Synthesizing Minimal Tile Sets for Patterned DNA Self-Assembly

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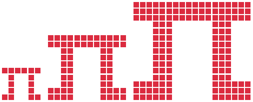
Outline

1. Previous Study
2. Problem Definition
3. Approach of Ma & Lombardi
4. Our Contributions

Previous Study

Shapes modulo Scale

[Soloveichik & Winfree 2004]



Unsolvable

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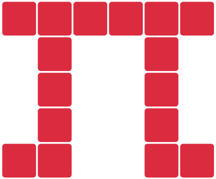
[Adleman et al. 2002]



NP-hard

Previous Study

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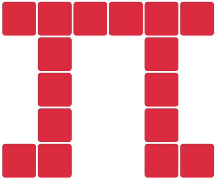
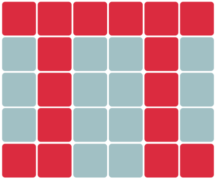


NP-hard

Patterns

[Ma & Lombardi 2008]

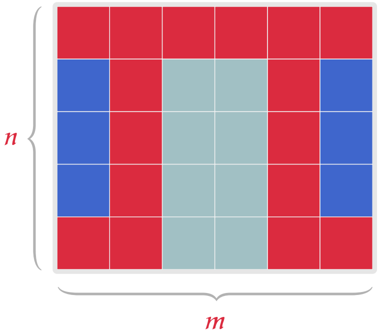


Not known?

Pattern self-Assembly Tile set Synthesis (PATS)

Input

A k-colouring $c : [m] \times [n] \to [k]$



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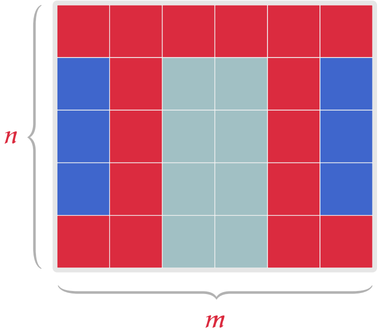

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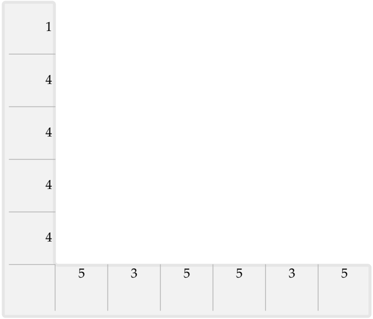

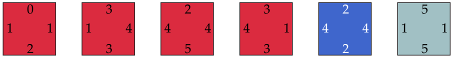

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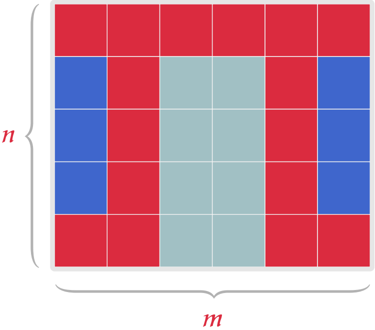

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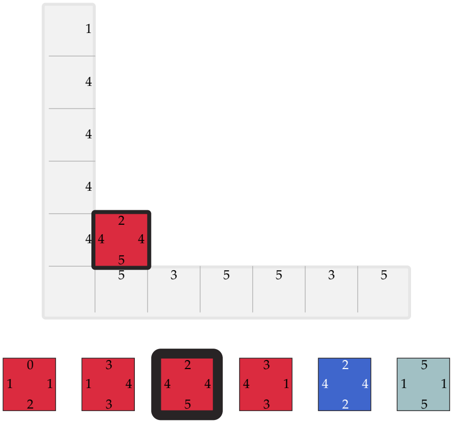

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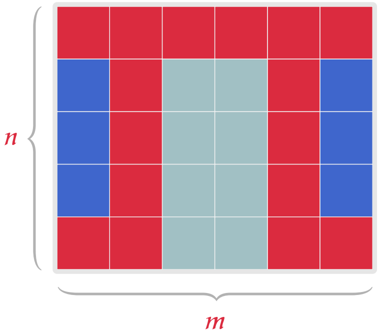

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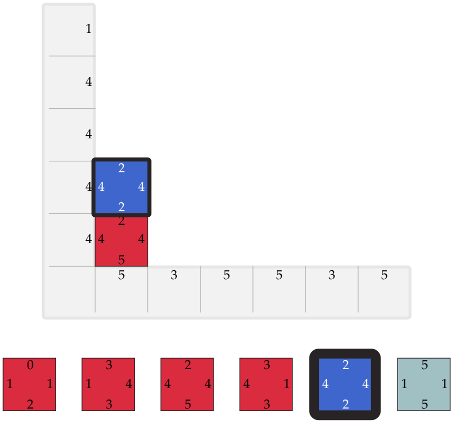

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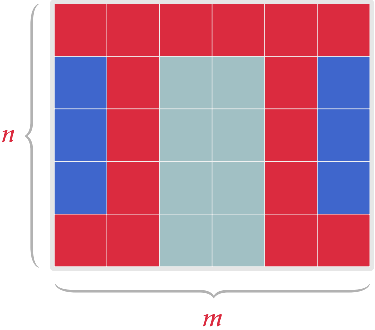

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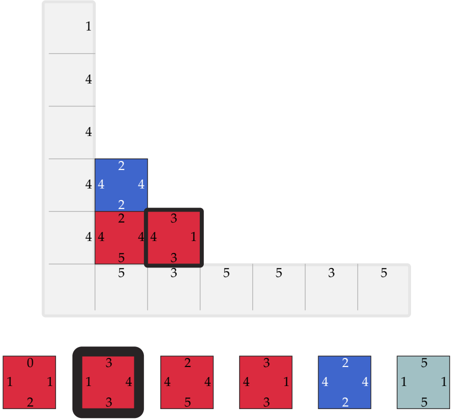

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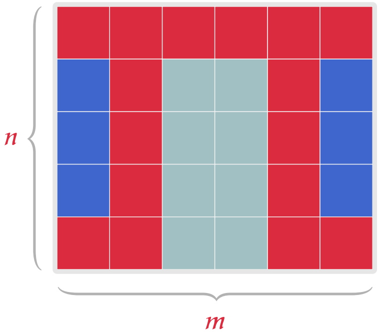

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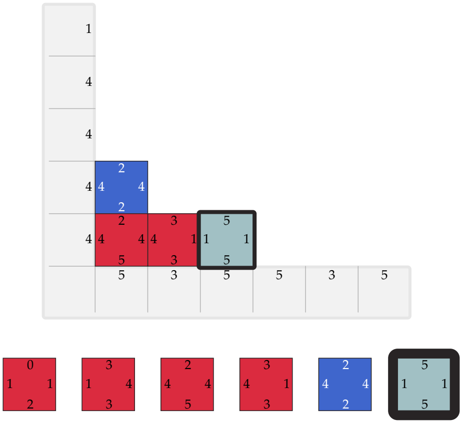

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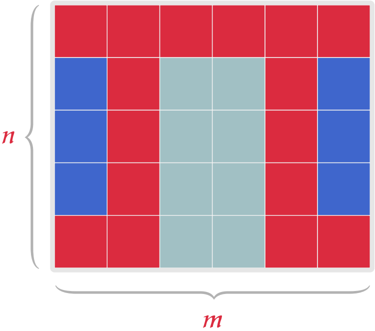

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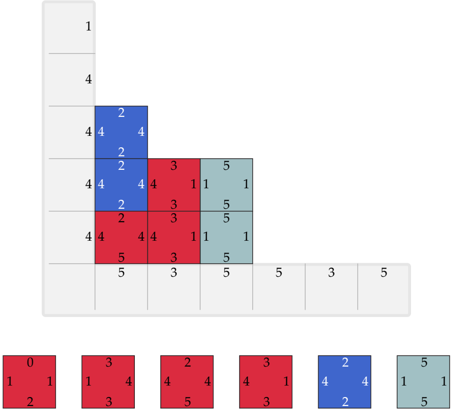

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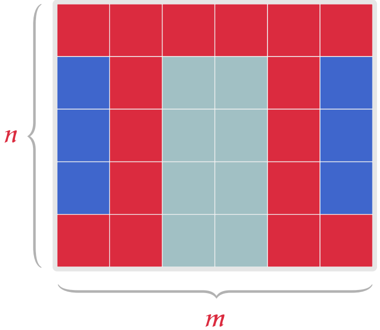

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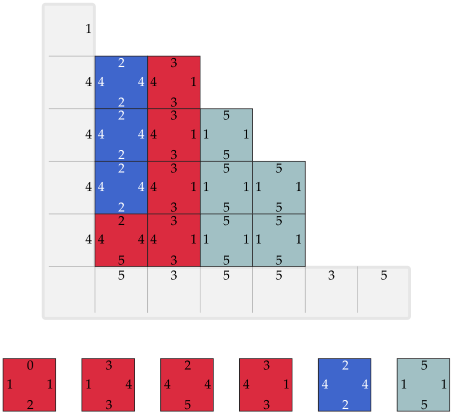

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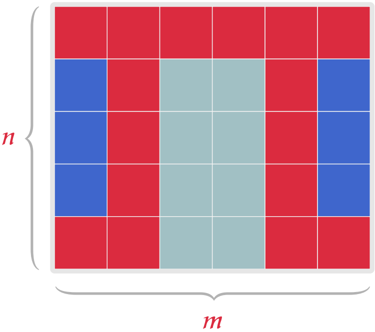

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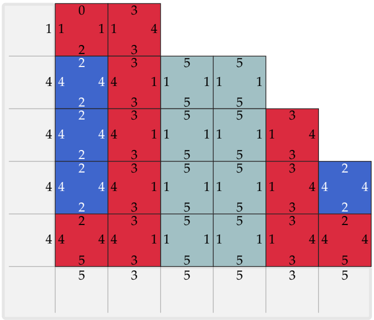

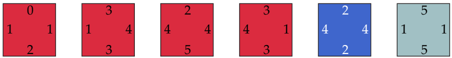

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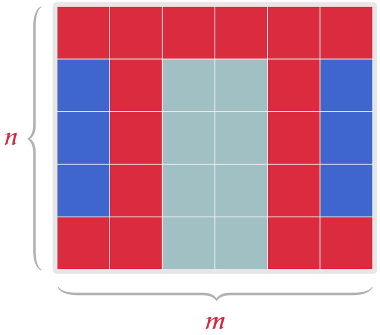

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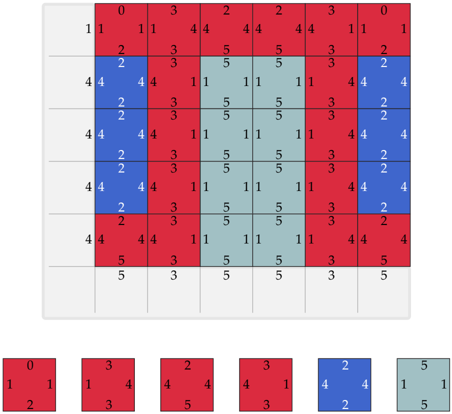


Pattern self-Assembly Tile set Synthesis (PATS)

Given: A k-colouring $c : [m] \times [n] \to [k]$.

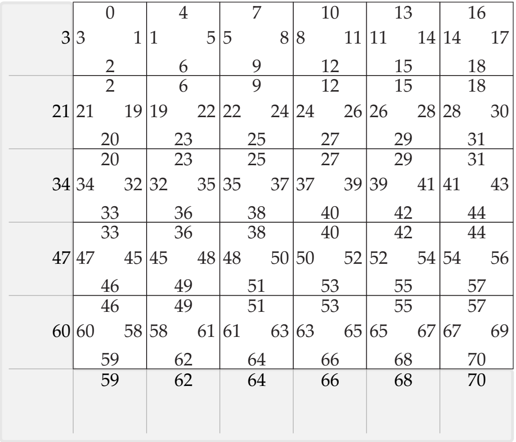
Find: A tile assembly system $\mathscr{T} = (T, \mathcal{S}, s, 2)$ s.t.

P1. The tiles in T have bonding strength 1.

P2. The domain of $\mathcal{S}$ is $[0, m] \times \{0\} \cup \{0\} \times [0, n]$ and all the terminal assemblies have the domain $[0, m] \times [0, n]$.

P3. There exists a colouring $d : T \to [k]$ such that for each terminal assembly $\mathcal{A} \in \mathrm{Term}\,\mathscr{T}$ we have $d(\mathcal{A}(x, y)) = c(x, y)$ for all $(x, y) \in [m] \times [n]$.

Approach of Ma & Lombardi



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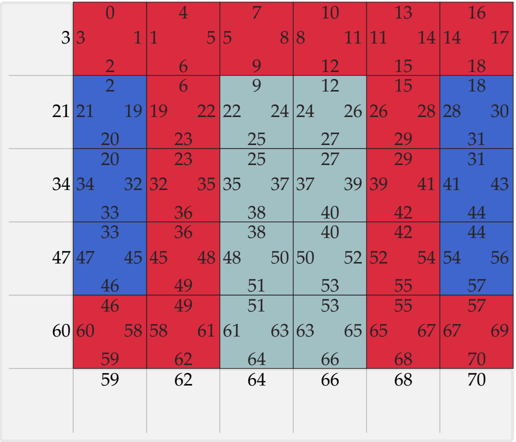

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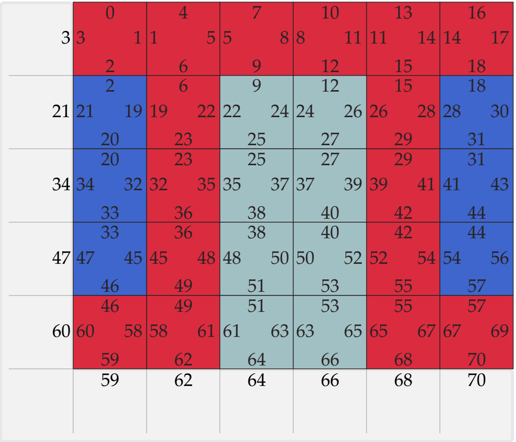


To minimize Tile set size:

- Merge glues
- Merge tiles

If conflicts arise:

- Continue merging!

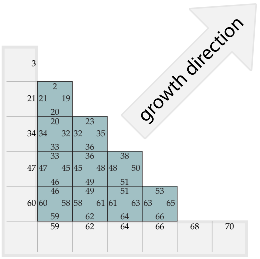
Our Contributions

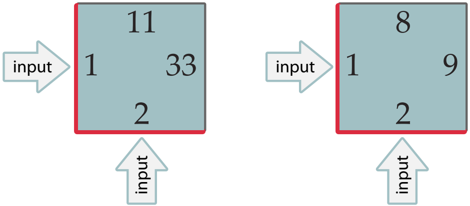
We present

1. Extension of the work of Ma & Lombardi
2. Branch & Bound algorithm
3. Pruning heuristics

Determinism

Lemma: **Minimal solutions to the PATS problem are** ***deterministic***





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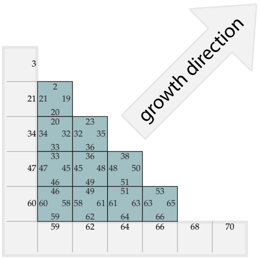
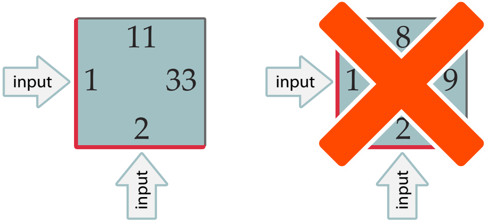
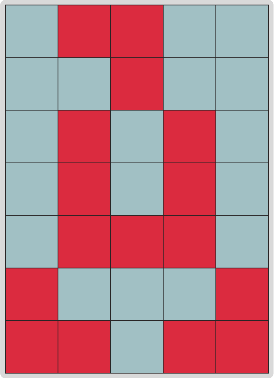




Partition Centric View



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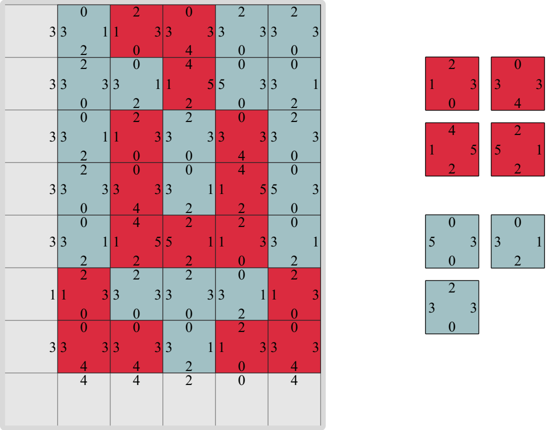

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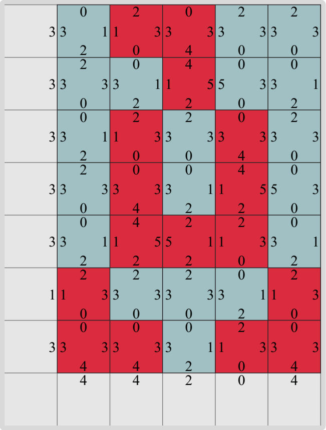
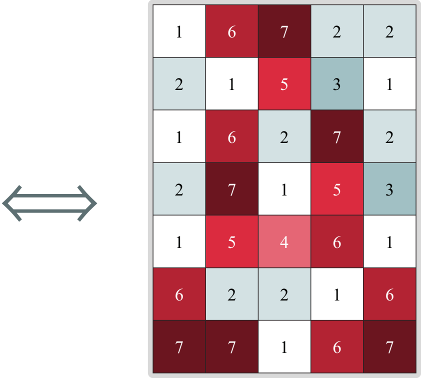
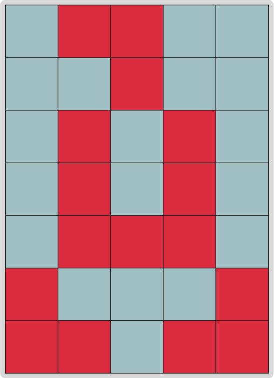


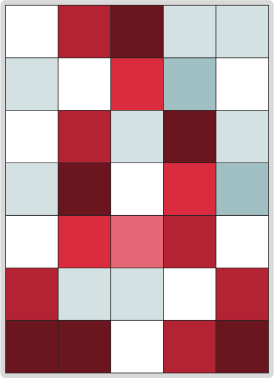


Contructible partition of $[m] \times [n]$

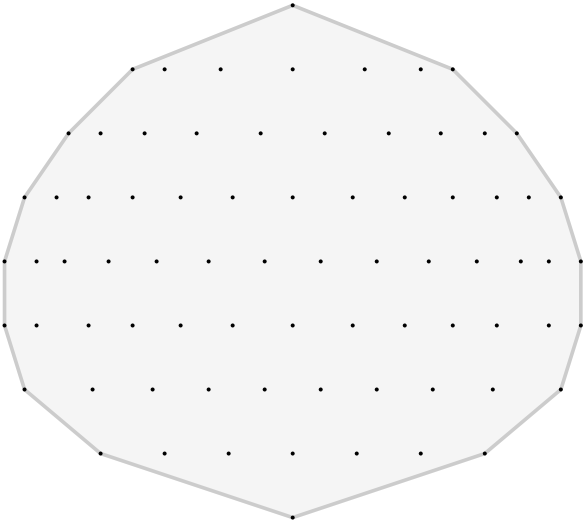
Partition Centric View



is **coarser** than



Searching the Lattice of Partitions



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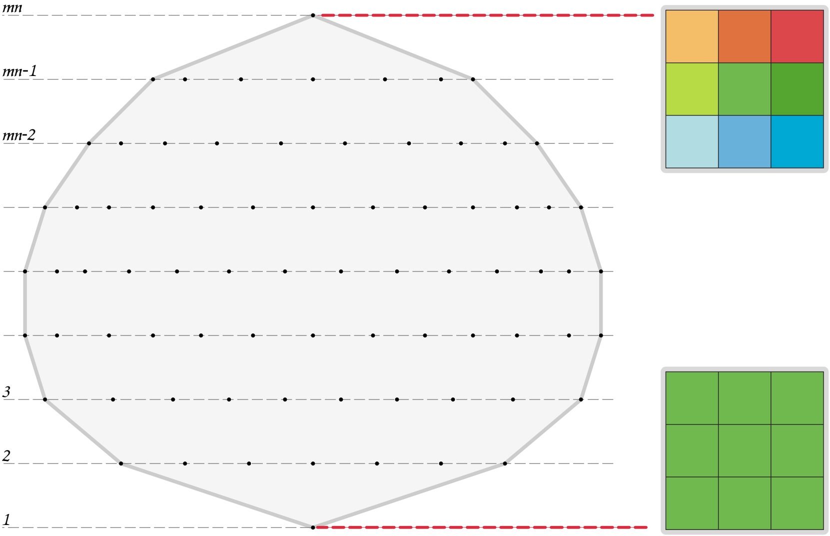

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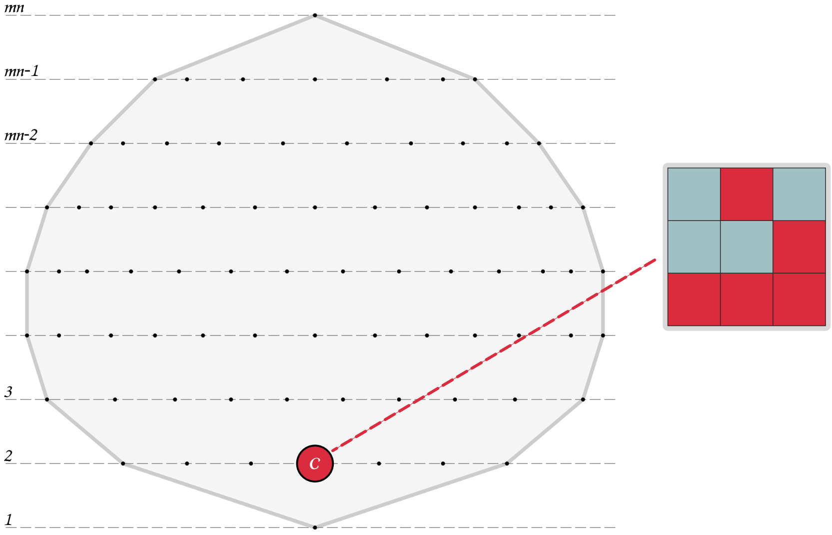

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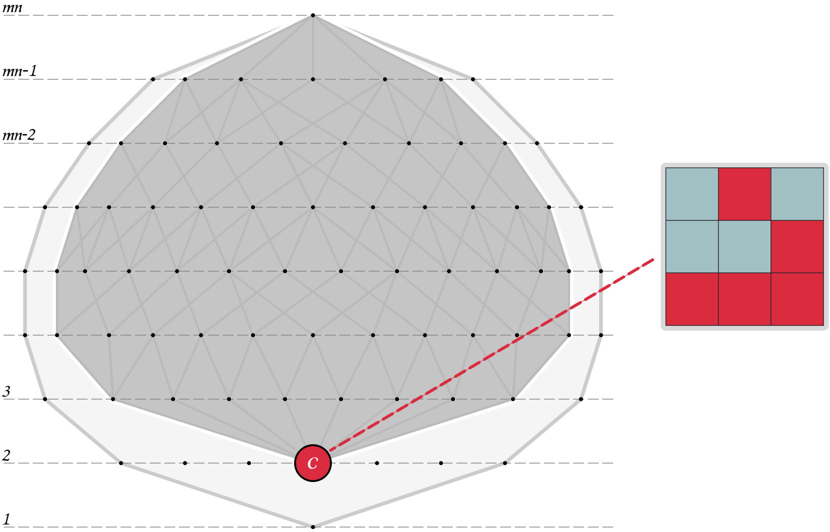

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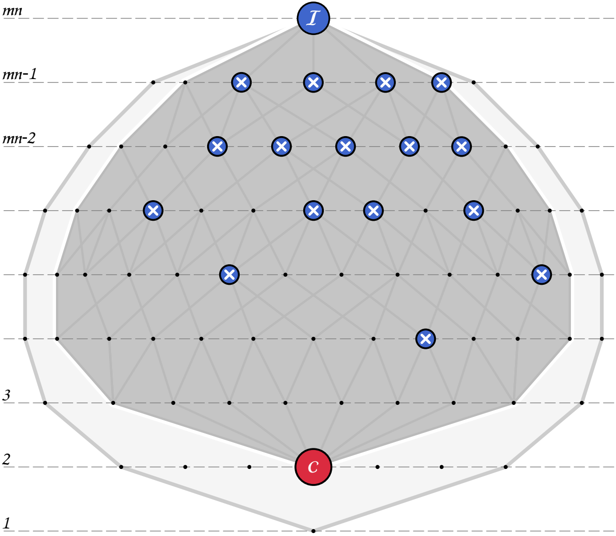

Contructible
partition

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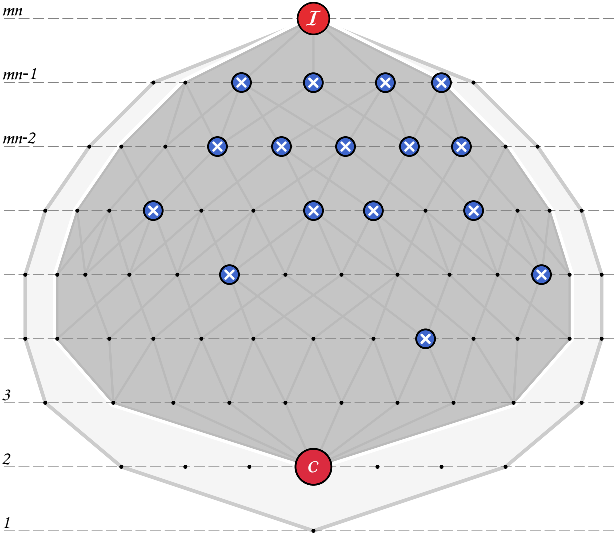

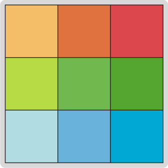

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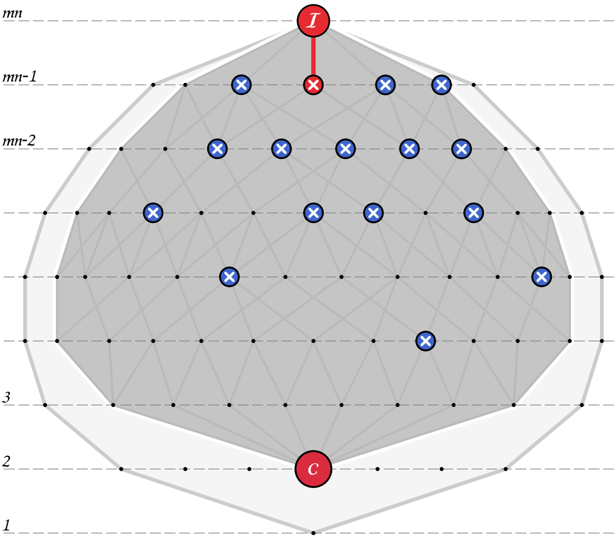

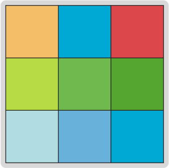

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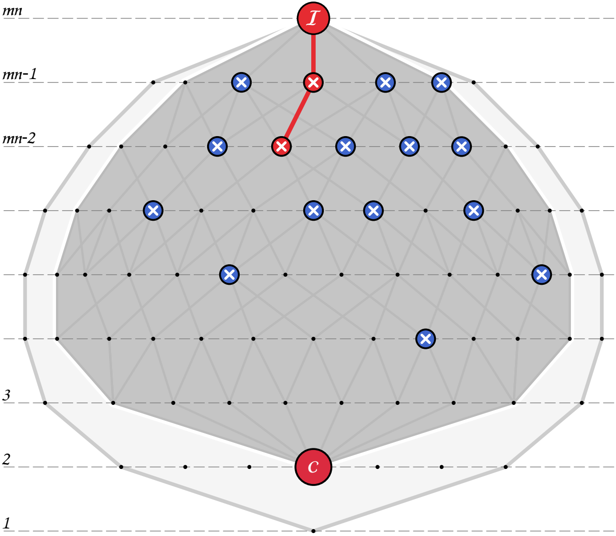

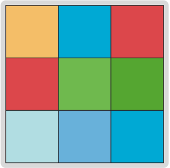

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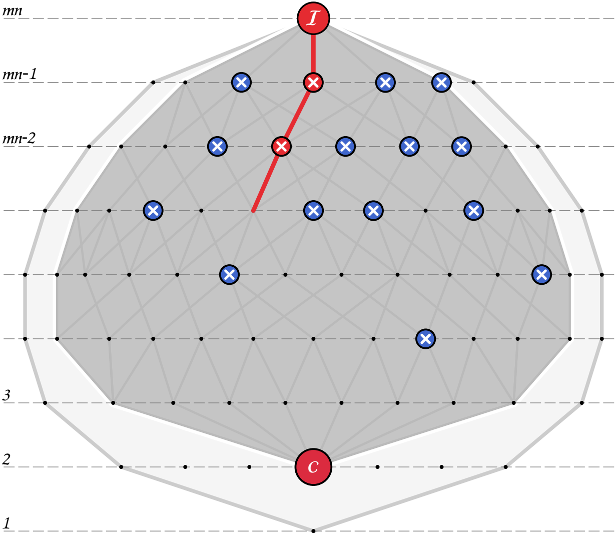

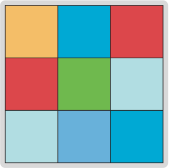

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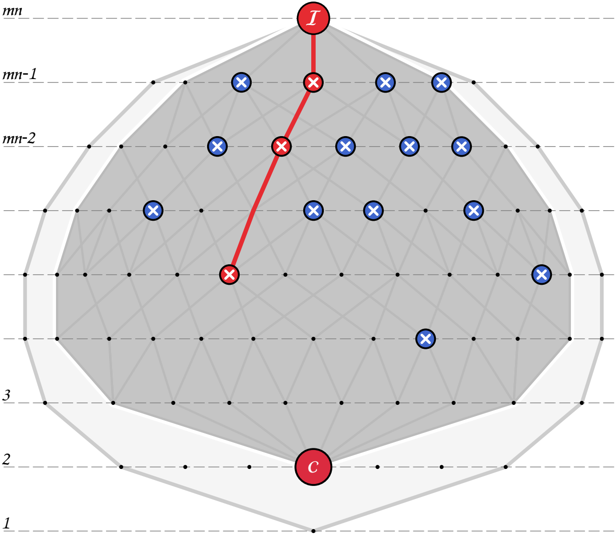

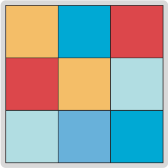

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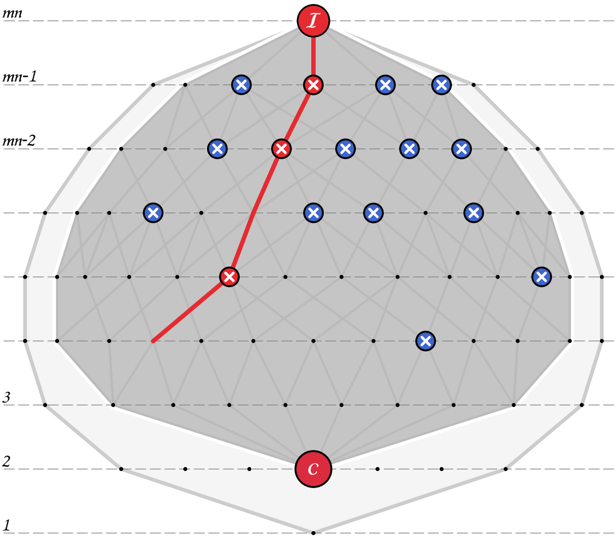

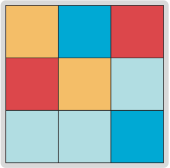

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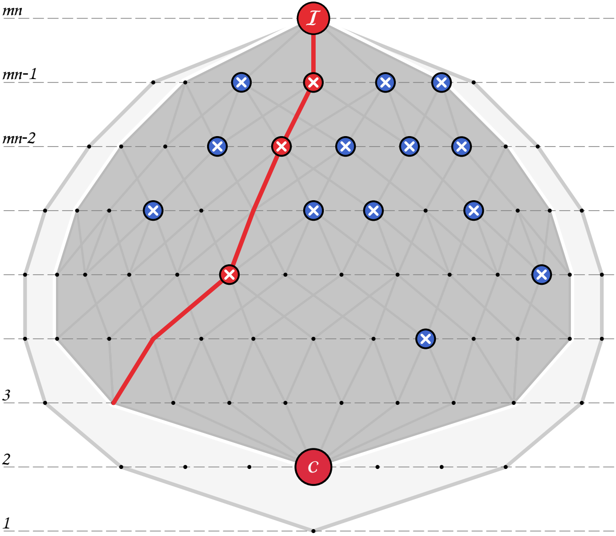

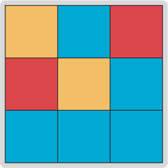

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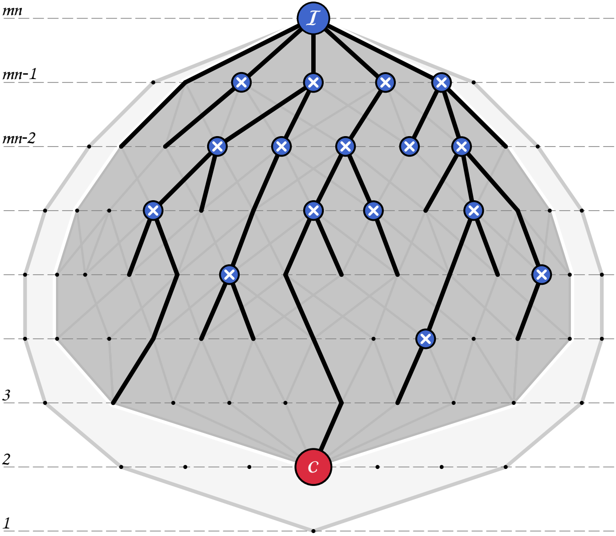

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1. Node-disjoint search tree
2. Uses memory $\mathbf{poly}(mn)$
3. Branching *only* on constructible partitions

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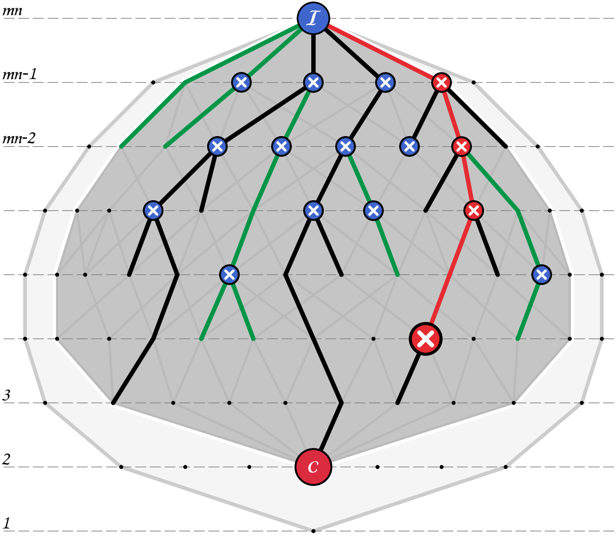

Our **B&B algorithm**

1. Node-disjoint search tree
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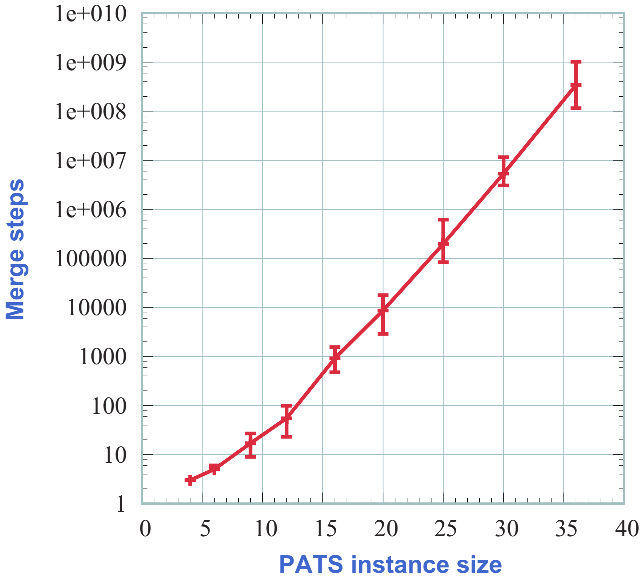
3. Branching *only* on constructible partitions
4. Cheap bounding function

Running time on random 2-coloured instances



$\sim 2^{mn}$

PATS problem remains challenging

- Open Problems:
  1. Is it **NP**-hard?
  2. Faster algorithms?
  3. Generalize to infinite finite-period patterns
- PATS is of practical importance

Thank you!