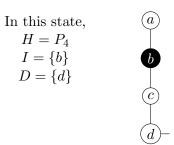
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A slice H is in **state** (H, I, D) if I is independent and D is the set of vertices that must be covered by the next slice.

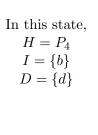


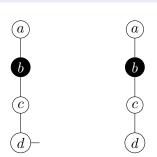
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In this state,  $H = P_4$   $I = \{b\}$  $D = \emptyset$ 

# **State Relationships**

#### Definition

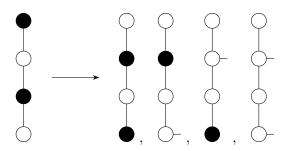
State  $s_2$  follows state  $s_1$  if a slice in state  $s_2$  can be pasted to the right of a slice in state  $s_1$  while maintaining an MIS.

# **State Relationships**

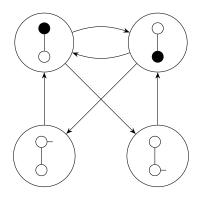
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For example,



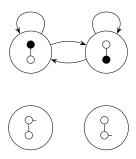
We can construct a directed graph with states as vertices and an arc from  $s_1$  to  $s_2$  if  $s_2$  follows  $s_1$ . For example:



 $P_2$  Map Digraph

# **Ticket Digraph**

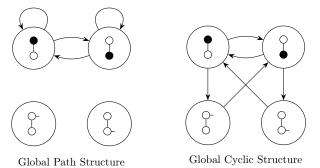
MIS's correspond to walks in the map digraph. We construct the *ticket digraph* to encode whether the endpoints of a walk in the map digraph are valid on a shape with a certain global structure:



Global Path Structure

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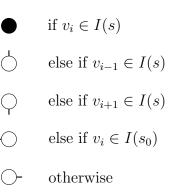
#### Properties of map digraph we know:

Let  $P_m$  or  $C_m$  be the slice of the grid-like graph and M be the map digraph.

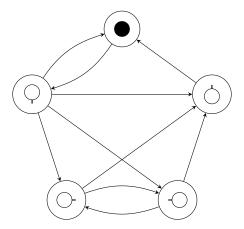
- Very strongly connected
- Number of vertices
- Number of edges
- $d^+(v)$  is a power of 2 for each  $v \in M$
- $\Delta^+(M) = 2^{\lceil \frac{m}{2} \rceil}$

#### Counting Map Digraph Vertices

Consider some slice, either  $P_m$  or  $C_m$ . All vertices on a slice are covered by some vertex in the MIS. s is the current state.  $s_0$  is the state which comes before s if it exists. Define the following 'vertex labels' below.



We can form a digraph to model which vertex labels can lie above each other vertex labels.



We can form a digraph to model which vertex labels can lie above each other vertex labels. Call the matrix below A. A(i,j) indicates if vertex label i can lie below label j in a state.

	•	$\bigcirc$	$\bigcirc$	-	<u></u>	
•	0	1	1	0	0	
$\bigcirc$	1	0	0	0	0	
$\bigcirc$	0	1	0	1	1	
-	0	1	0	0	1	
<u></u>	0	1	0	1	0 _	

The minimal polynomial of A yields the recurrence relation for the number of walks our vertex label map digraph. We determine the base cases by hand.

Minimal Polynomial:

$$x^4 - x^3 - x^2 - 1$$

Recurrence:

$$s(m) = s(m-1) + s(m-2) + s(m-4)$$

with

$$s(0) = 1, s(1) = 3, s(2) = 4, s(3) = 8.$$

We use the same technique to count the number of **edges** in the map digraph.

Recurrence:

$$f(m) = 3f(m-2) + 2f(m-3) + 3f(m-4) + 2f(m-5)$$

with

$$f(1) = 4, f(2) = 6, f(3) = 14, f(4) = 30, f(5) = 66, f(6) = 142$$

#### **Metro Pairs**

Our method for counting MIS's in grid-like graphs comes down to computing sequences that can be described by walks on the map digraph that satisfy tickets, so we created notation to condense this idea.

#### **Definition**

A **metro pair** is a pair of directed graphs (M,T) sharing a vertex set S such that for any sufficiently large n, for any  $u,v\in S$ , there exists a uv-walk along M of length n, and E(T) is nonempty. Define the **travel sequence** of (M,T) to be  $\tau(n)=$  the number of uv-walks of length n such that  $(u,v)\in E(T)$ .

#### **Metro Pairs**

We can express the travel sequence in terms of linear algebra with

$$\tau(n) = A_T \bullet A_M^n,$$

where  $A_M$  and  $A_T$  are the (transposes of the) adjacency matrices of M and T and  $\bullet$  is the vector dot product.

Using the Perron-Frobenius Theorem, we know that

$$\lim_{n \to \infty} \frac{\tau(n)}{r^n} = A_T \bullet \frac{\vec{v}\vec{w}^\top}{\vec{w}^\top \vec{v}},$$

where r is the principle eigenvalue of  $A_M$  and  $\vec{w}^{\top}, \vec{v}$  are the principle left and right eigenvectors of  $A_M$ .

### **Globally Cyclic Structures**

#### **Theorem**

Let H be a graph, and let  $\phi$  be a graph automorphism of H. Let r be the principle eigenvalue of the map digraph M of H. Then

$$\lim_{n \to \infty} \frac{|\operatorname{MIS}((H \square P_{n+1})/\phi)|}{r^n} = 1.$$

In particular, this is a generalization of the result that

$$\lim_{n \to \infty} \frac{|\operatorname{MIS}(M_{m \times n})|}{|\operatorname{MIS}(FC_{m \times n})|} = 1.$$

# **Globally Cyclic Structures**

#### Proof sketch:

- 1. The vertices of M are pairs of subsets of H, so an automorphism  $\phi$  of H gives us and automorphism  $\phi^*$  of M.
- 2. The eigenvectors of  $A_M$  are determined the graph structure of M, so if two vectors are sent to each other by an automorphism, their entries of the eigenvectors must be the same.
- 3. The ticket graph consisting of tickets  $(i, \phi^*(i))$  must give the same result as the one consisting of tickets (i, i) when dotted with  $\frac{\vec{v}\vec{w}^{\top}}{\vec{v}\vec{i}^{\top}\cdot\vec{v}}$ .

4.

$$I \bullet \frac{\vec{v} \vec{w}^\top}{\vec{w}^\top \vec{v}} = \frac{\vec{w}^\top \vec{v}}{\vec{w}^\top \vec{v}} = 1.$$

Seungsang Oh defined and proved the existence of what he called the maximal hard square entropy constant:

$$\kappa := \lim_{m,n \to \infty} |\operatorname{MIS}(G_{m \times n})|^{\frac{1}{mn}}.$$

This constant plays a large role in all of the limits we are trying to compute, as the above limit yields the same result for each structure we are studying. In particular, if  $r_H$  is the principle eigenvalue of the adjacency matrix of the map digraph of H, we have

$$\lim_{m \to \infty} (r_{P_m})^{\frac{1}{m}} = \kappa = \lim_{m \to \infty} (r_{C_m})^{\frac{1}{m}}.$$

Oh proved that the limit existed by showing it was equal to

$$\sup_{m,n} |\operatorname{MIS}(G_{m\times n})|^{\frac{1}{(m+1)(n+1)}},$$

which he bounded above by 16. He also estimated the value of  $\kappa$  to be a little over

$$|\operatorname{MIS}(G_{8\times380})|^{\frac{1}{(8+1)(380+1)}} \approx 1.225084.$$

We have improved on both of these bounds. For a lower bound, we calculated

$$\kappa = \sup_{m,n} |\operatorname{MIS}(G_{m \times n})|^{\frac{1}{(m+1)(n+1)}} \ge \lim_{n \to \infty} |\operatorname{MIS}(G_{10 \times n})|^{\frac{1}{(10+1)(n+1)}}$$
$$= \sqrt[11]{r_{P_{10}}} \approx 1.230538.$$

For an upper bound, we calculated first that

$$\kappa = \lim_{m,n\to\infty} |\operatorname{MIS}(G_{m\times n})|^{\frac{1}{mn}} \le \lim_{m,n\to\infty} |\mathcal{P}(V(G_{m\times n}))|^{\frac{1}{mn}} = 2.$$

We then improved again on this upper bound by more tightly bounding the number of MIS's total.

In an MIS, each slice must be in a state, so given some local structure with s states, there are at most  $s^n$  MIS's of that structure with n slices. This gives  $\kappa \leq (s^n)^{\frac{1}{mn}} = (s)^{\frac{1}{m}}$ .

If there are  $s_l$  walks in the map digraph of length l, that that would similarly give us  $\kappa \leq (s_l^{\frac{n}{l}})^{\frac{1}{mn}} = (s)^{\frac{1}{lm}}$ .

We have found a way to compute  $s_l$  for large local structures and small values of l, and as such were able to give an upper bound with l = 7 of  $\kappa < 1.311534$ .

#### **Theorem**

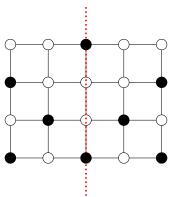
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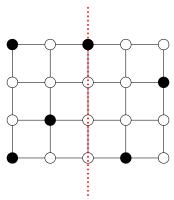
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Consider the set of MISs on some  $G_{m \times n}$ . Some of these MIS's have symmetry. Some do not.

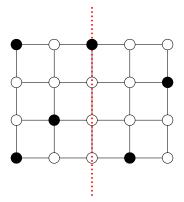


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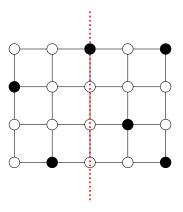
#### **Asymmetric Case**

Consider some MIS which does **not** have symmetry over this axis.



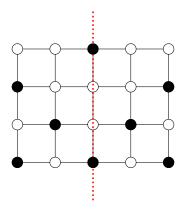
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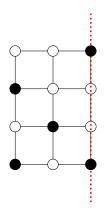
#### Symmetric Case - odd n

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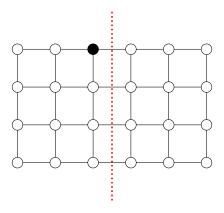


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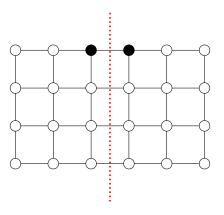
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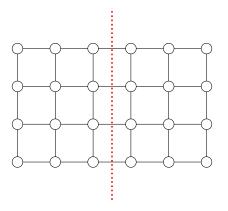
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There is no way for an MIS on  $G_{m \times n}$  to contain two empty slices.

### What is a Non-isomorphic MIS?

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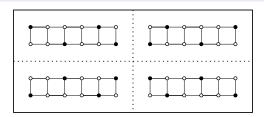


Figure: MIS  $G_{2\times 6}$ 

We found:

$$|\operatorname{NIMIS}(G_{2\times n})| = \begin{cases} \frac{F(n) + F(\frac{n}{2})}{2} & \text{if } n \text{ is even} \\ \frac{F(n) + F(\frac{n+3}{2})}{2} & \text{if } n \text{ is odd} \end{cases}$$

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#### Proof Sketch:

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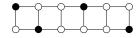
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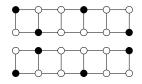
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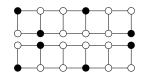
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- This pair of MIS's in  $G_{2\times 6}$  maps to 110101:



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- We count the amount of symmetrical strings, add them to F(n), and then divide by 2 to get rid of the double counting.

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$$|\operatorname{NIMIS}(G_{2\times n})| = \begin{cases} \frac{F(n) + F(\frac{n}{2})}{2} & \text{if } n \text{ is even} \\ \frac{F(n) + F(\frac{n+3}{2})}{2} & \text{if } n \text{ is odd} \end{cases}$$

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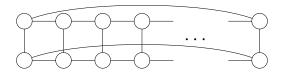
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Consider the set of MISs on  $FC_{2\times n}$  below.



For each MIS on  $FC_{2\times n}$ , generate the corresponding cyclic binary string.

- no consecutive 0s
- even number of 1s

Each string corresponds to a pair of isomorphic MISs, which can be obtained by reflection over horizontal axis between row 1 and 2.

The problem is now translated to finding the number of distinguishable cyclic strings in our set.

#### Example:

011010111 is not distinguishable among:

$$101101011, 110110101, \dots$$
(rotational symmetry)

110101101, 101011011, . . . 
$$\left(\text{reflection symmetry over index } \frac{n+1}{2}\right)$$

#### Collapsed Strings

To make life easier, each binary string can be collapsed into a smaller string.

 $\{011010111, 101101011, 110110101\} \rightarrow `213'$ 

#### How many collapsed strings can we have?

The number of digits of the collapsed string + the sum of the digits must be n. Let  $P_n(k)$  be the number of nonnegative integer partitions of n into k parts.

#### How many collapsed strings can we have?

For an even non-collapsed string b of length n, b must have an even number 2k of 0s. Each index of a collapsed string must be at least 1. Thus, for each value of 2k, the set of collapsed strings is  $P_{n-4k}(2k)$ .

$$\geq 1 \quad | \quad \geq 1 \quad | \quad \geq 1 \quad | \quad \cdots \quad | \quad \geq 1 \quad |$$

The group of symmetries of a cyclic string of length n is equivalent to the group of symmetries of an n-gon:  $D_n$ .

#### Burnside's Lemma

#### Theorem

Let G be a finite group acting on X, and let X/G be the set of orbits of X. Then,

$$|X/G| = \frac{1}{|G|} \sum_{g \in G} |X^g|$$

where  $X^g$  is the set of fixed points of X with respect to  $g \in G$ .

Therefore, with the help of Burnside's Lemma,

$$|\operatorname{NIMIS}(FC_{2\times n})| = \begin{cases} 1 + \sum_{k=1}^{\lfloor \frac{n}{4} \rfloor} |P_{n-4k}(2k)/D_{4k}| & \text{if } n \text{ is even} \\ \sum_{k=1}^{\lfloor \frac{n-2}{4} \rfloor} |P_{n-4k-2}(2k+1)/D_{4k+1}| & \text{if } n \text{ is odd} \end{cases}$$

## Average Size of MIS's

#### Definition

Let G be a graph. Then the **total MIS size** is

$$T(G) := \sum_{I \in \text{MIS}(G)} |I|.$$

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$$A(G) := \frac{T(G)}{|\operatorname{MIS}(G)|}.$$

We found that

$$T(G_{2\times n}) = 2\sum_{i=1}^{n} F(i)F(n+1-i).$$

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- Note that each 1 splits the string into two valid substrings
- Example:

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- Example:

#### **1**0101**1**01**1**

• Use that each substring is counted by F(i)

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Barbossa showed that the MIS sizes in  $FC_{2\times n}$  range from  $\frac{n}{2}$  to n. Since  $\frac{\varphi}{\sqrt{5}} \approx 0.724$ , the average MIS is a bit under the midpoint.

### **General Case**

Let G be an  $m \times n$  grid-like graph. We can use transfer matrices to obtain T(G). The reasoning is similar to in the  $G_{2\times n}$  case.

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Let H be the local structure of G,  $s_1, \ldots, s_N \in S(H)$  the states, A the transfer matrix of H, and T the ticket matrix of G. Then,

$$T(G) = \sum_{ij \in E(T)} \sum_{k=1}^{N} |I(s_k)| \sum_{m=1}^{n} (A^{m-1})_{(k,i)} (A^{n-m})_{(j,k)}.$$

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