Seminar, WS 22/23

Constructions in combinatorics via neural networks

Based on (Wagner, 2021)

Sandro Roch

Article

Advancing mathematics by guiding human intuition with AI

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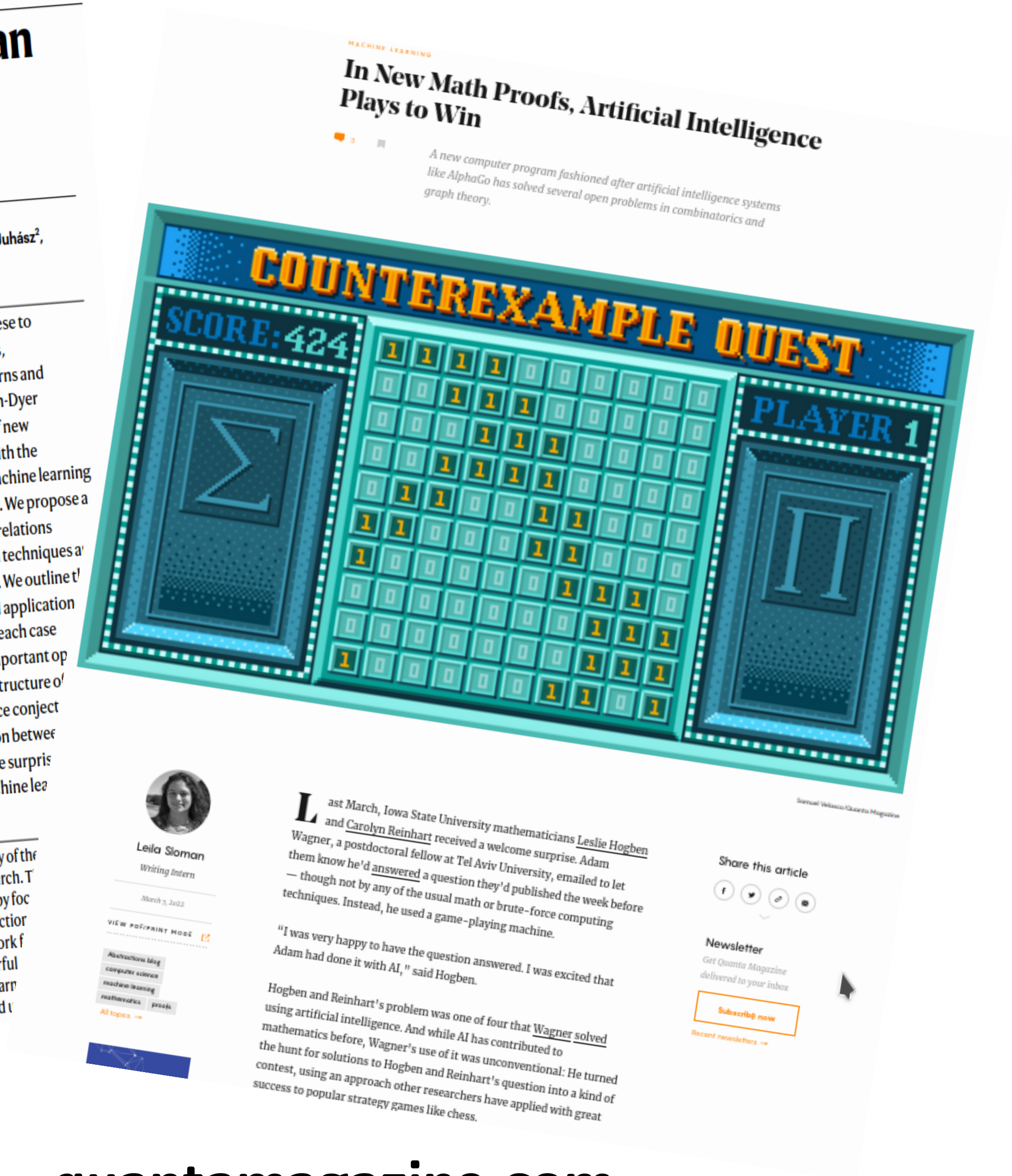
The practice of mathematics involves discovering patterns and using these to formulate and prove conjectures, resulting in theorems. Since the 1960s, mathematicians have used computers to assist in the discovery of patterns and formulation of conjectures[1], most famously in the Birch and Swinnerton-Dyer conjecture[2], a Millennium Prize Problem[3]. Here we provide examples of new fundamental results in pure mathematics that have been discovered with the assistance of machine learning—demonstrating a method by which machine learning can aid mathematicians in discovering new conjectures and theorems. We propose a process of using machine learning to discover potential patterns and relations between mathematical objects, understanding them with attribution techniques a using these observations to guide intuition and propose conjectures. We outline t machine-learning-guided framework and demonstrate its successful application current research questions in distinct areas of pure mathematics, in each case showing how it led to meaningful mathematical contributions on important op problems: a new connection between the algebraic and geometric structure o and a candidate algorithm predicted by the combinatorial invariance conject symmetric groups[4]. Our work may serve as a model for collaboration betwe fields of mathematics and artificial intelligence (AI) that can achieve surpris by leveraging the respective strengths of mathematicians and machine lea

One of the central drivers of mathematical progress is the discovery of patterns and formulation of useful conjectures: statements that are suspected to be true but have not been proven to hold in all cases. Mathematicians have always used data to help in this process—from the early hand-calculated prime tables used by Gauss and others that led to the prime number theorem[5], to modern computer-generated data[1,5] in cases such as the Birch and Swinnerton-Dyer conjecture[2]. The introduction of computers to generate data and test conjectures

that AI can also be used to assist in the discovery of the jectures at the forefront of mathematical research. T using supervised learning to find patterns[20–24] by foc mathematicians to understand the learned functior mathematical insight. We propose a framework f standard mathematician's toolkit with powerful and interpretation methods from machine learr its value and generality by showing how it led t

nature

Article citing Wagner



MACHINE LEARNING

In New Math Proofs, Artificial Intelligence Plays to Win

A new computer program fashioned after artificial intelligence systems like AlphaGo has solved several open problems in combinatorics and graph theory.

Leila Sloman

Writing Intern

March 7, 2022

Last March, Iowa State University mathematicians Leslie Hogben and Carolyn Reinhart received a welcome surprise. Adam Wagner, a postdoctoral fellow at Tel Aviv University, emailed to let them know he'd answered a question they'd published the week before — though not by any of the usual math or brute-force computing techniques. Instead, he used a game-playing machine.

"I was very happy to have the question answered. I was excited that Adam had done it with AI," said Hogben.

Hogben and Reinhart's problem was one of four that Wagner solved using artificial intelligence. And while AI has contributed to mathematics before, Wagner's use of it was unconventional: He turned the hunt for solutions to Hogben and Reinhart's question into a kind of contest, using an approach other researchers have applied with great success to popular strategy games like chess.

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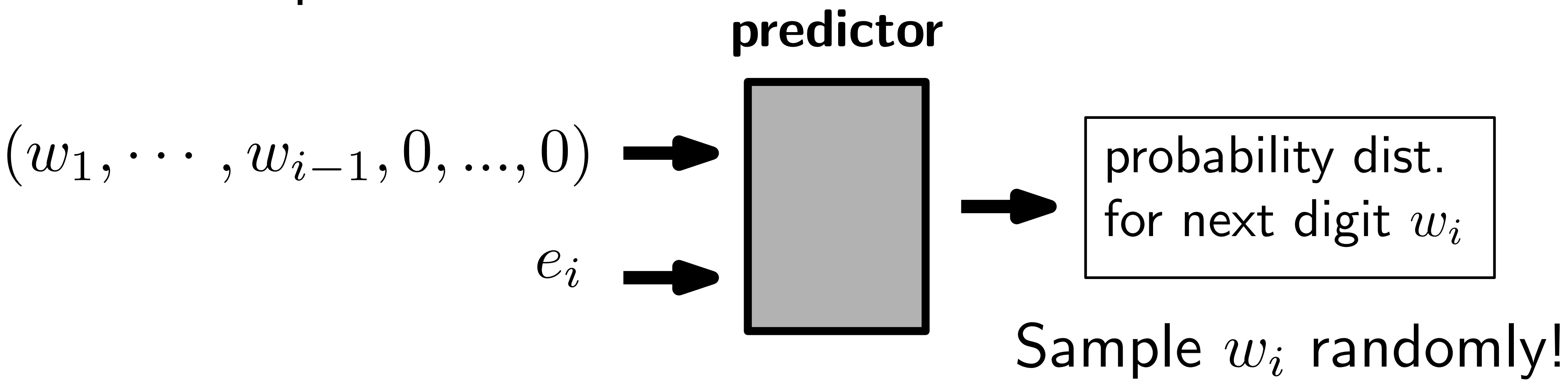
Article dedicated to Wagner's work

Generating structures using reinforcement learning

- Encode instances by fixed length word w over fin. alphabet

  Example: Graph on n vertices as $w \in \{0,1\}^{\binom{n}{2}}$

- Start with empty word
- In i-th step:



Generating structures using reinforcement learning

Deep cross-entropy method:

- Generate $N > 0$ instances
- For each instance: Evaluate score function
  Ex.: „*How close is instance to conjectured bound?*“
- For top y percentage of instances:

  Training: Fit predictor on pairs

  $$((w_1, ..., w_{i-1}, 0, ..., 0),\ \ e_i) \ \ \rightarrow \ \ e_{w_i}$$

- Keep top $x < y$ percentage of instances
  for next iteration(s)

Generating structures using reinforcement learning

Architecture of predictor

- Neural network with three hidden layers:
  dense layers with 128 / 64 / 4 nodes
  activation function: ReLU
- Output layer: sigmoid (binary case)
- Loss function: Cross entropy
- Optimizer: SGD

Example

M. Aouchiche and P. Hansen, *A survey of automated conjectures in spectral graph theory*, 2010:

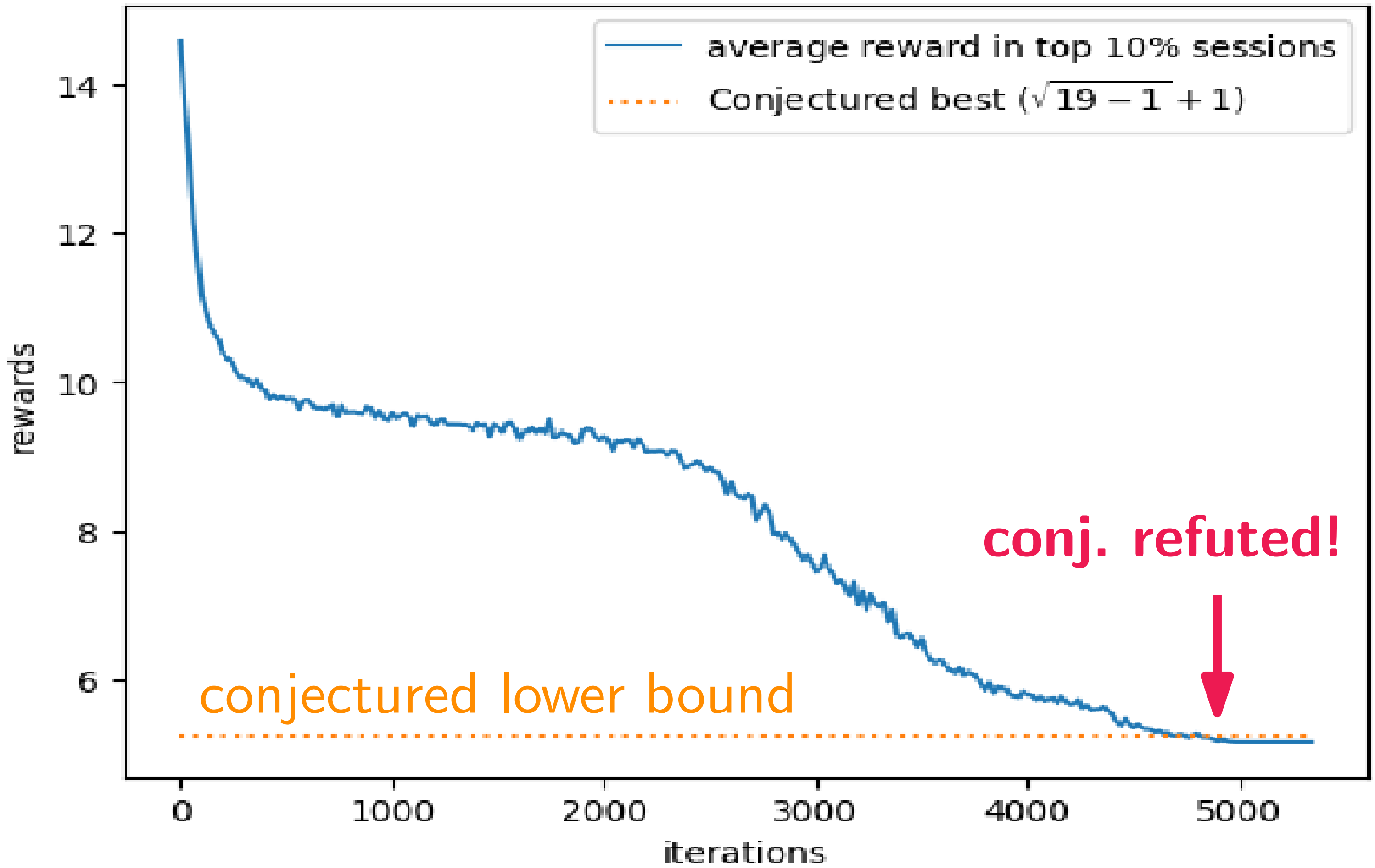
Conjecture: G connected graph, $n \geq 3$, largest eigenvalue λ_1, matching number μ. Then:

$$\lambda_1 + \mu \geq \sqrt{n-1} + 1$$

Apply cross-entropy method:
Fix n, minimize score function $\lambda_1 + \mu$

Example

For $n = 19$, average score after many iterations:



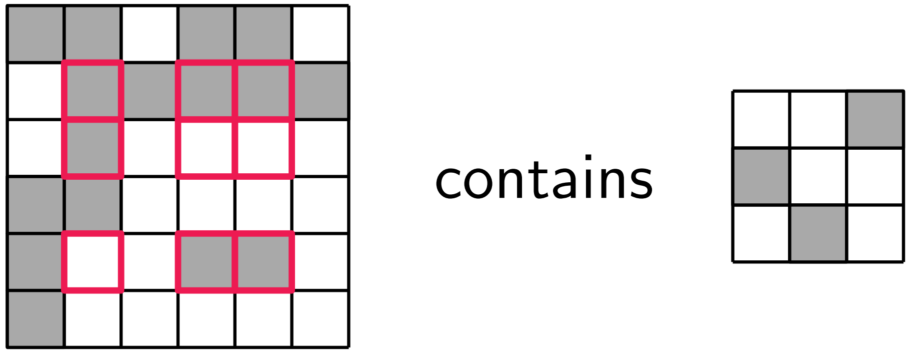
Pattern avoiding 0-1-matrices

Definition: 0-1-matrix patterns

The 0-1-matrix $A \in \{0,1\}^{r \times s}$ *contains* 0-1-matrix $P \in \{0,1\}^{k \times l}$, if there exists a submatrix $D \in \{0,1\}^{k \times l}$ with $P \leq D$.

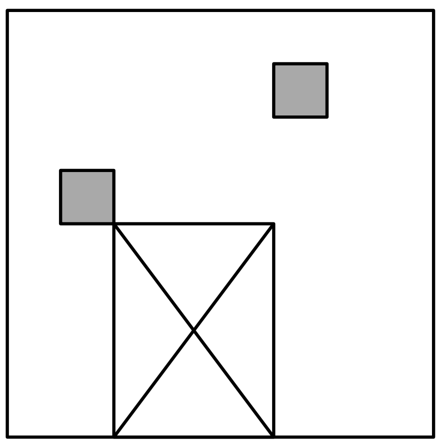
Otherwise, A *avoids* P.

Example:



Pattern avoiding 0-1-matrices

- $P_\pi := [\delta_{j,\pi(i)}]_{i,j} \in \{0,1\}^{n\times n}$ permutation matrix of $\pi \in S_n$
- **Def:** 0-1-matrix M *contains* (resp. *avoids*) $\pi \in S_k$,
  if M avoids (resp. contains) P_π.
- **Example:** 312-avoiding 0-1-matrices:



- **Obs.:** P_π avoids P_σ iff π avoids σ as permutation pattern.

Permanent in pattern avoiding 0-1-matrices

Motivation: If $A \in \{0,1\}^{n\times n}$ avoids π, then the permanent

$$\mathrm{per}(A) := \sum_{\sigma\in S_n} \prod_{i=1}^{n} a_{i,\sigma(i)}$$

counts (π-avoiding) permutations S_n contained in A.

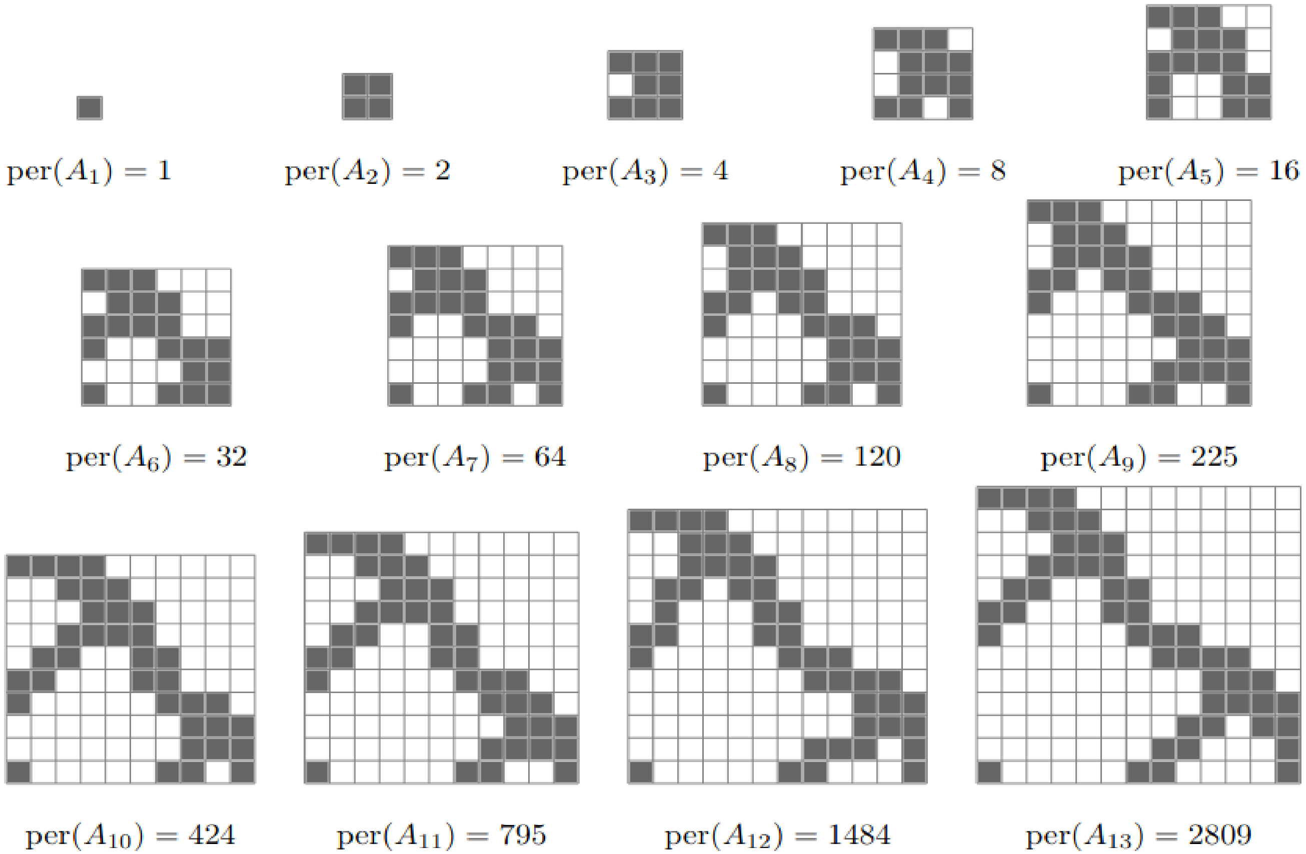
Question (Brualdi & Cao, 2020):
Given $n \in \mathbb{N}$ and $\pi \in S_k$, what is the value of

$$f_\pi(n) := \max\left\{\mathrm{per}(A) : A \in \{0,1\}^{n\times n}, A \text{ avoids } \pi\right\}$$

Here: Wagner finds bounds on f_{312}.

Permanent in pattern avoiding 0-1-matrices

Using the cross-entropy method, find 312-avoiding matrices with high permanent:



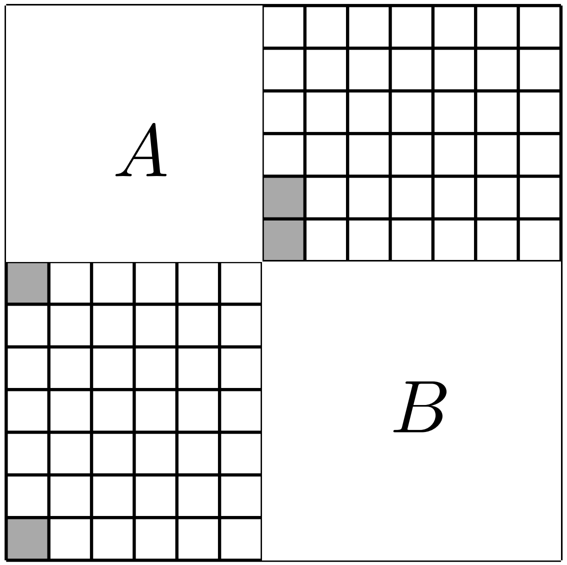
Breaks conjectured value $f_{312}(5) = 12$ by Brualdi and Cao!

Permanent in pattern avoiding 0-1-matrices

Theorem:

$$2^{0.88n} \leq f_{312}(n) \leq 24^{n/4} \approx 2^{1.15n}$$

Proof of lower bound:

$A * B :=$ 

Observation:

- $\mathrm{per}(A * B) \geq \mathrm{per}(A) \cdot \mathrm{per}(B)$
- $f_{312}(n + m) \geq f_{312}(n) \cdot f_{312}(m)$

Idea: Use $\mathrm{per}(A_{13}) = 2809 > 2^{0.88 \cdot 13}$ and Fekete's Lemma.

$\square$

Proof of upper bound:

Theorem (Bregman & Minc, 1973):
For $A \in \{0,1\}^{n \times n}$ with row sums $r_1, \ldots, r_n$:

$$\mathrm{per}(A) \leq \prod_{i=1}^{n} (r_i!)^{1/r_i}$$

Proposition (Brualdi & Cao, 2020):
At most $4n - 4$ one entries in 312-avoiding matrix $M \in \{0,1\}^{n \times n}$.

Idea: rhs. expression maximized when all $r_i = 4$. $\square$

Organization of the seminar

For obtaining 6 LP:

- Read Wagner's paper, understand the method
- Pick a problem and think of an AI-attack:
  - Encoding of instances
  - Variation of Wagner's method
- Send me a short draft of your approach
- Set up the environment, implement your approach (and modifications of it)
- Give a short presentation in the end of the semester about the problem, the approach and the result.

Don't avoid questions!