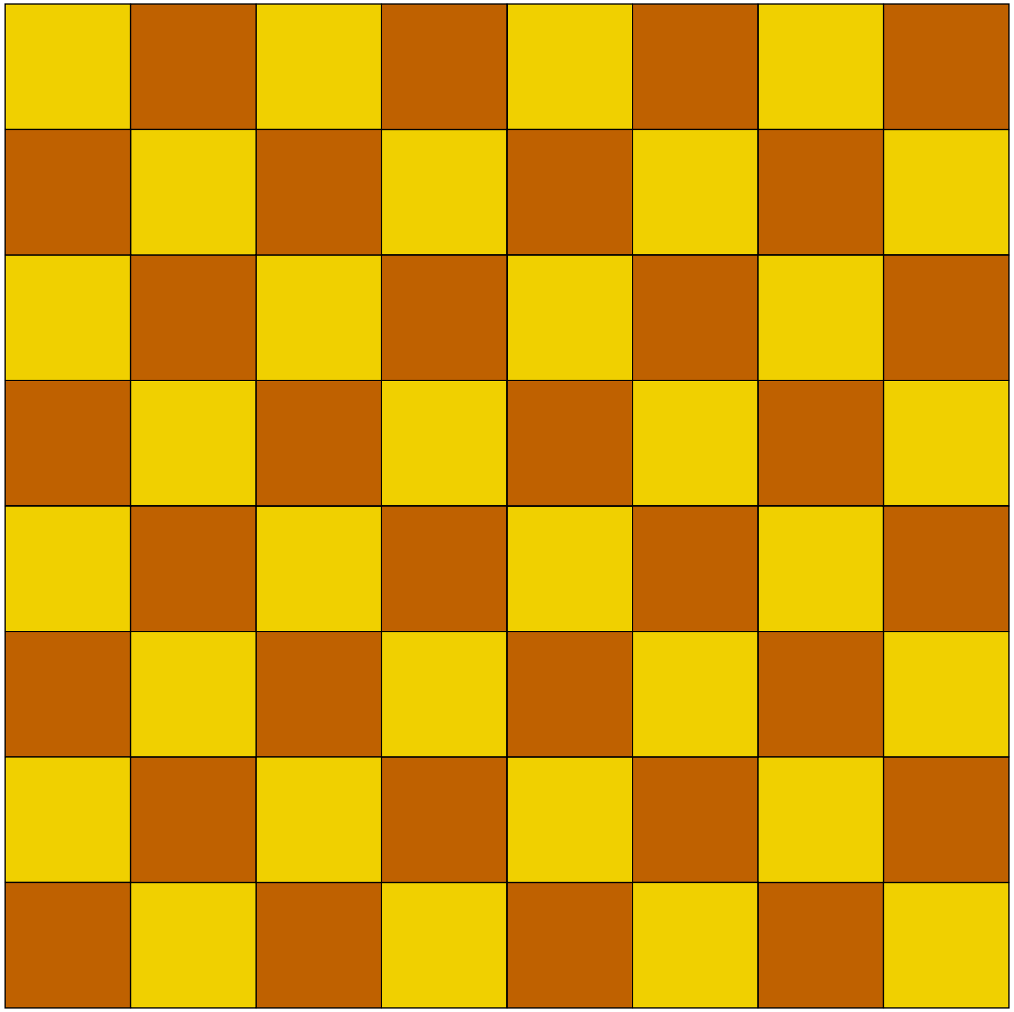
Fast Approximate Counting by Loopy Belief Propagation

Pascal O. Vontobel

Talk at CUHK, Hong Kong, December 16, 2013

Chess Board



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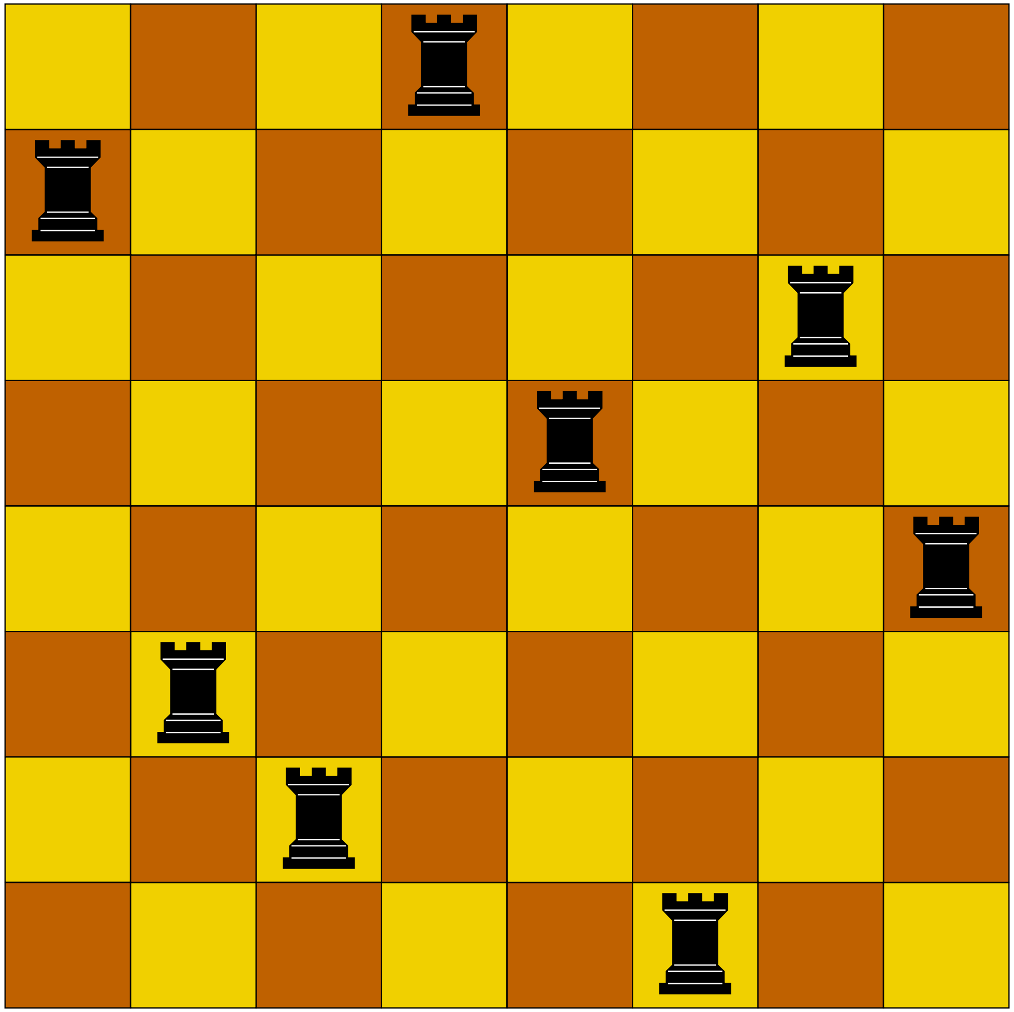

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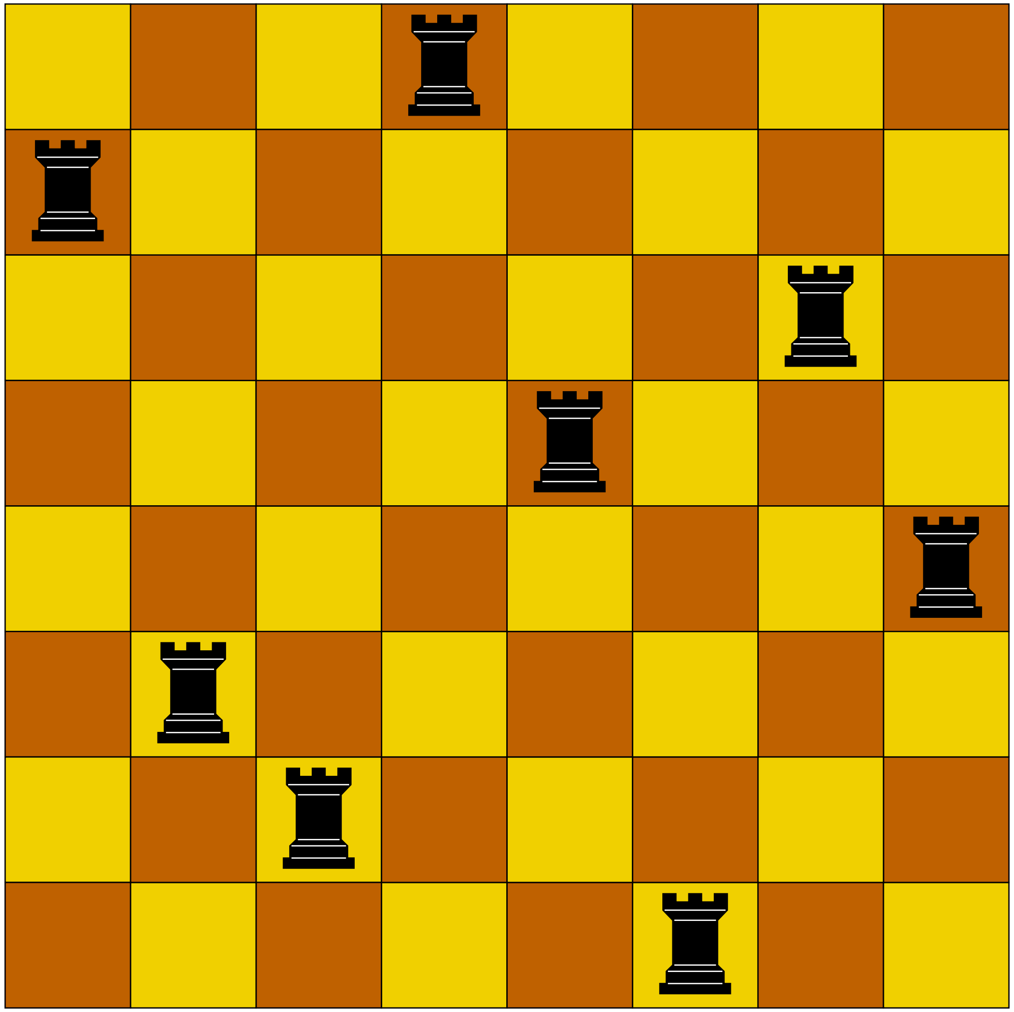
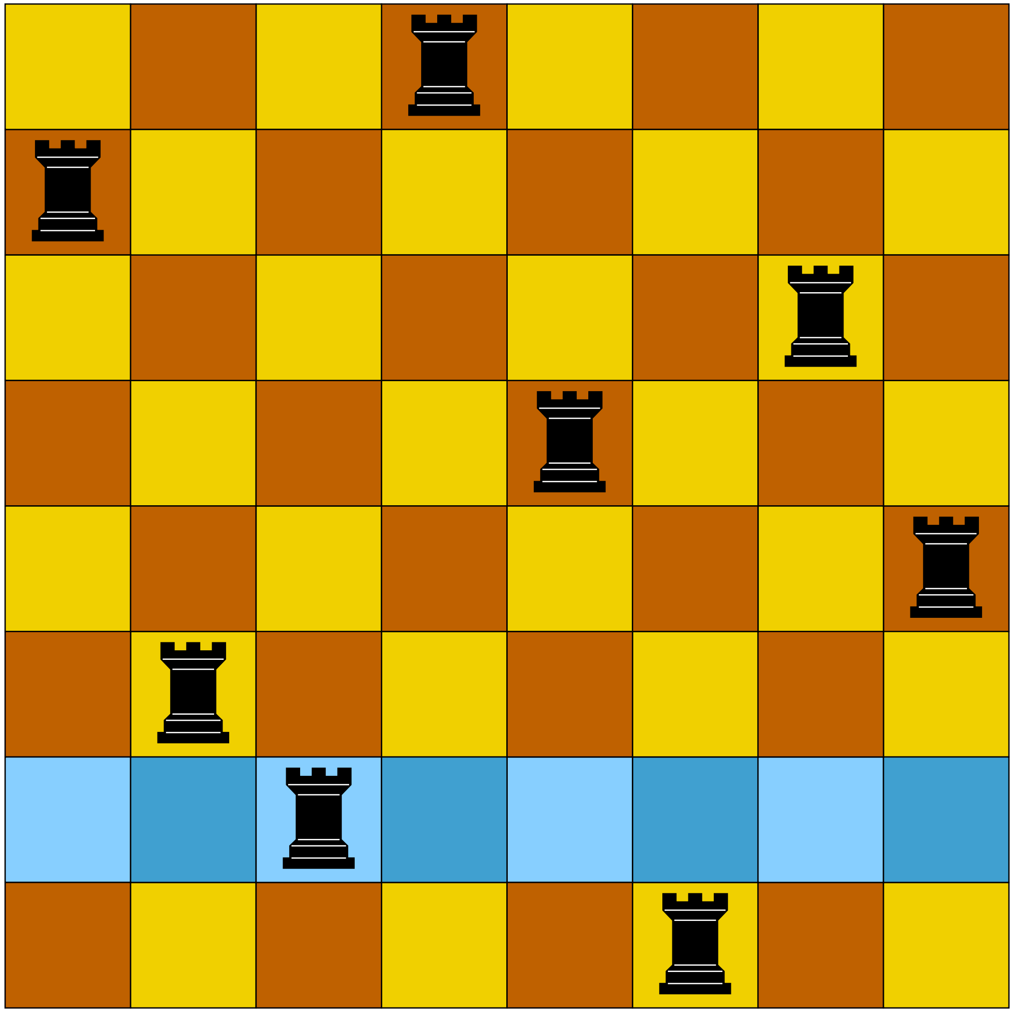


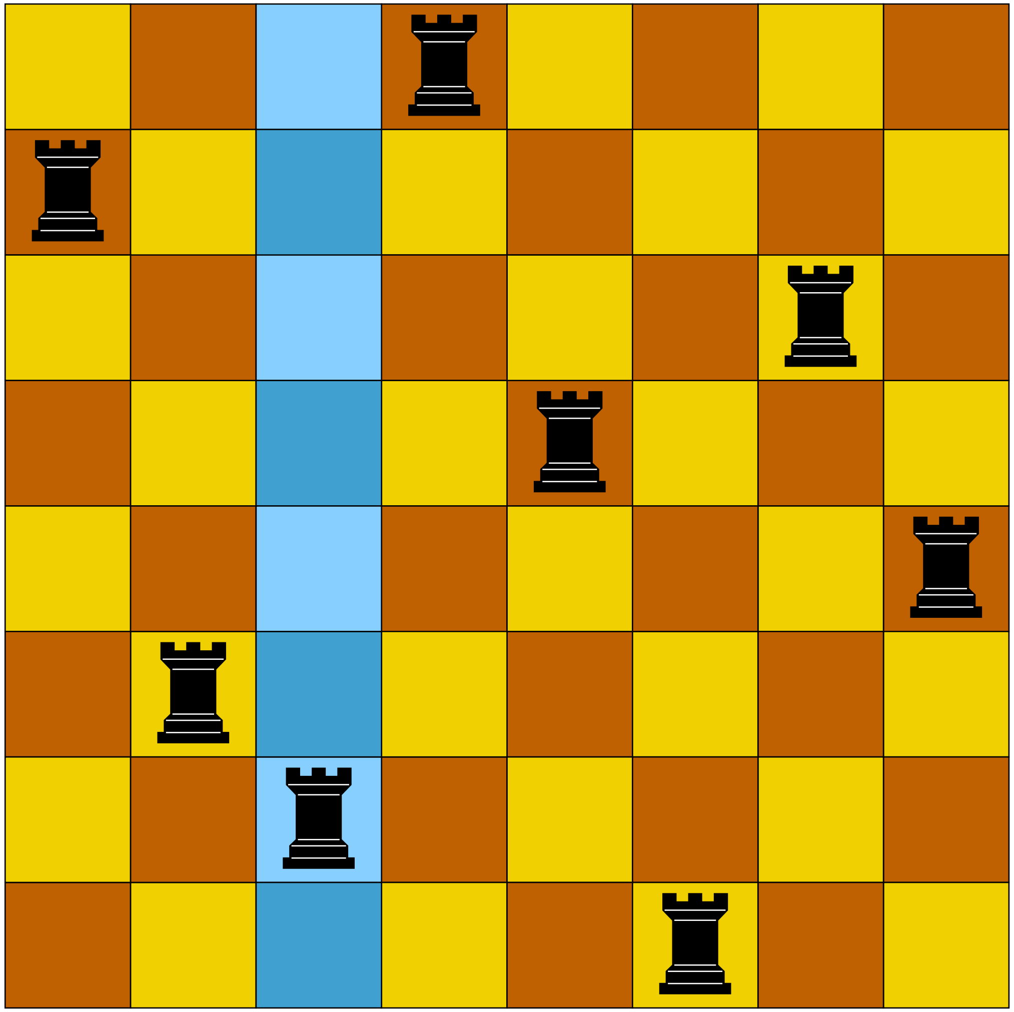
Question: in how many ways can we place 8 non-attacking rooks on a chess board?

Chess Board



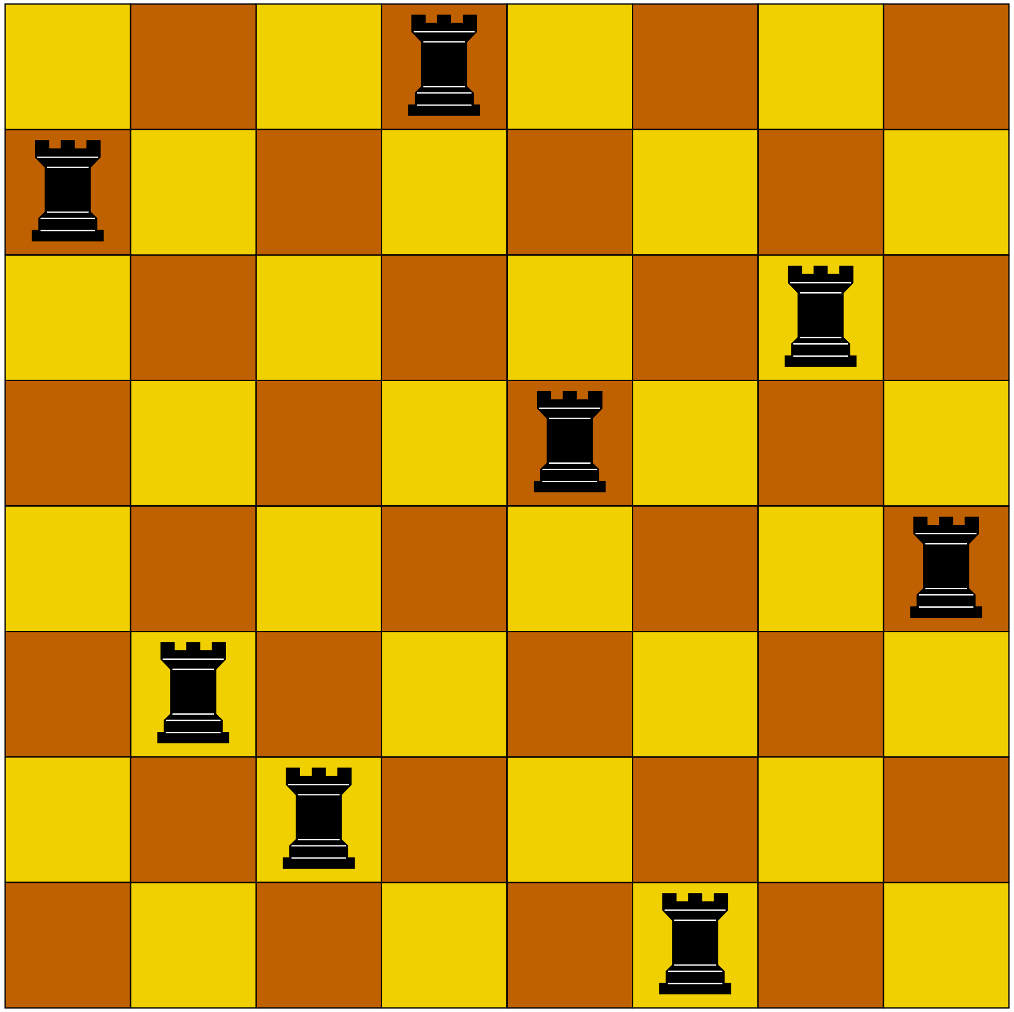
Row condition: exactly one rook per row.

Chess Board



Column condition: exactly one rook per column.

Chess Board



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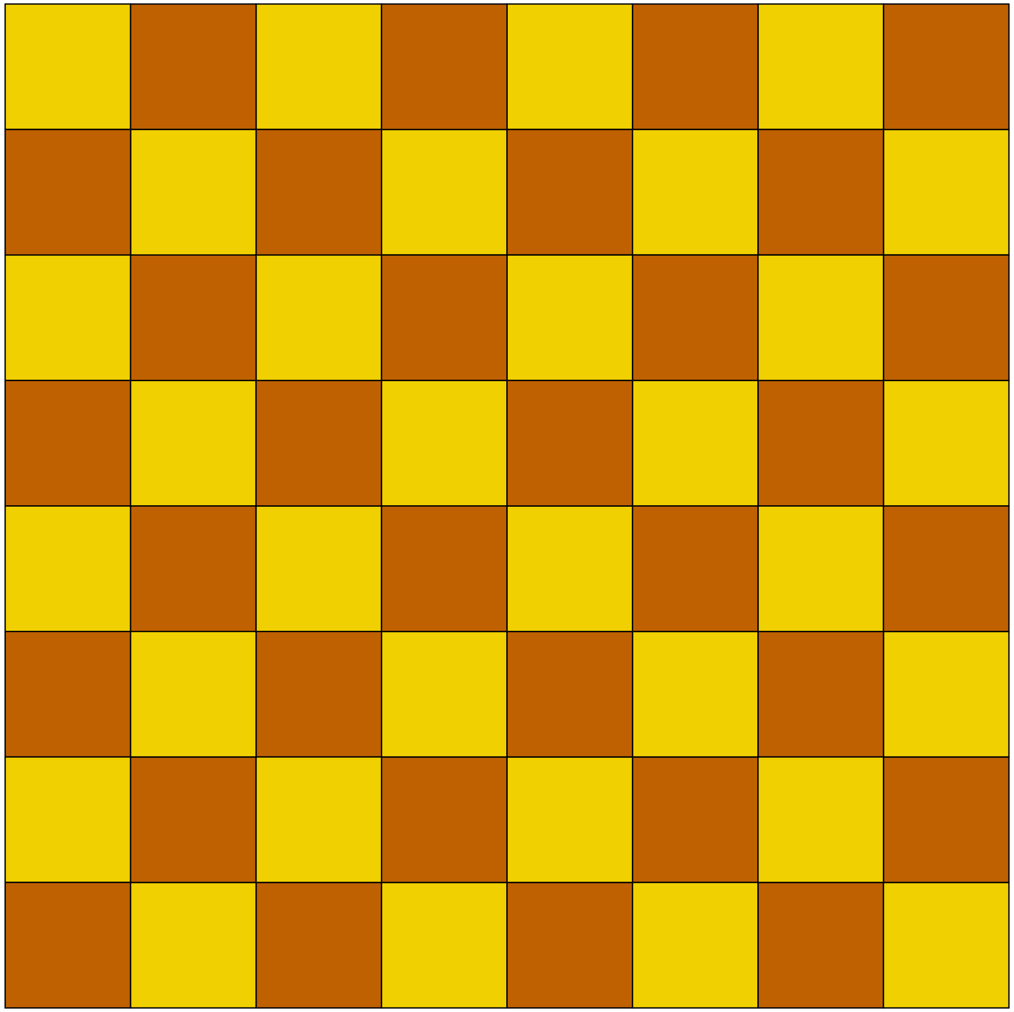

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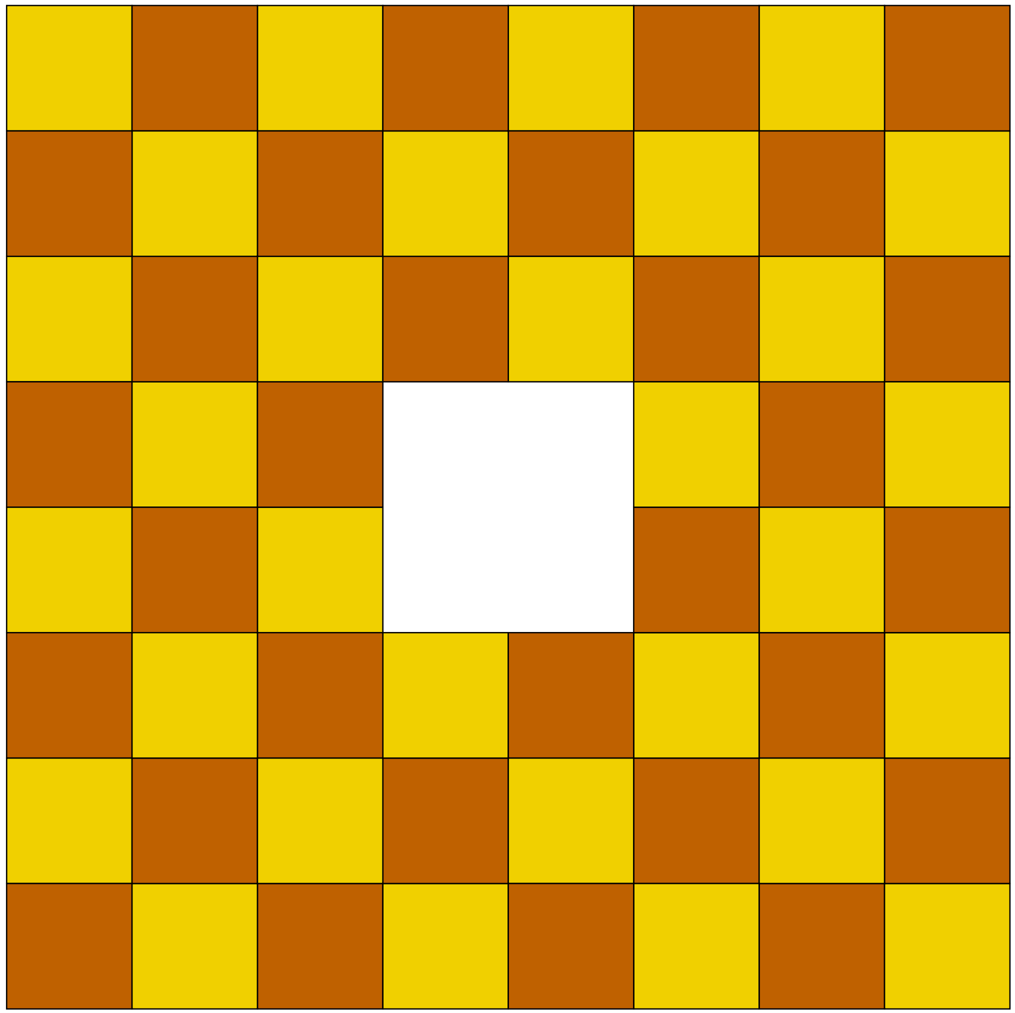

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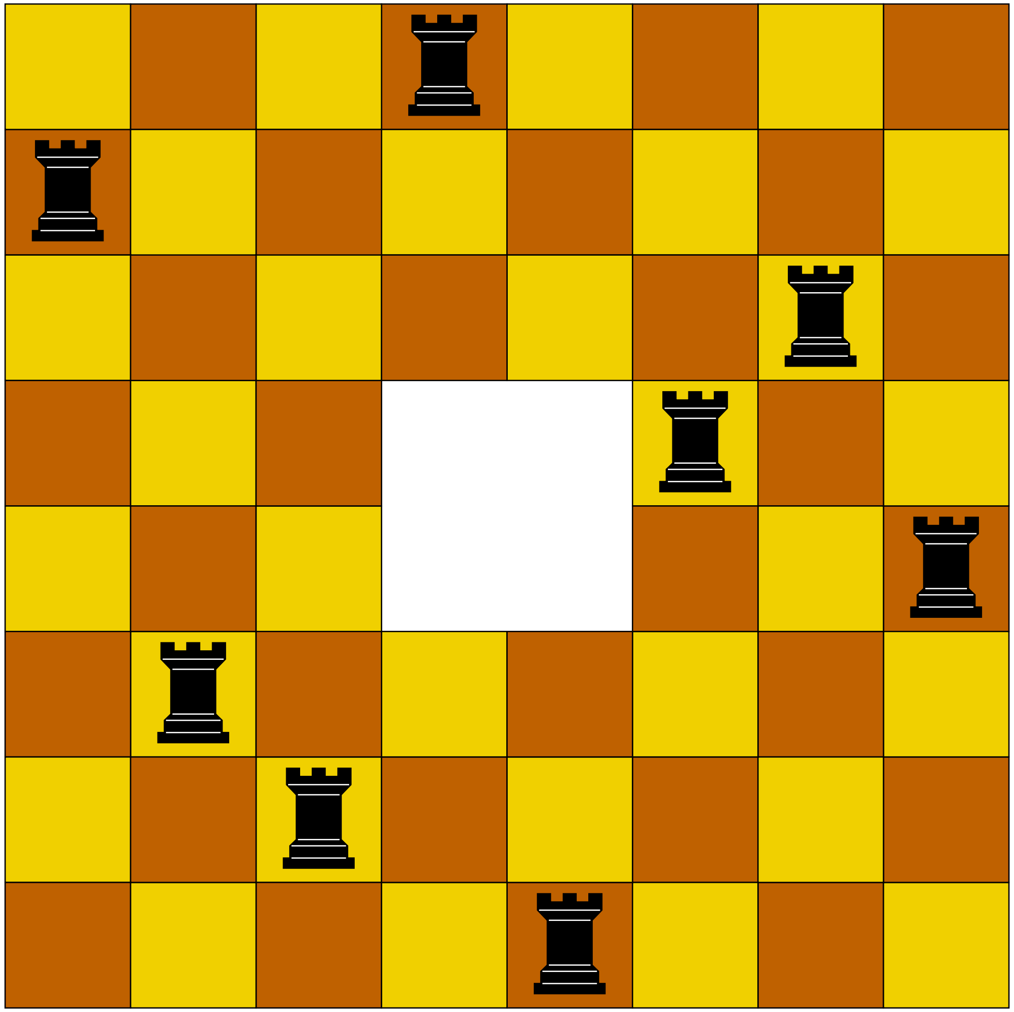
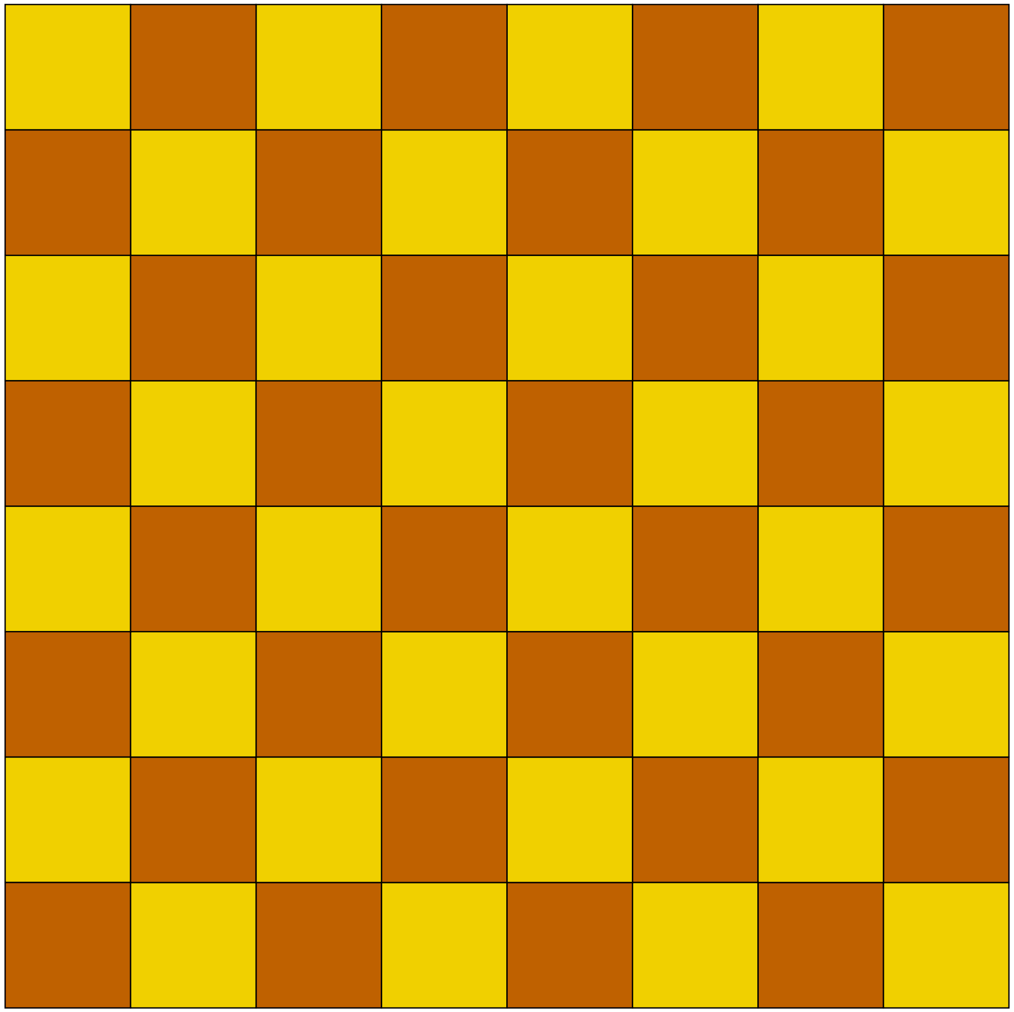


Question: in how many ways can we place 8 non-attacking rooks on this modified chess board?

Chess Board



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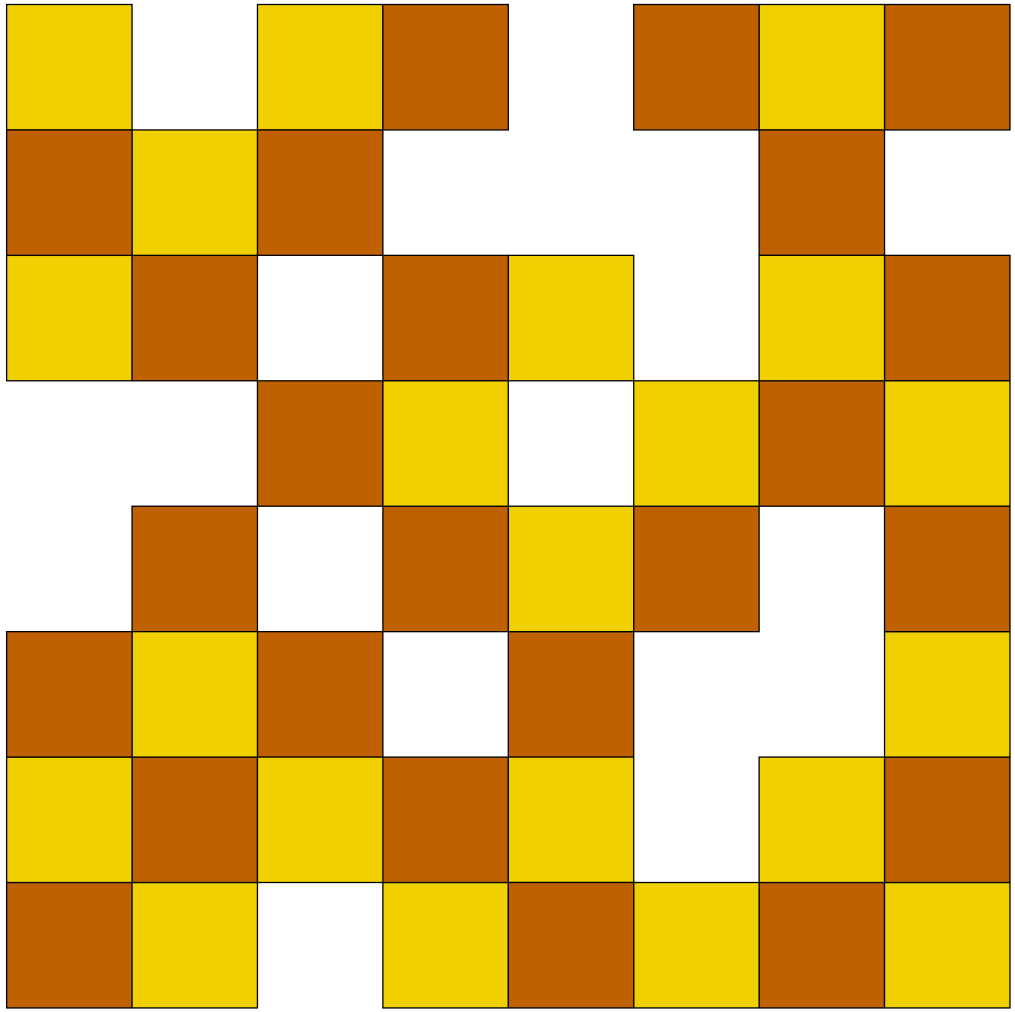

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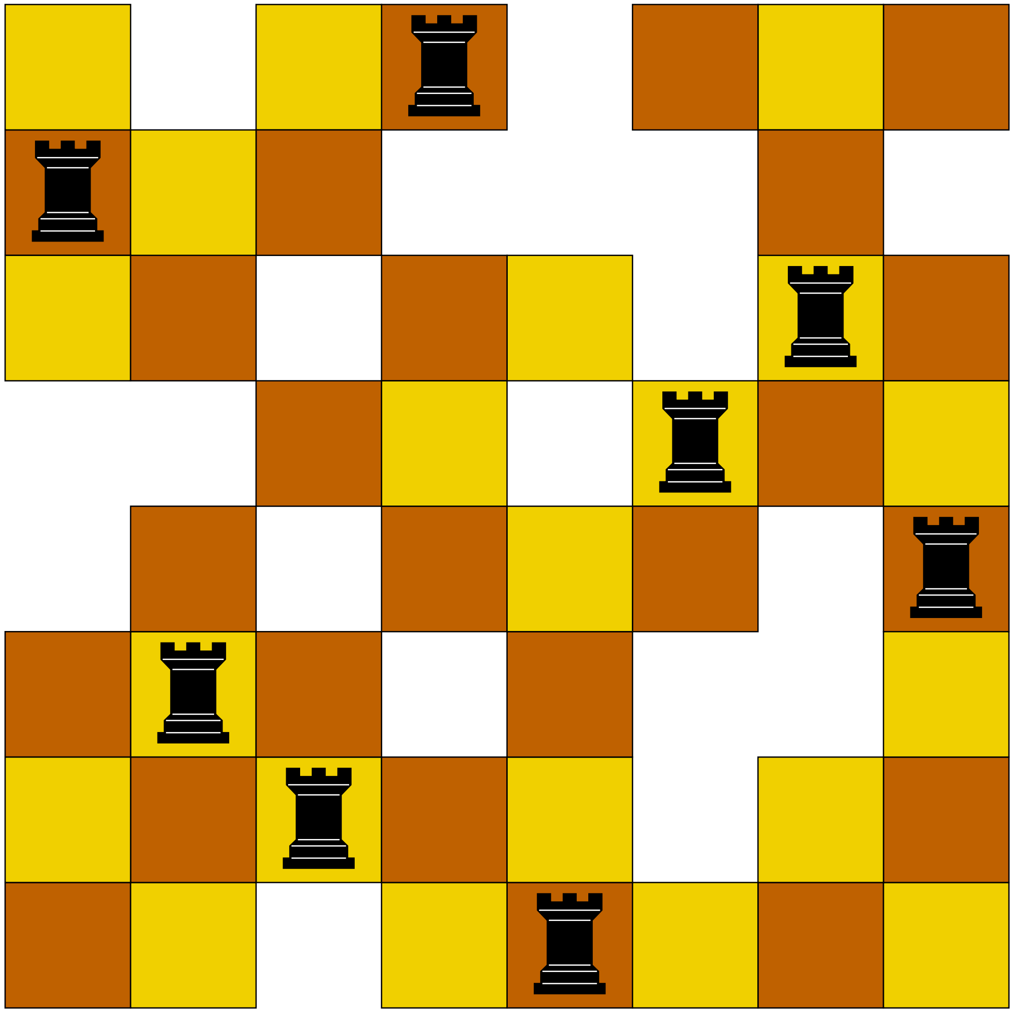

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Sudoku

Sudoku

1	2	5	3	9	6	8	7	4
4	6	3	8	7	5	2	9	1
7	9	8	2	4	1	5	3	6
5	4	7	6	1	2	9	8	3
2	3	9	5	8	4	1	6	7
8	1	6	9	3	7	4	2	5
6	8	1	7	5	9	3	4	2
3	7	4	1	2	8	6	5	9
9	5	2	4	6	3	7	1	8

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2	3	9	5	8	4	1	6	7
8	1	6	9	3	7	4	2	5
6	8	1	7	5	9	3	4	2
3	7	4	1	2	8	6	5	9
9	5	2	4	6	3	7	1	8

Question: how many Sudoku arrays are there?

(More technically: how many valid configurations are there?)

Sudoku

1	2	5	3	9	6	8	7	4
4	6	3	8	7	5	2	9	1
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6	8	1	7	5	9	3	4	2
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Row condition: numbers $1, \ldots, 9$ appear exactly once.

Sudoku

1	2	5	3	9	6	8	7	4
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2	3	9	5	8	4	1	6	7
8	1	6	9	3	7	4	2	5
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Column condition: numbers $1, \ldots, 9$ appear exactly once.

Sudoku

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7	9	8	2	4	1	5	3	6
5	4	7	6	1	2	9	8	3
2	3	9	5	8	4	1	6	7
8	1	6	9	3	7	4	2	5
6	8	1	7	5	9	3	4	2
3	7	4	1	2	8	6	5	9
9	5	2	4	6	3	7	1	8

Sub-block condition: numbers $1, \ldots, 9$ appear exactly once.

Sudoku

1	2	5	3	9	6	8	7	4
4	6	3	8	7	5	2	9	1
7	9	8	2	4	1	5	3	6
5	4	7	6	1	2	9	8	3
2	3	9	5	8	4	1	6	7
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Other Sudoku Setups

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3	5	8	1	9	6	2	7	4
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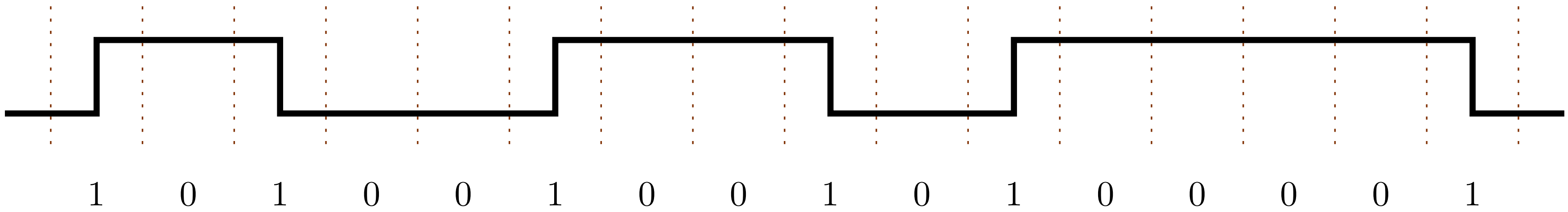
7	3	4	6	1	5	9	8	2
5	6	1	2	8	9	3	4	7

1D constraints in communications

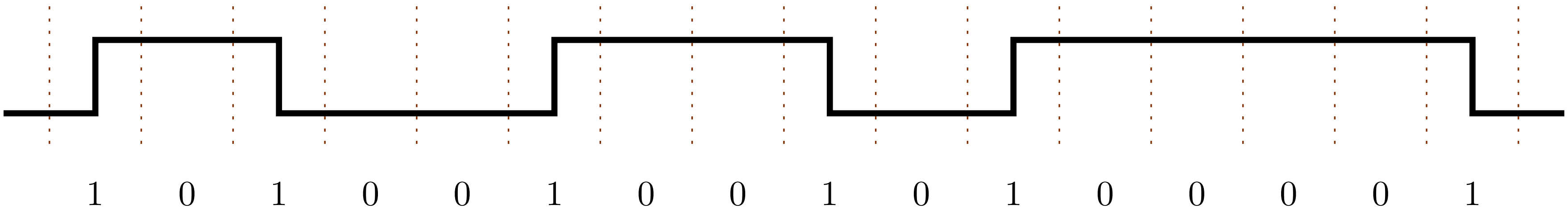
RLL Constraints



A (d, k) RLL constraint imposes:

- At least d zero symbols between two ones.
- At most k zero symbols between two ones.

RLL Constraints



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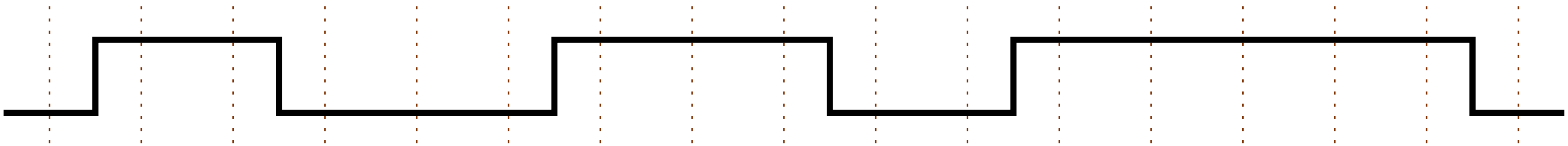

1 0 1 0 0 1 0 0 1 0 1 0 0 0 0 1

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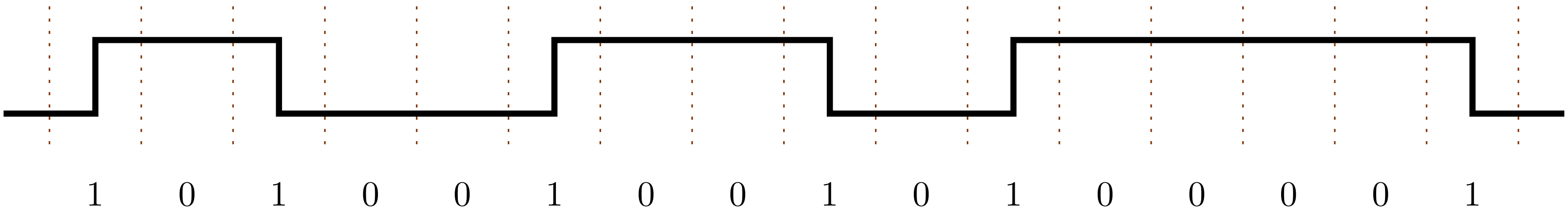
Answer: typically, the answer to such questions looks like

$$N(T) = \exp\big(C \cdot T + o(T)\big).$$

RLL Constraints



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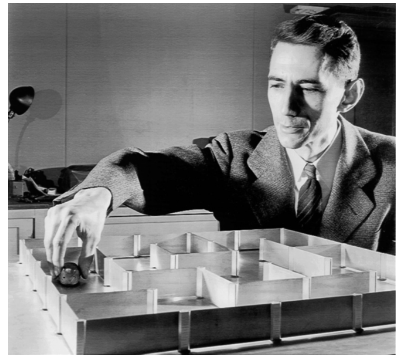
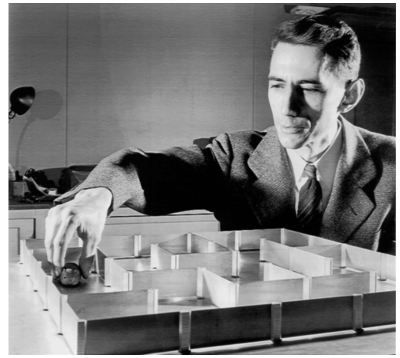
C: “capacity” or “entropy.”

Shannon (1948), Figure 2



Shannon (1948), Figure 2



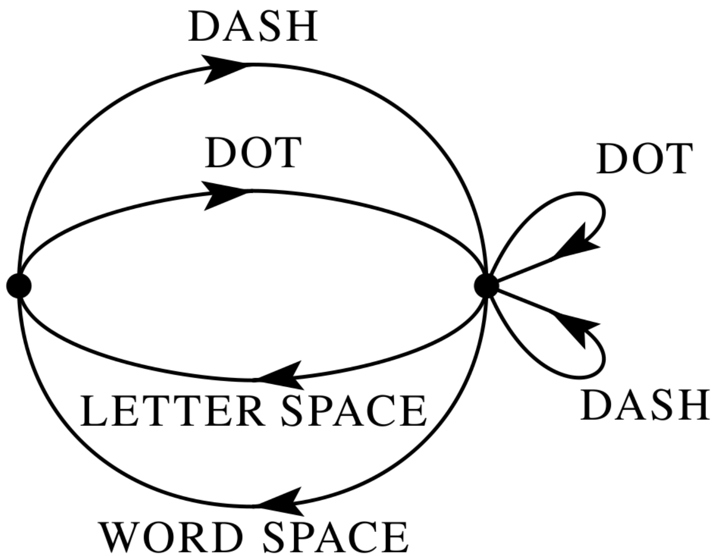
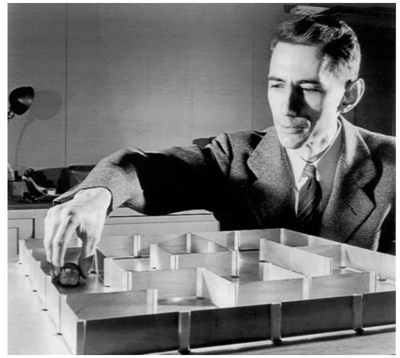


Fig. 2—Graphical representation of the constraints on telegraph symbols.

Shannon (1948)



Definition: The capacity C of a discrete channel is given by

$$C = \operatorname*{Lim}_{T\to\infty} \frac{\log N(T)}{T}$$

where $N(T)$ is the number of allowed signals of duration T.

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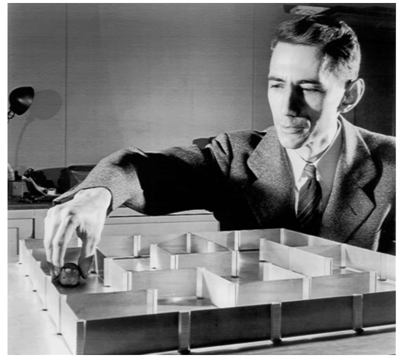

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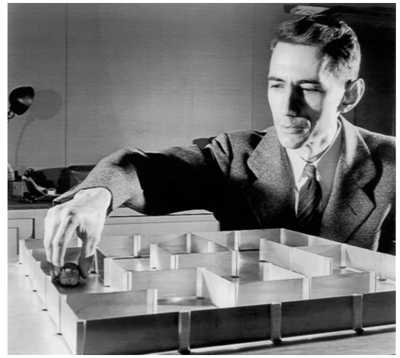
Theorem 1: Let $b_{ij}^{(s)}$ be the duration of the s^{th} symbol which is allowable in state i and leads to state j. Then the channel capacity C is equal to $\log W$ where W is the largest real root of the determinant equation:

$$\left|\sum_s W^{-b_{ij}^{(s)}} - \delta_{ij}\right| = 0$$

where $\delta_{ij} = 1$ if $i = j$ and is zero otherwise.

Shannon (1948)



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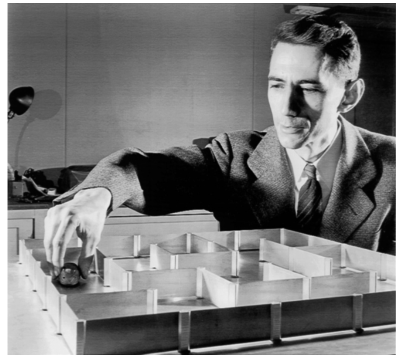


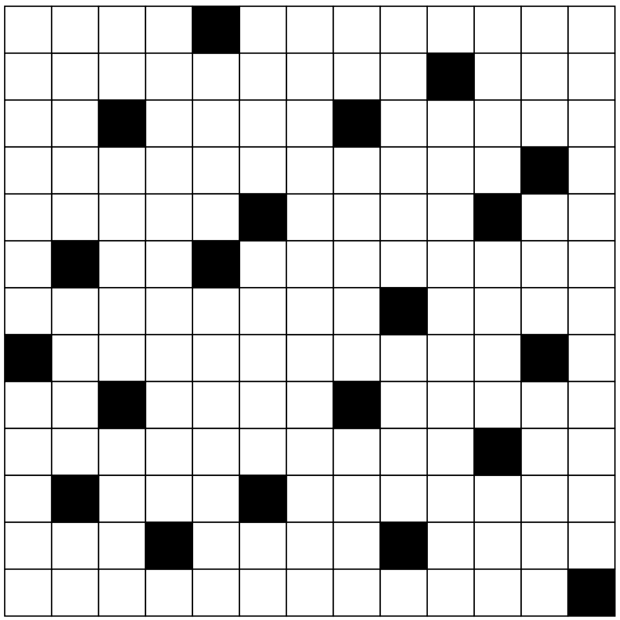
$$C = \lim_{T \to \infty} \frac{\log N(T)}{T}$$

i.e.,

$$N(T) = 2^{C \cdot T + o(T)}$$

2D constraints in communications

Two-Dimensional RLL Constraints



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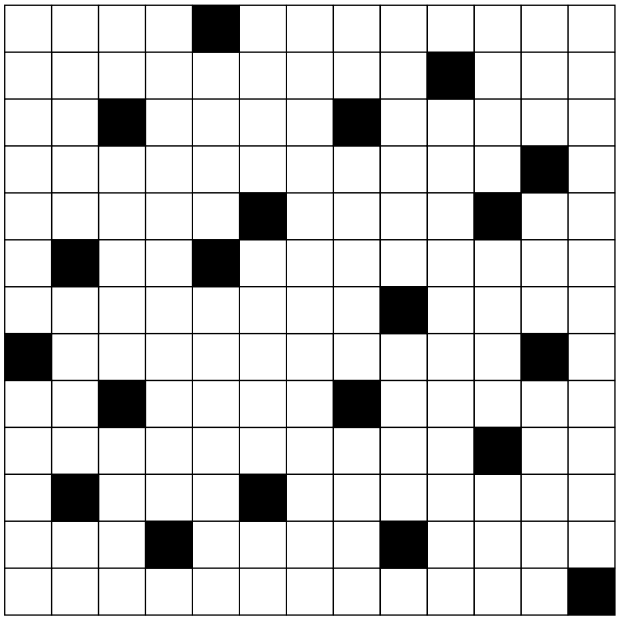

A $(d_1, k; d_2, k_2)$ RLL constraint imposes:

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- ...

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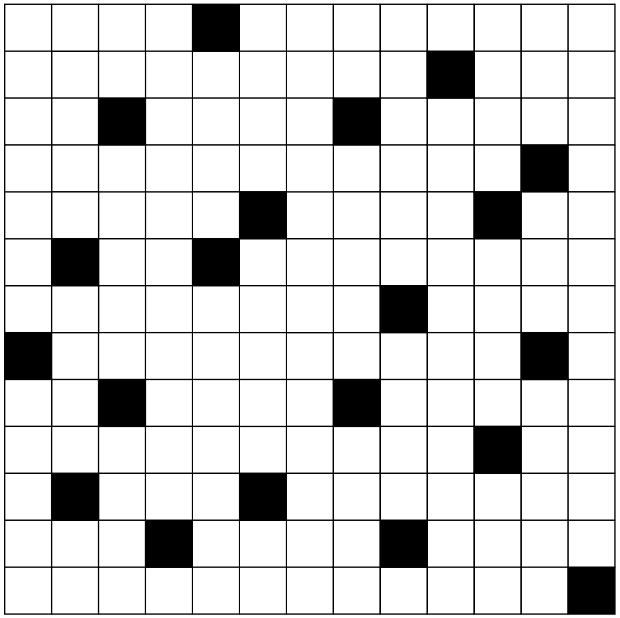

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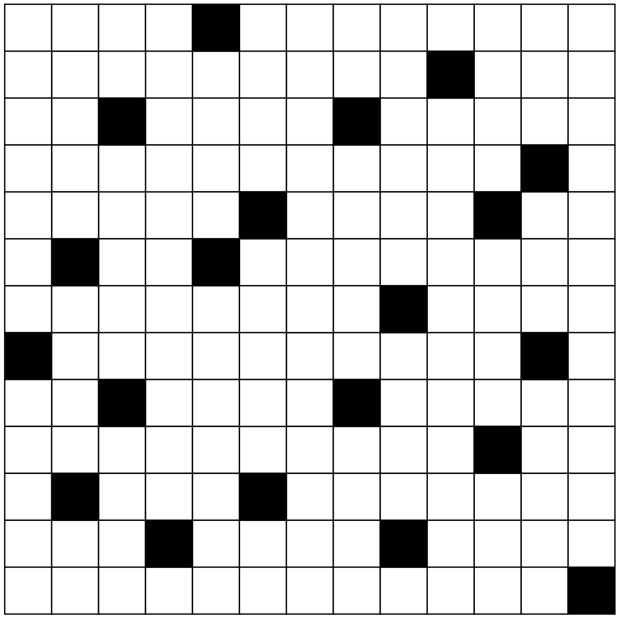
Two-Dimensional RLL Constraints



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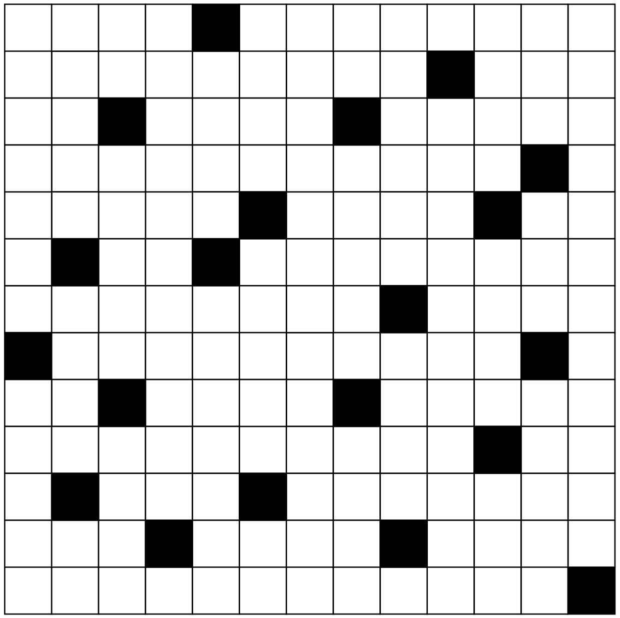

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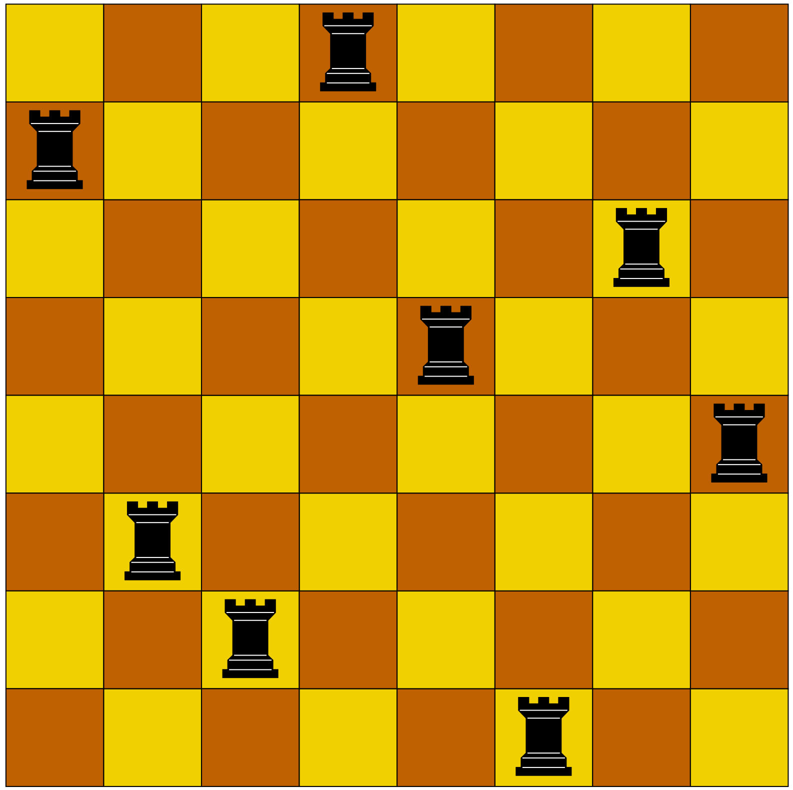
Overview

- Setting up a graphical model
- Permanent of a matrix
- Factor graphs and the sum-product algorithm
- The total sum of a factor graph and its Bethe approximation
- A combinatorial interpretation of the Bethe approximation
- Further comments
- Conclusions

Towards a graphical model

Towards a Graphical Model



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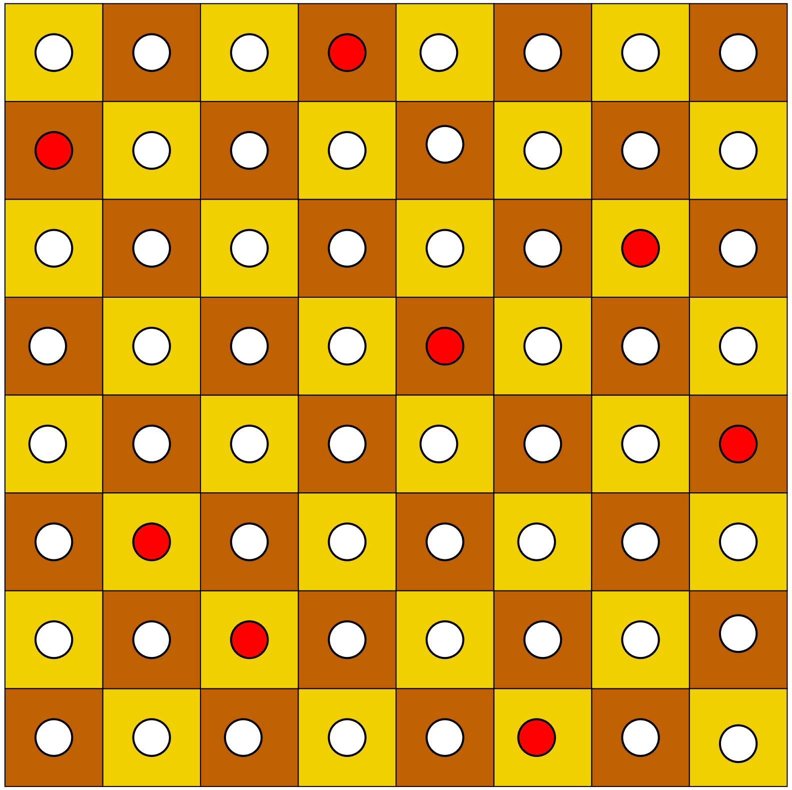
Towards a Graphical Model



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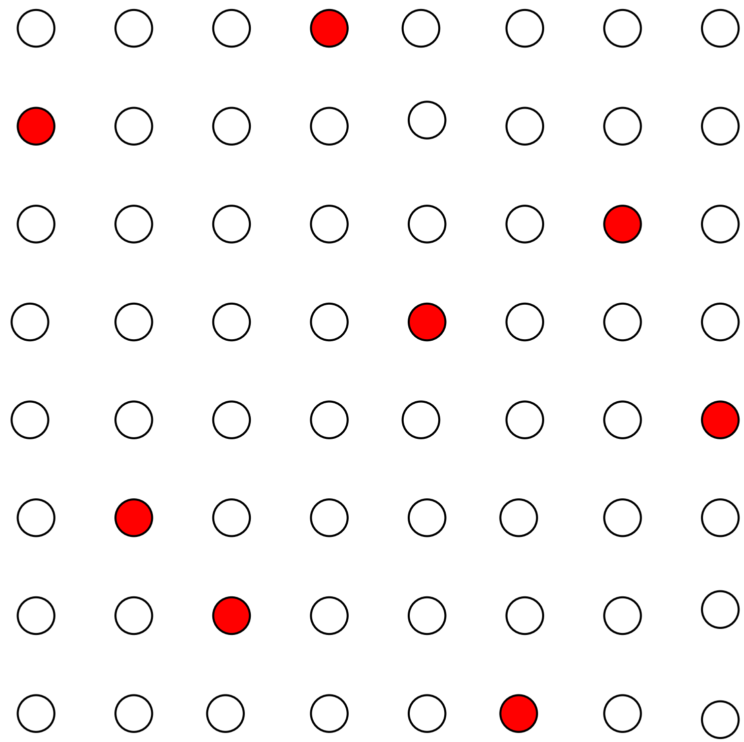

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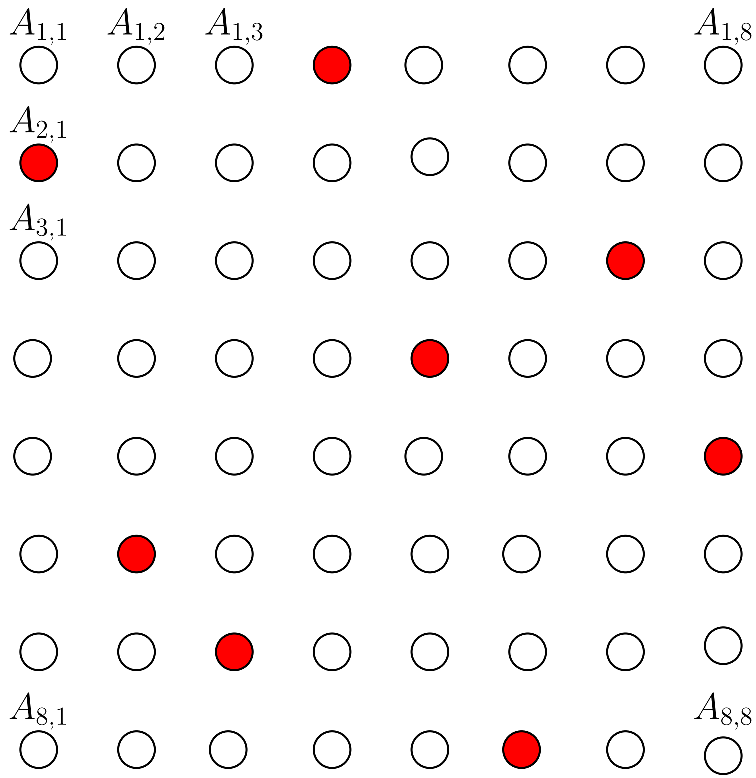

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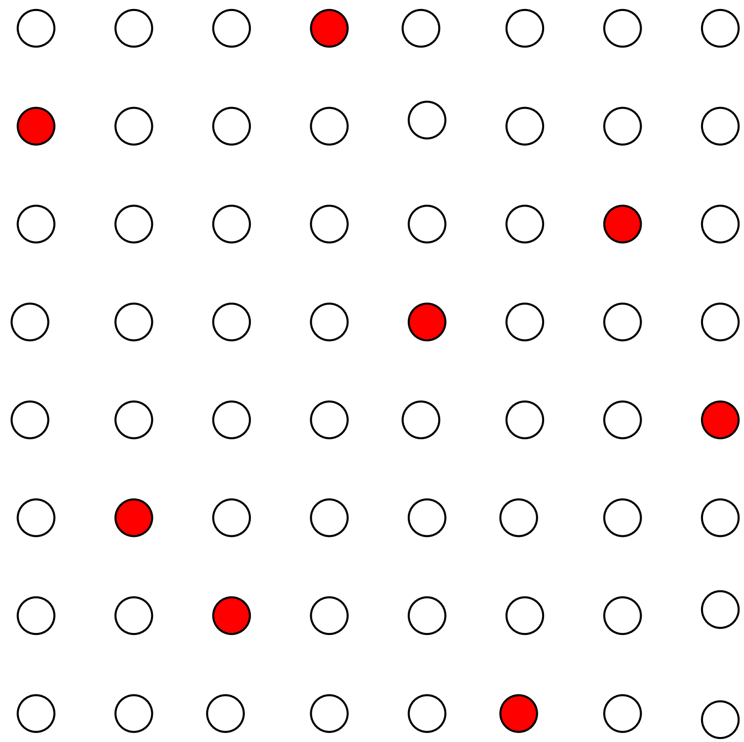

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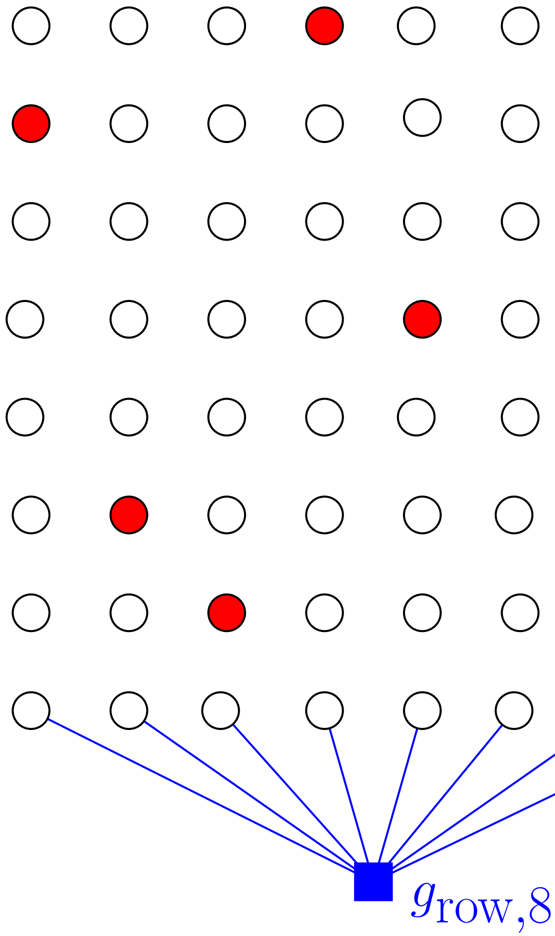
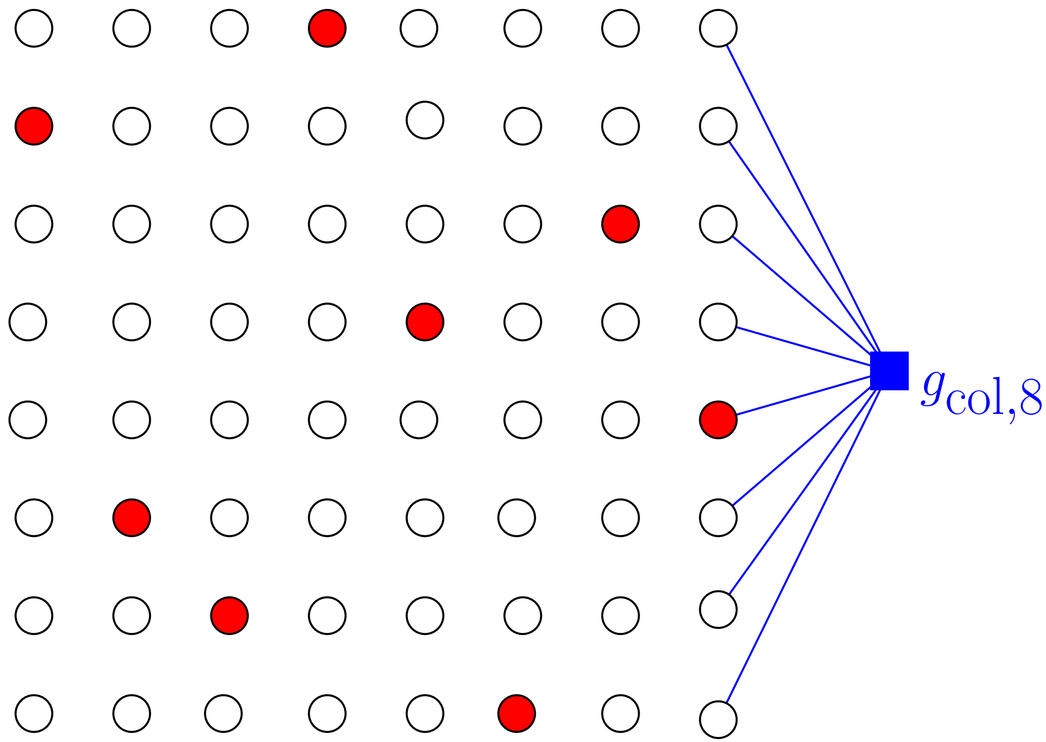


$$g_{\mathrm{row},8}(a_{8,1}, \ldots, a_{8,8}) \triangleq \begin{cases} 1 & \text{exactly one rook} \\ 0 & \text{otherwise} \end{cases}$$

Towards a Graphical Model



$$g_{\mathrm{col},8}(a_{1,8}, \ldots, a_{8,8}) \triangleq \begin{cases} 1 & \text{exactly one rook} \\ 0 & \text{otherwise} \end{cases}$$

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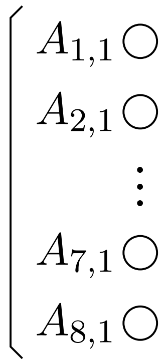

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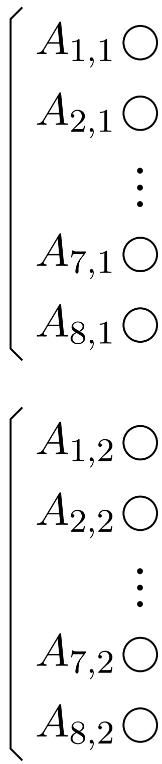

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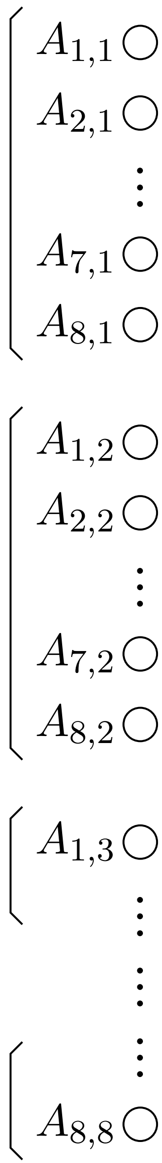

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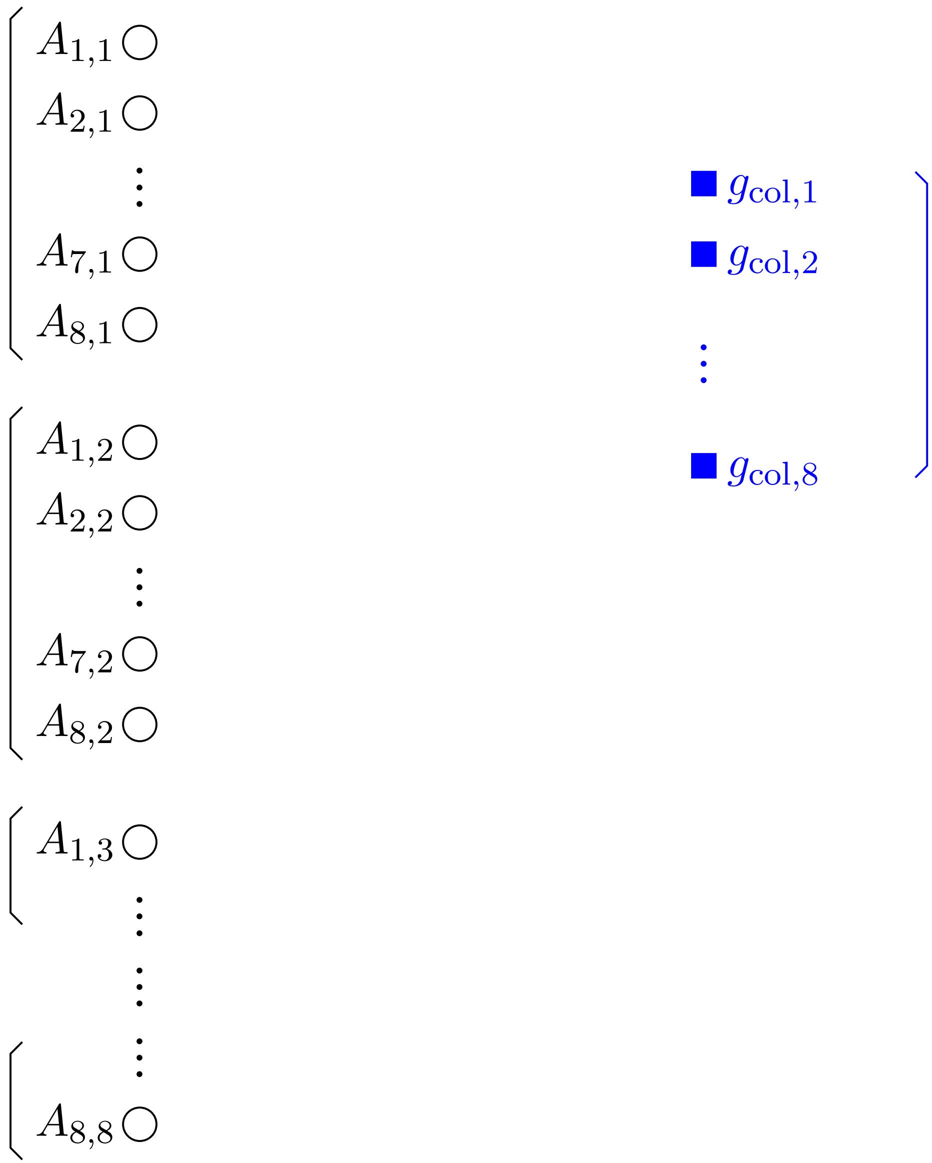

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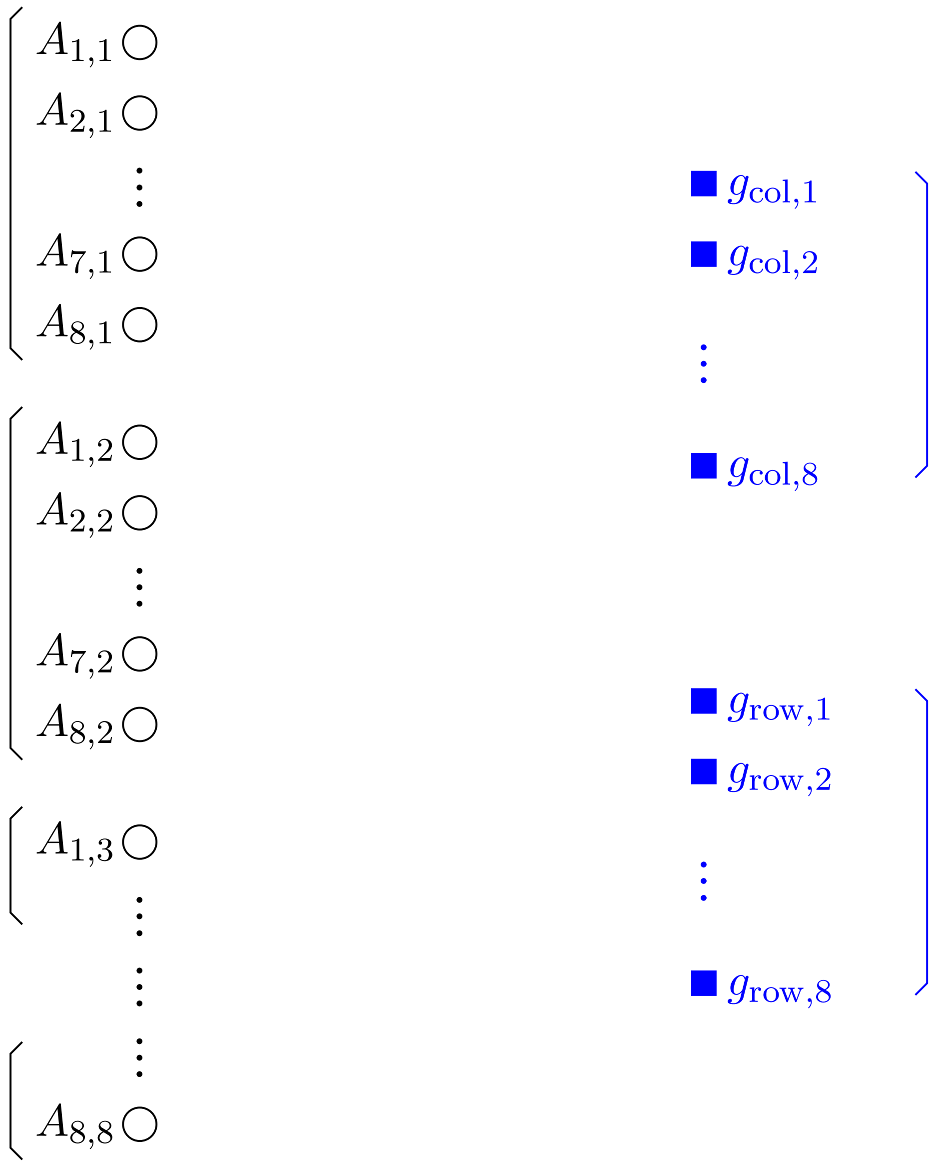

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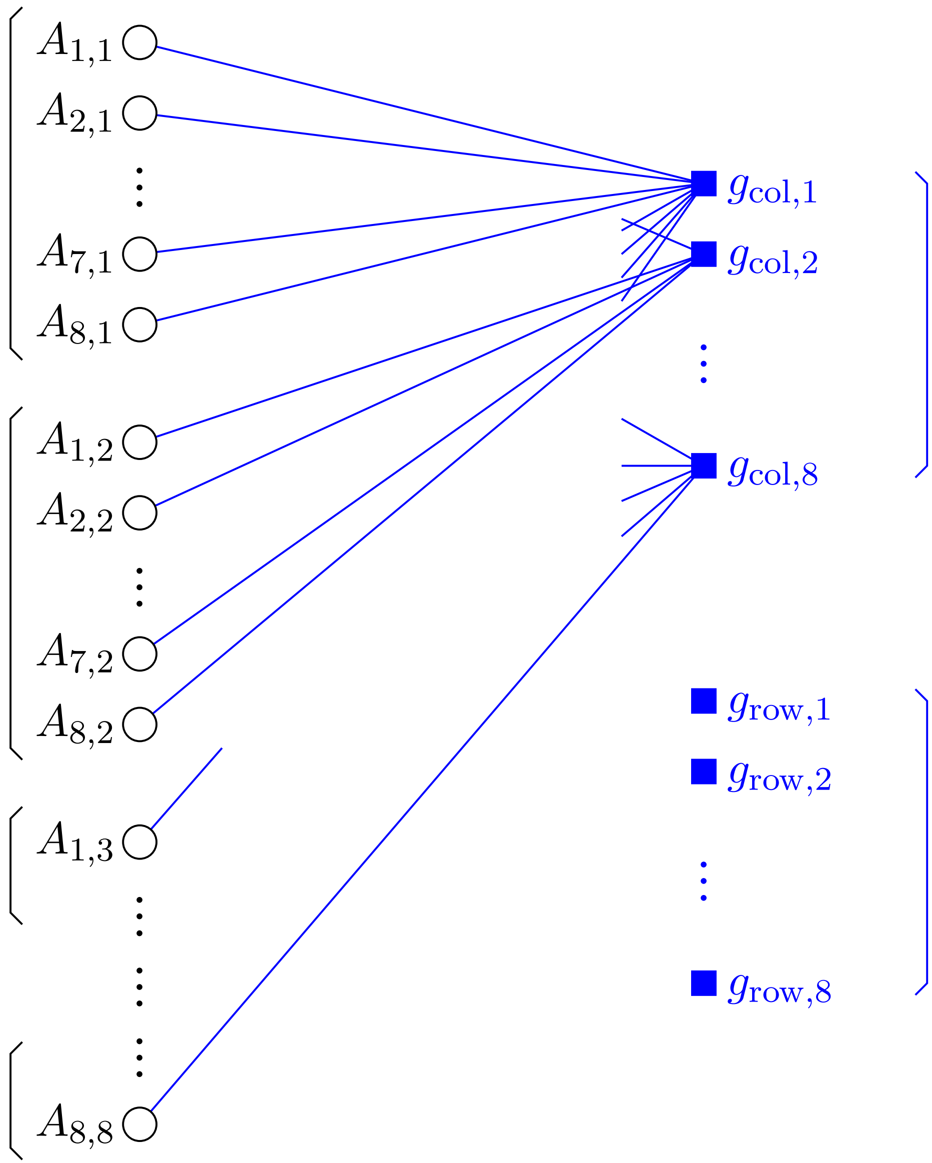

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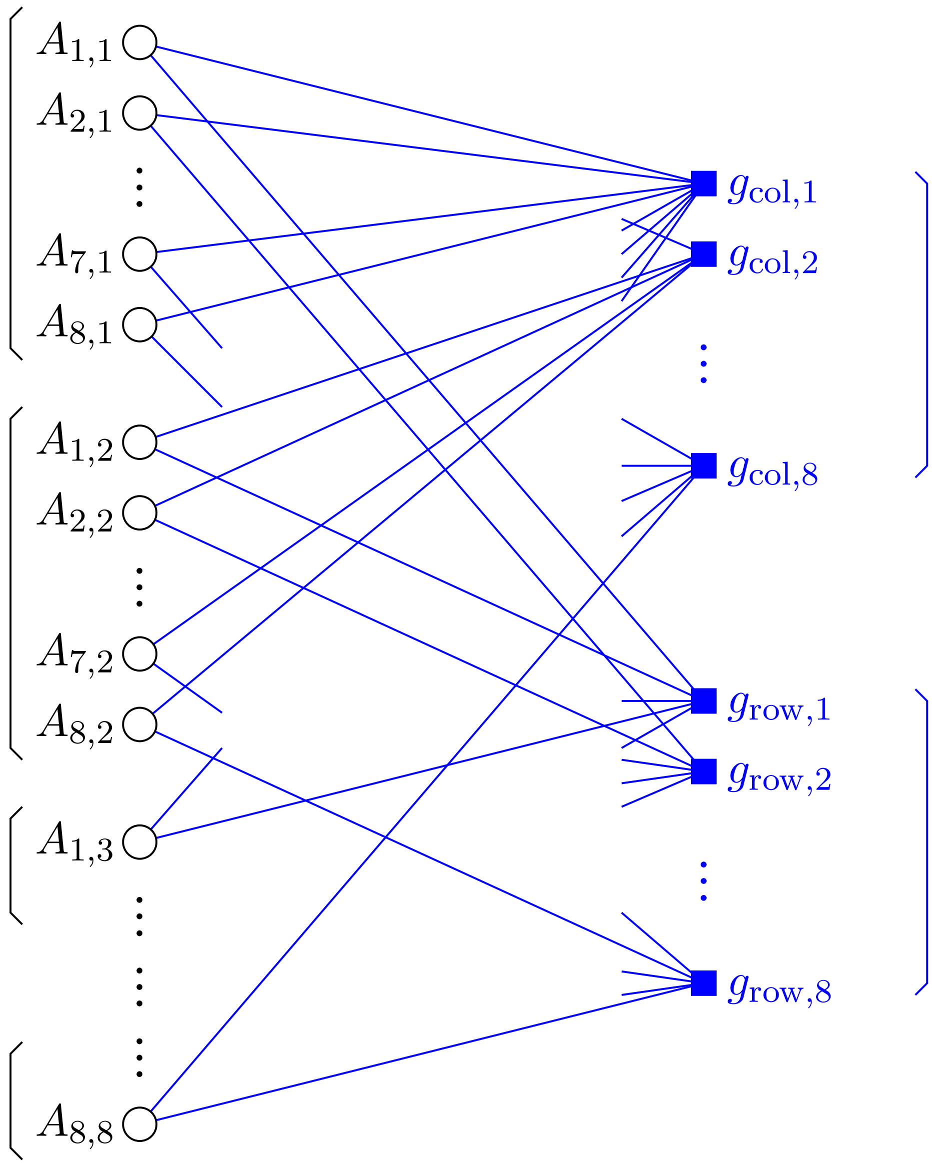

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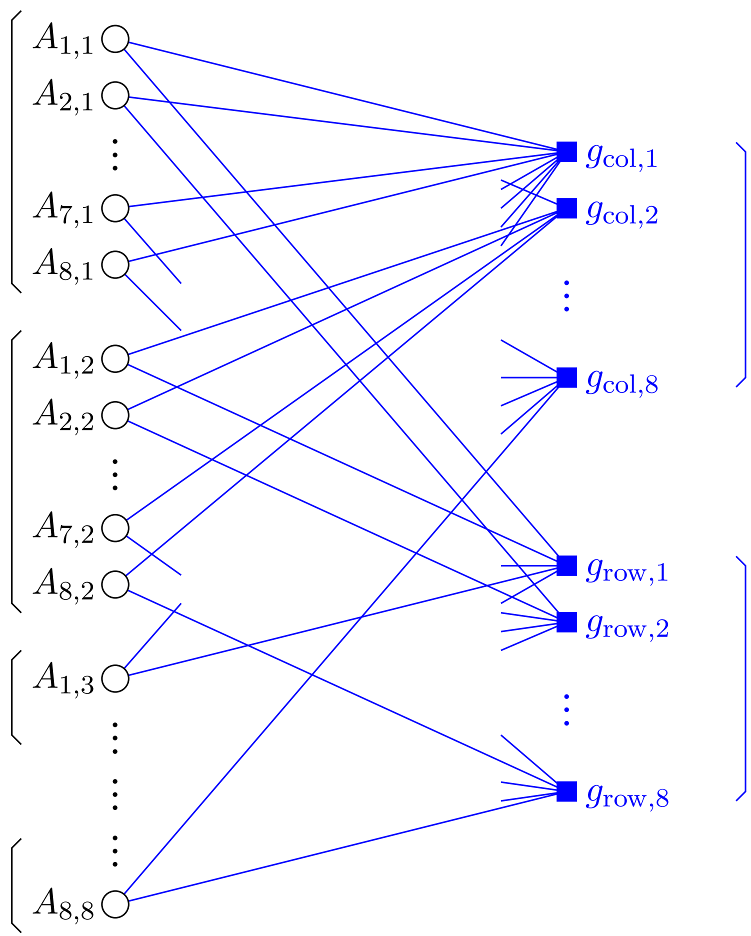

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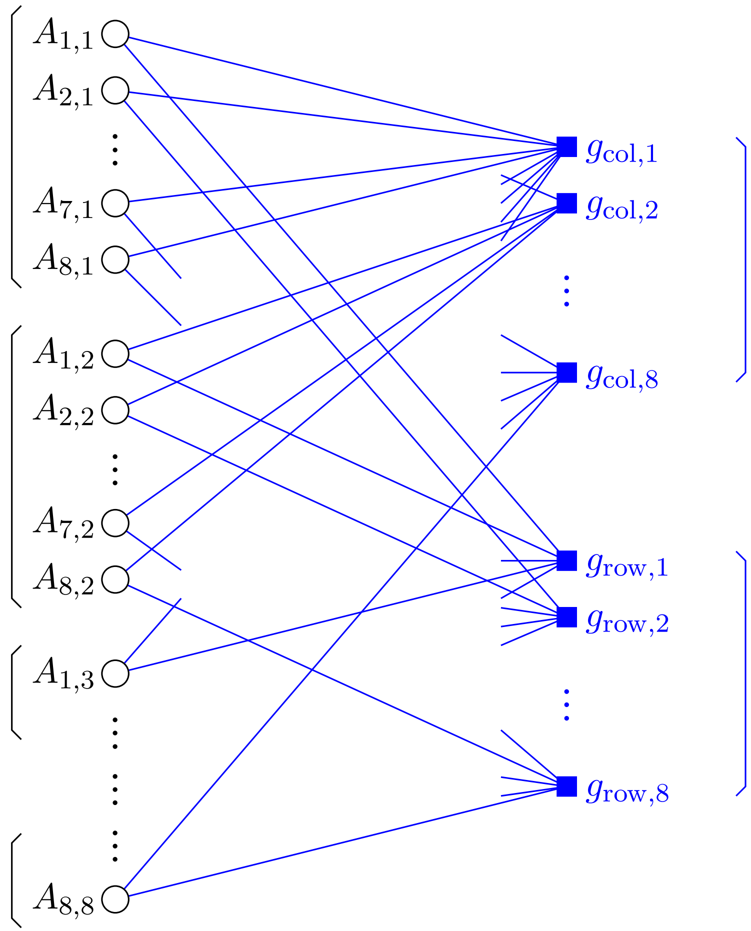
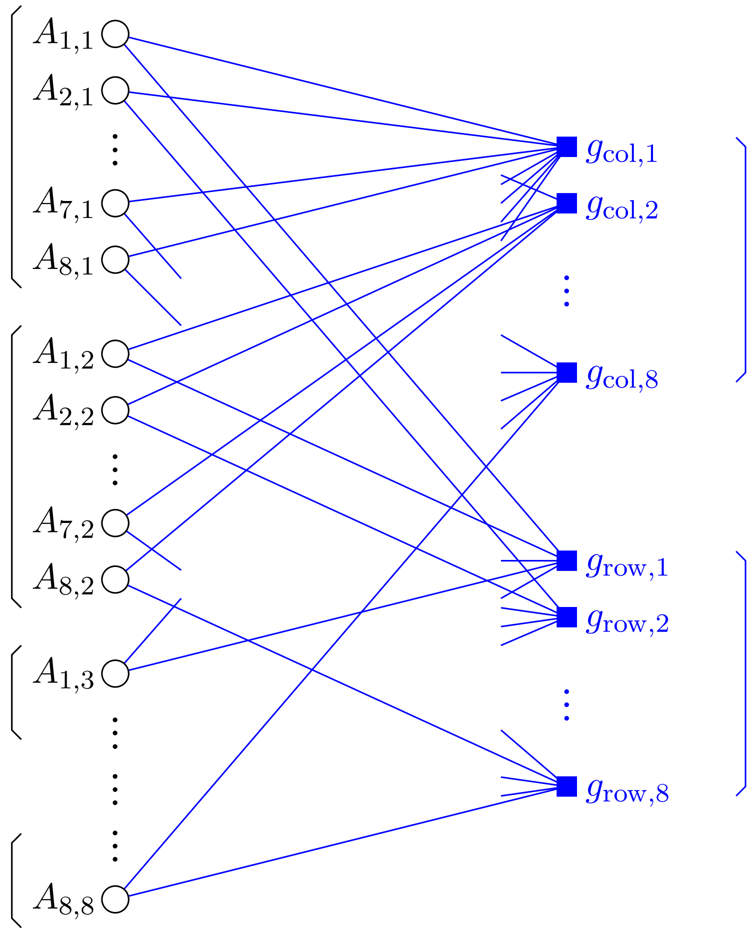


Global function:

$$
\begin{aligned}
g(a_{1,1},\ldots,a_{8,8}) &= \prod_j g_{\text{col},j}(a_{1,j},\ldots,a_{8,j}) \times \\
&\quad \prod_i g_{\text{row},i}(a_{i,1},\ldots,a_{i,8})
\end{aligned}
$$

Towards a Graphical Model



Global function:

$$g(a_{1,1}, \ldots, a_{8,8}) = \prod_j g_{\mathrm{col},j}(a_{1,j}, \ldots, a_{8,j}) \times \prod_i g_{\mathrm{row},i}(a_{i,1}, \ldots, a_{i,8})$$

Total sum:

$$Z = \sum_{a_{1,1}, \ldots, a_{8,8}} g(a_{1,1}, \ldots, a_{8,8})$$

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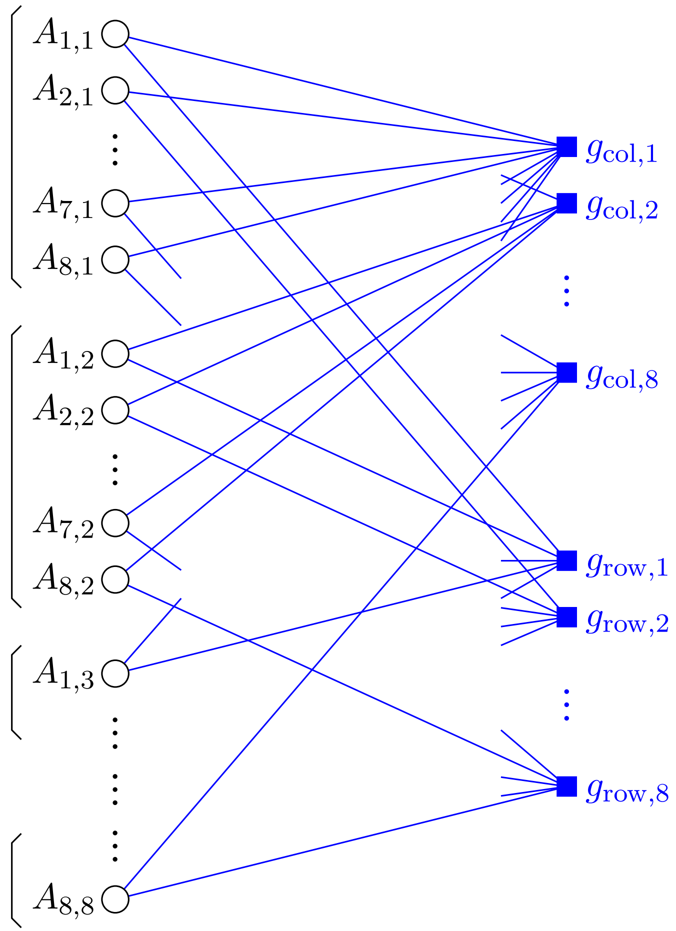

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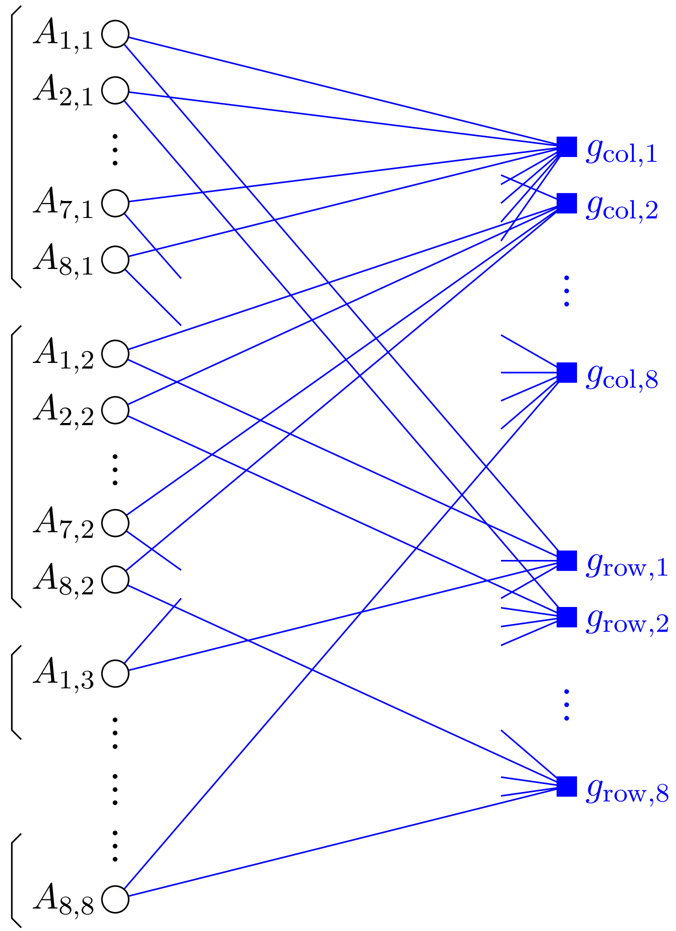
Total sum (partition function):

$$Z = \sum_{a_{1,1},\ldots,a_{8,8}} g(a_{1,1}, \ldots, a_{8,8})$$

Towards a Graphical Model



Global function:

$$g(a_{1,1}, \ldots, a_{8,8}) = \prod_j g_{\mathrm{col},j}(a_{1,j}, \ldots, a_{8,j}) \times \prod_i g_{\mathrm{row},i}(a_{i,1}, \ldots, a_{i,8})$$

Total sum (partition function):

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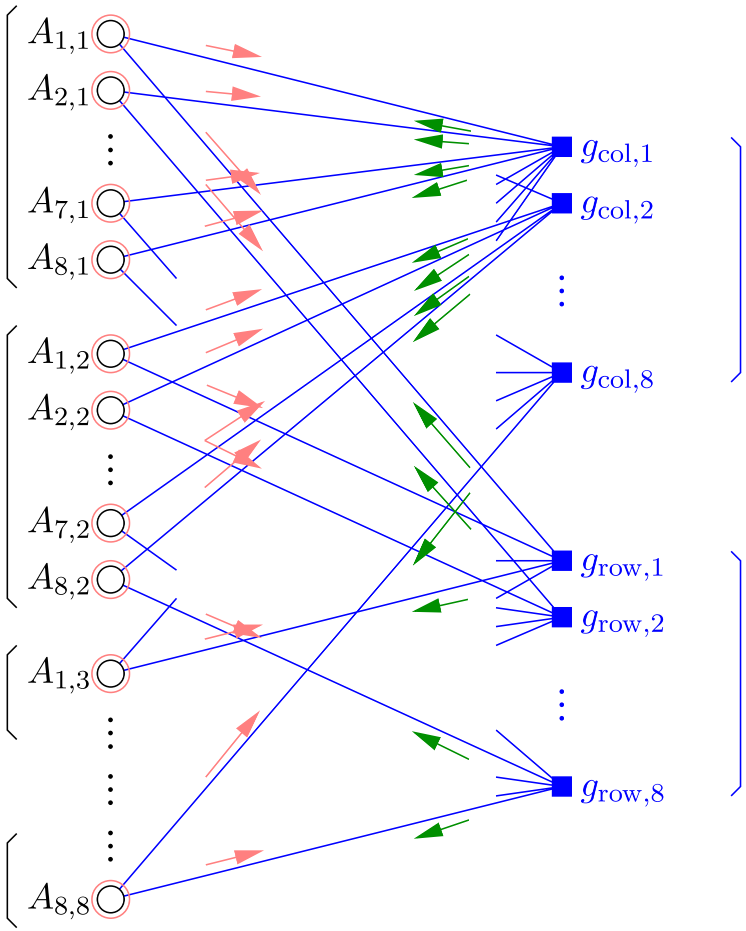
Use of loopy belief propagation for approximating Z?

Towards a Graphical Model



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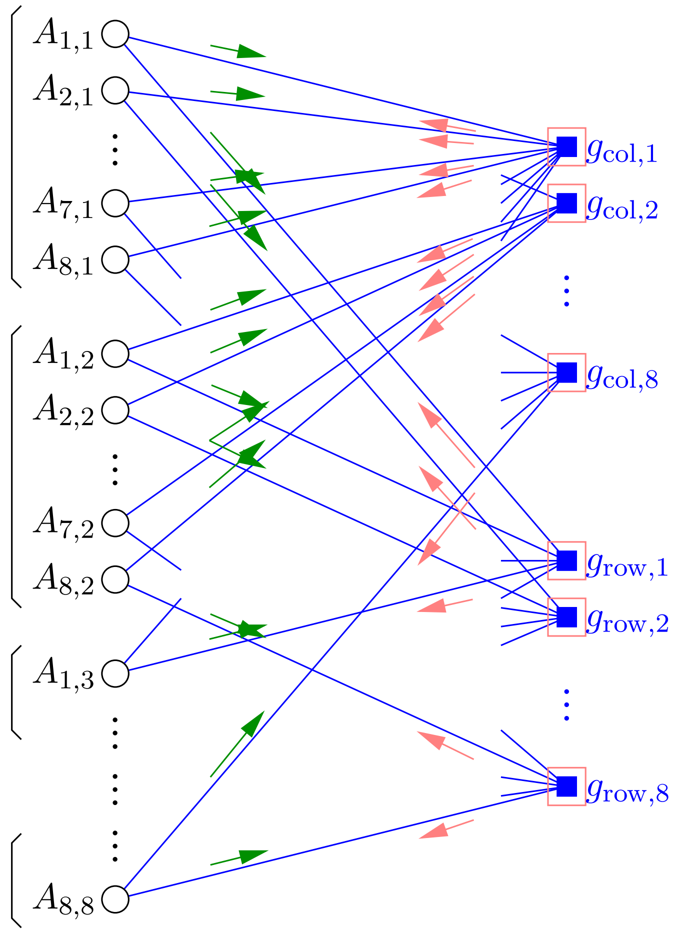

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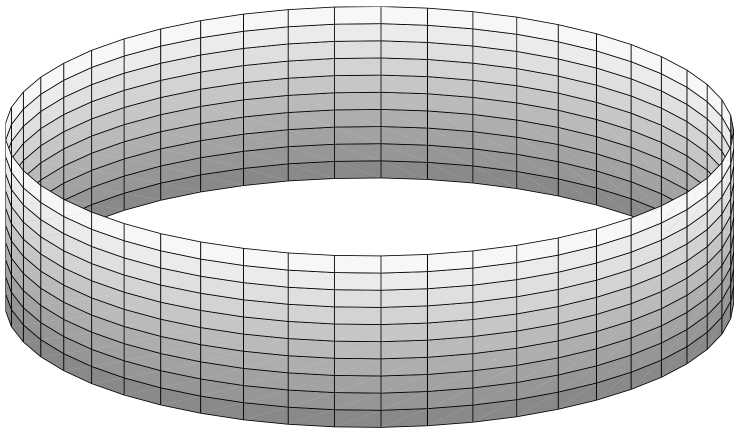
Some considerations on counting algorithms

Coloring the Surfaces of a Closed Strip



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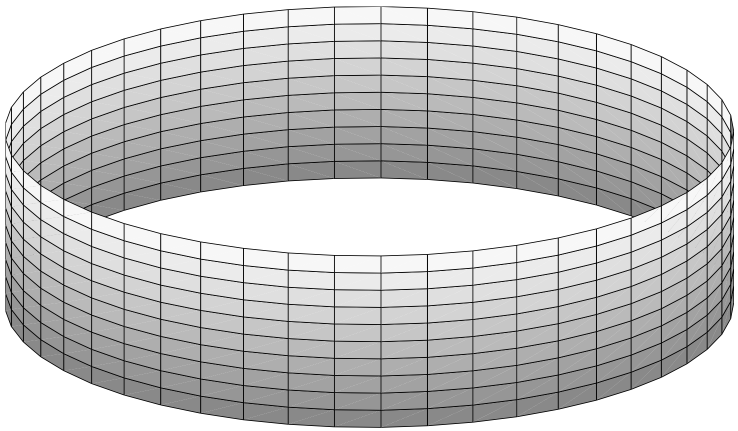

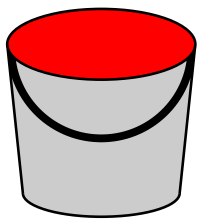

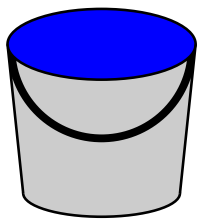

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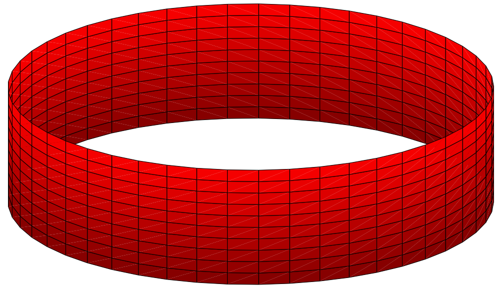

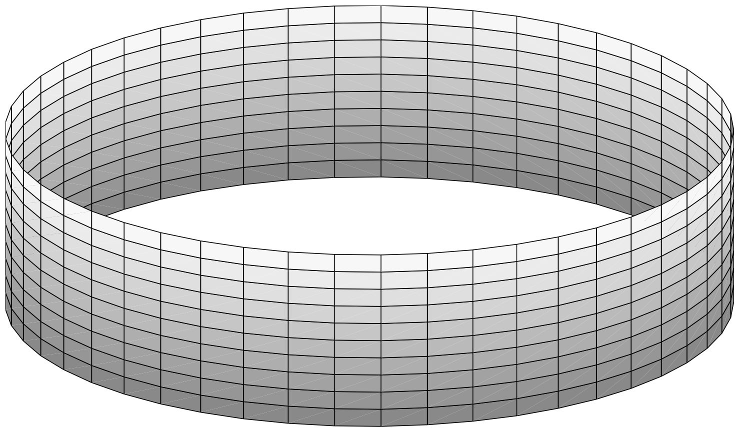

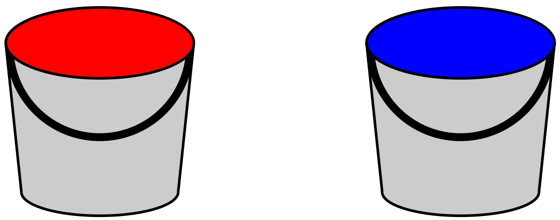

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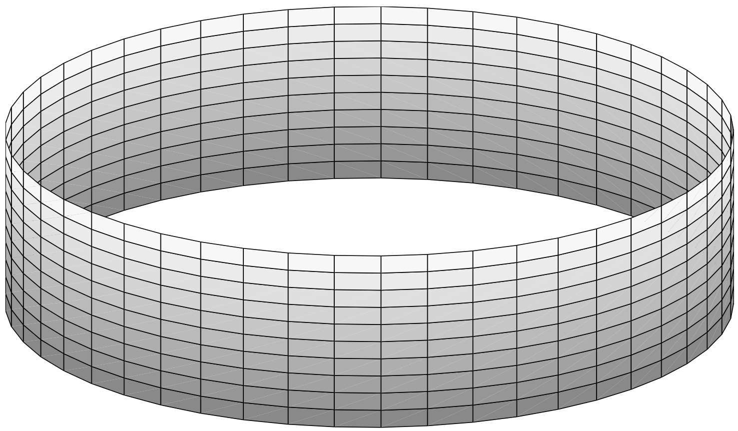

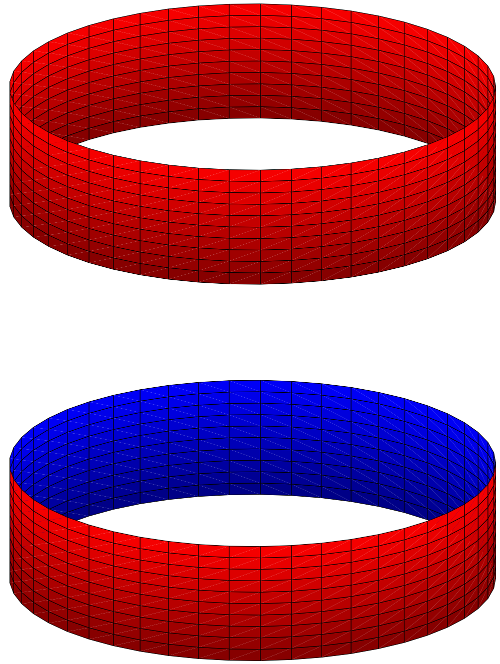

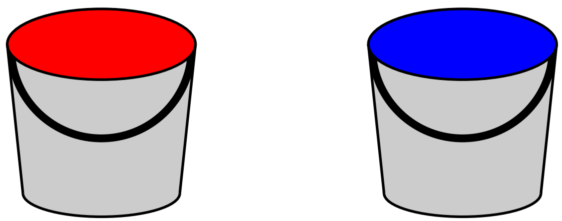

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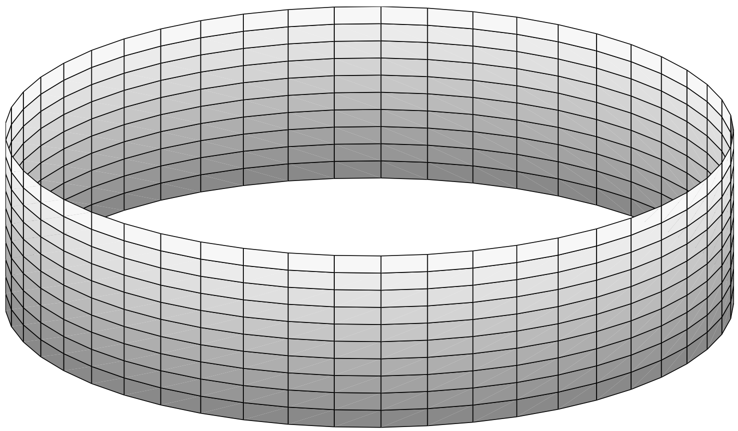

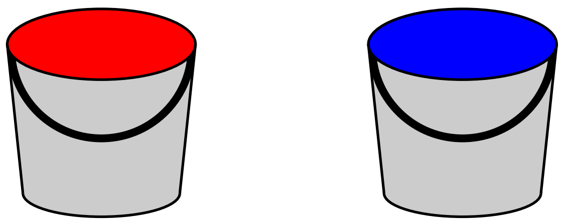

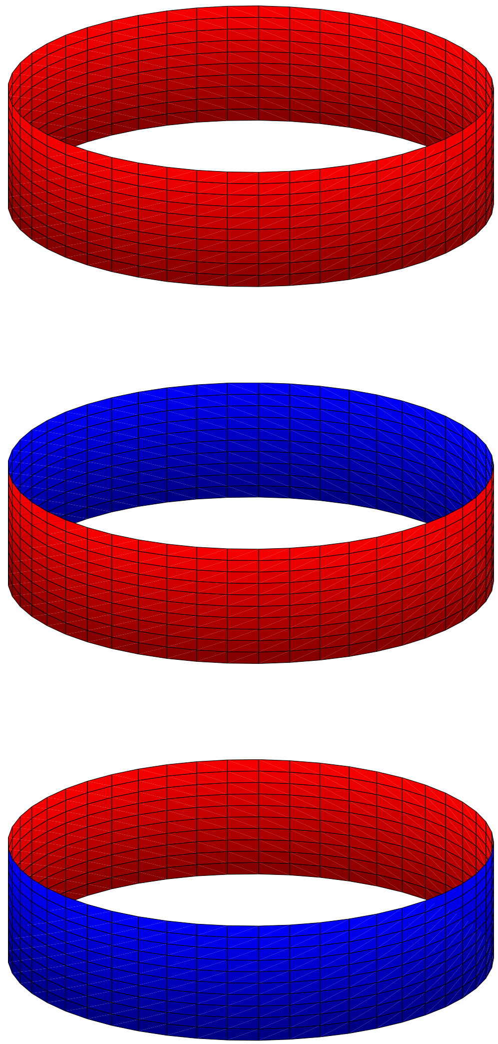

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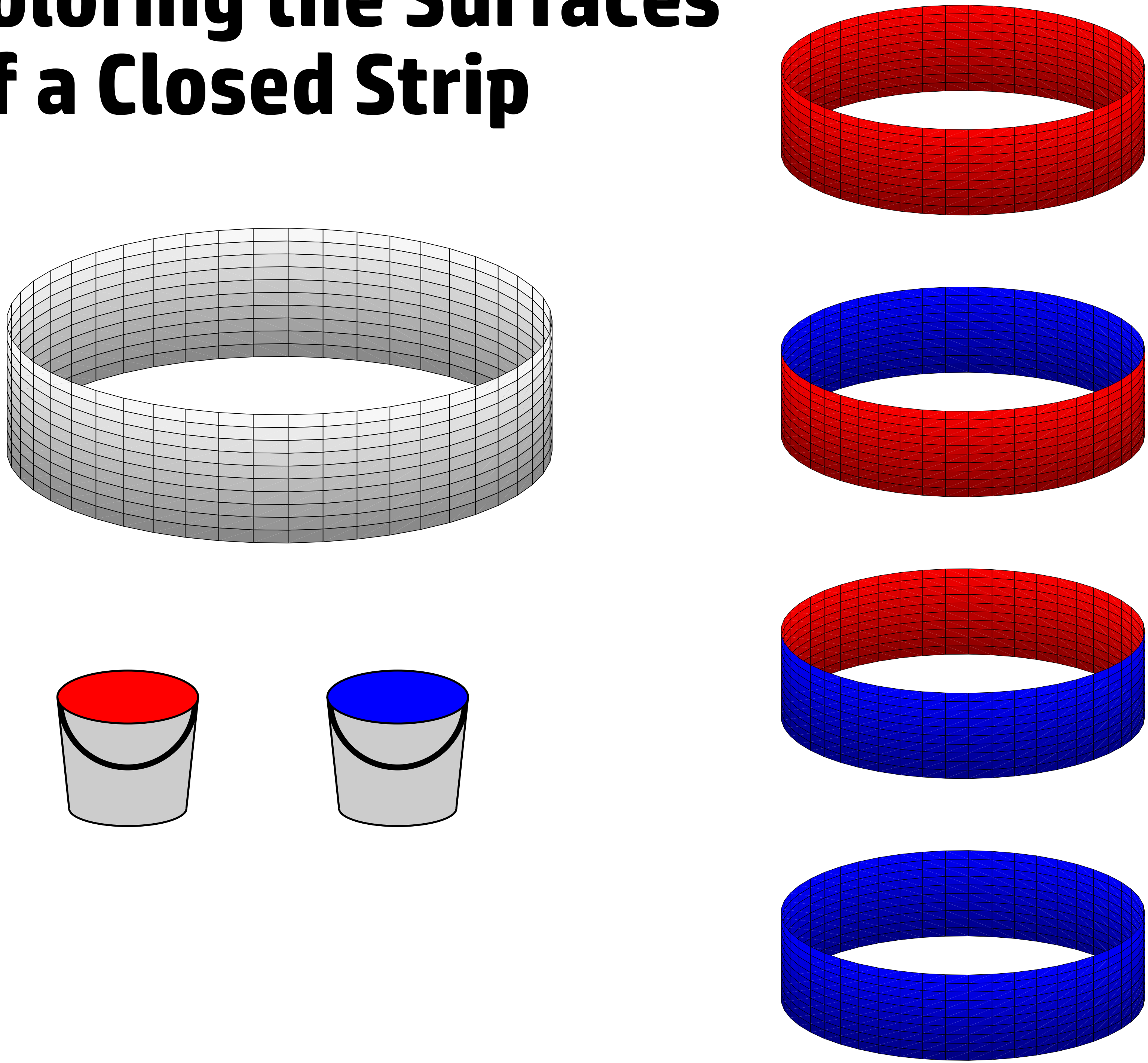

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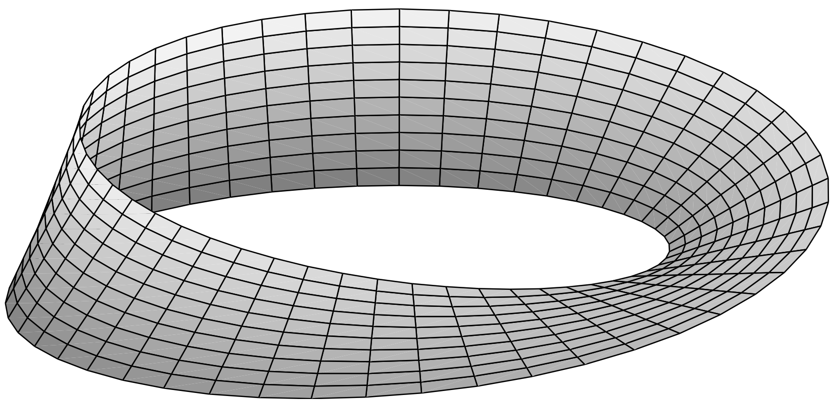

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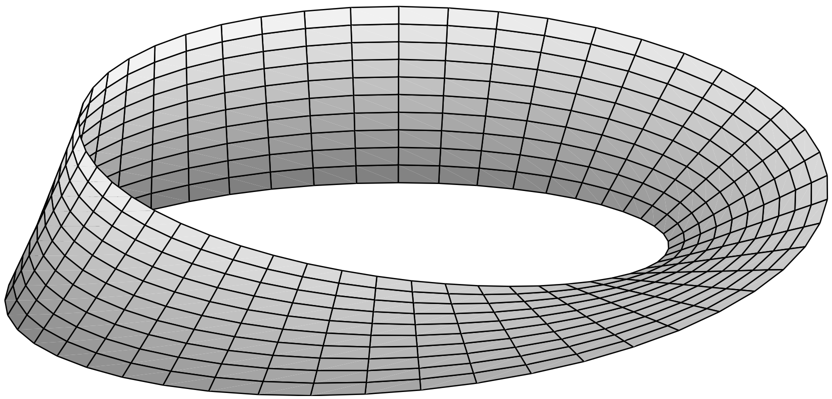

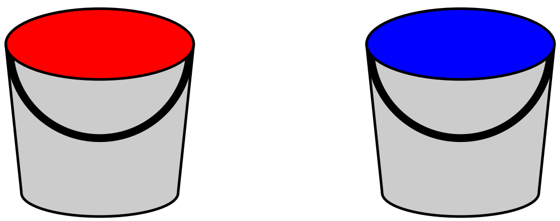

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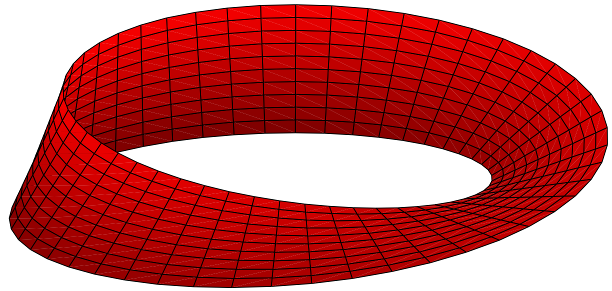

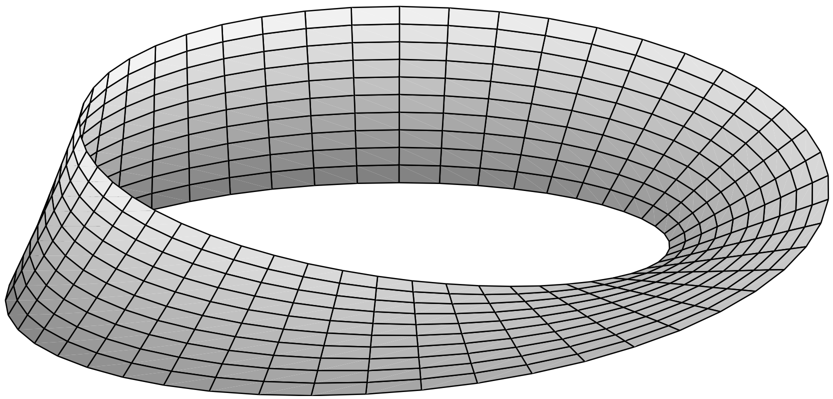

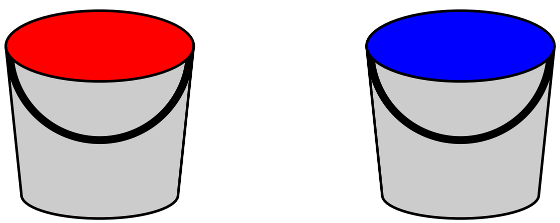

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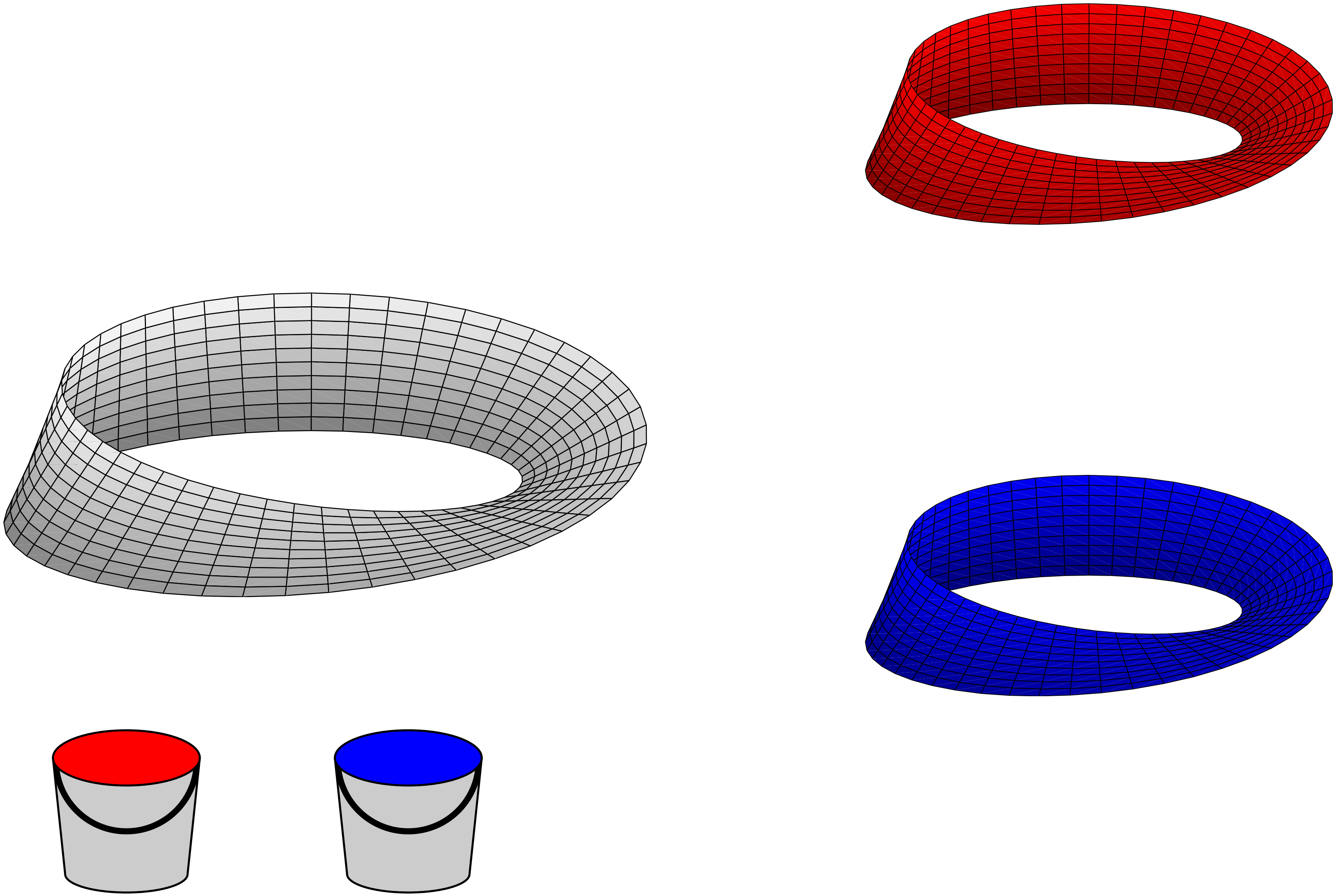
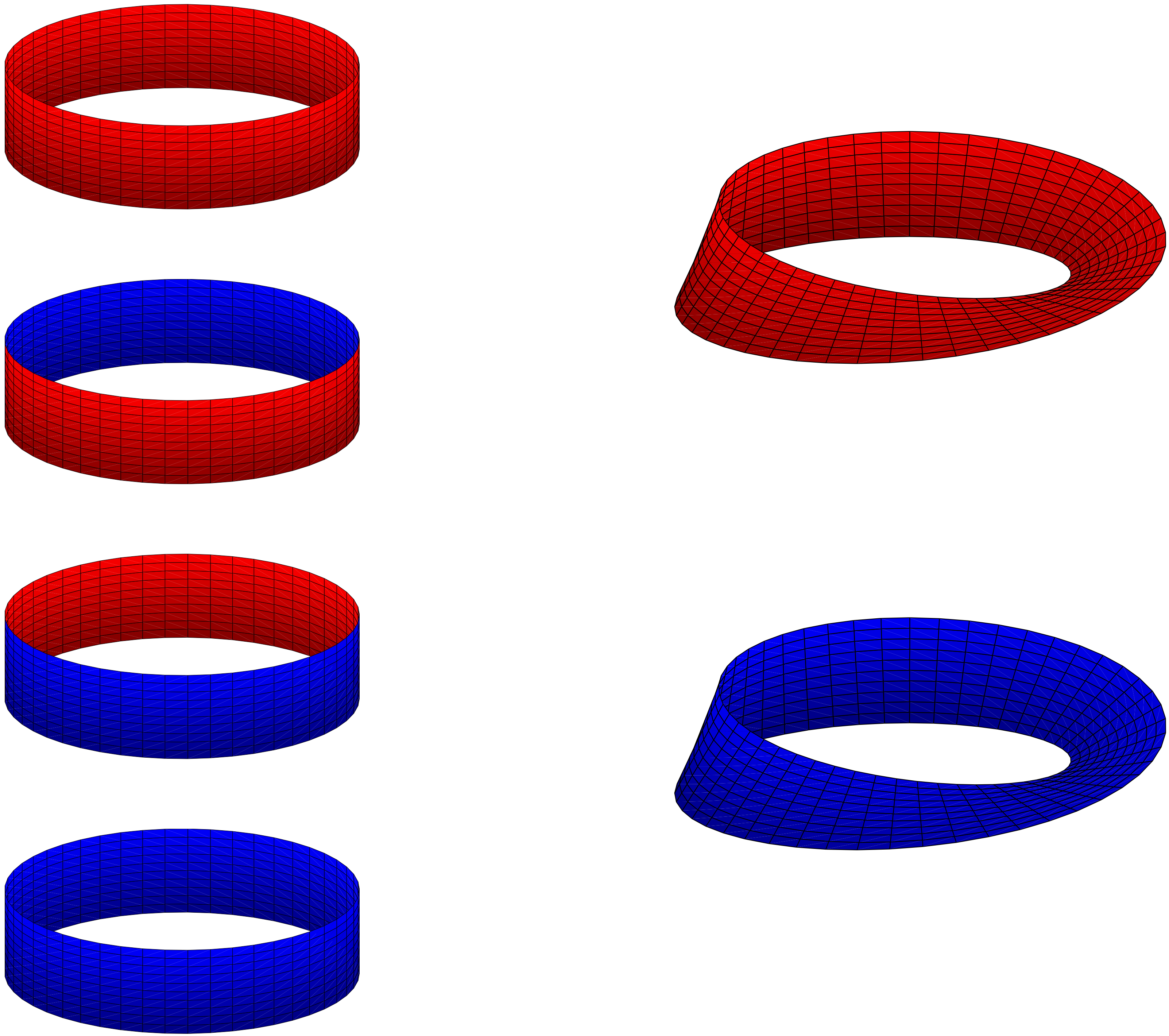
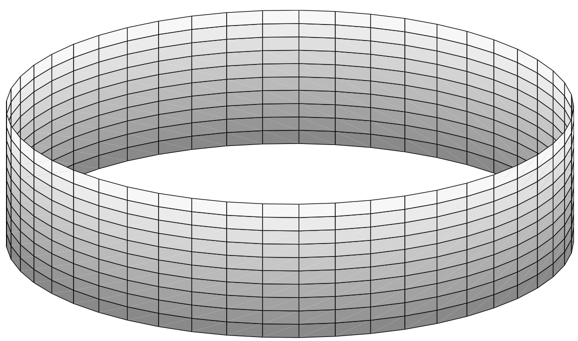
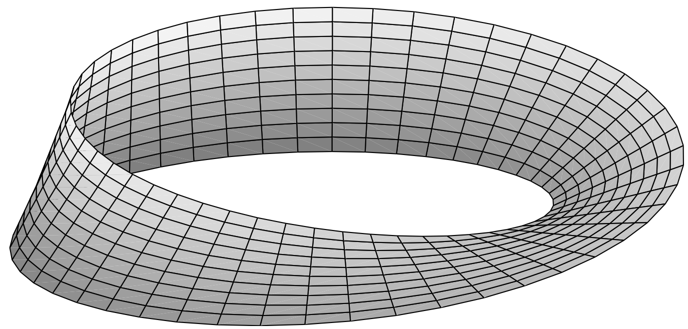
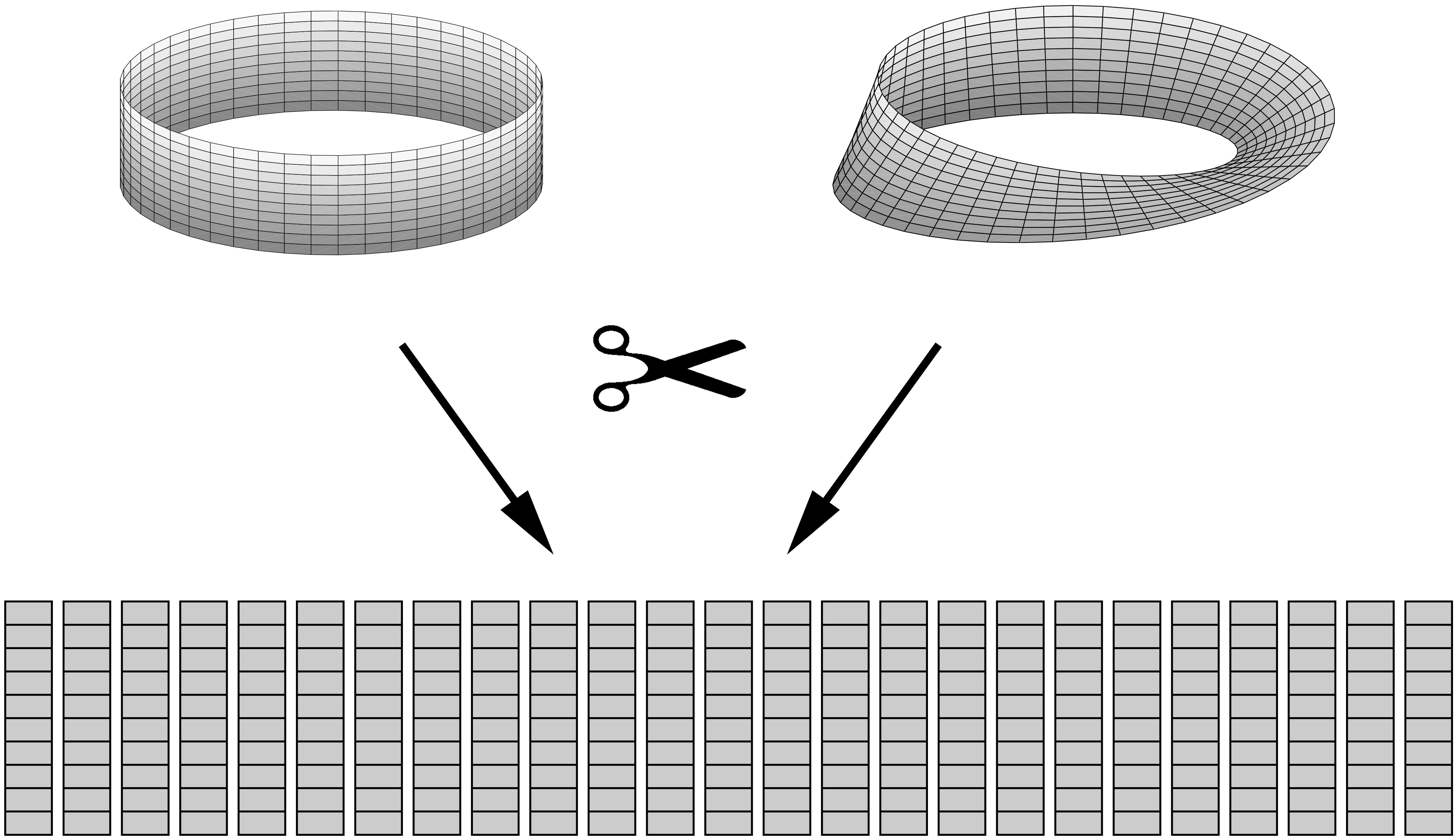
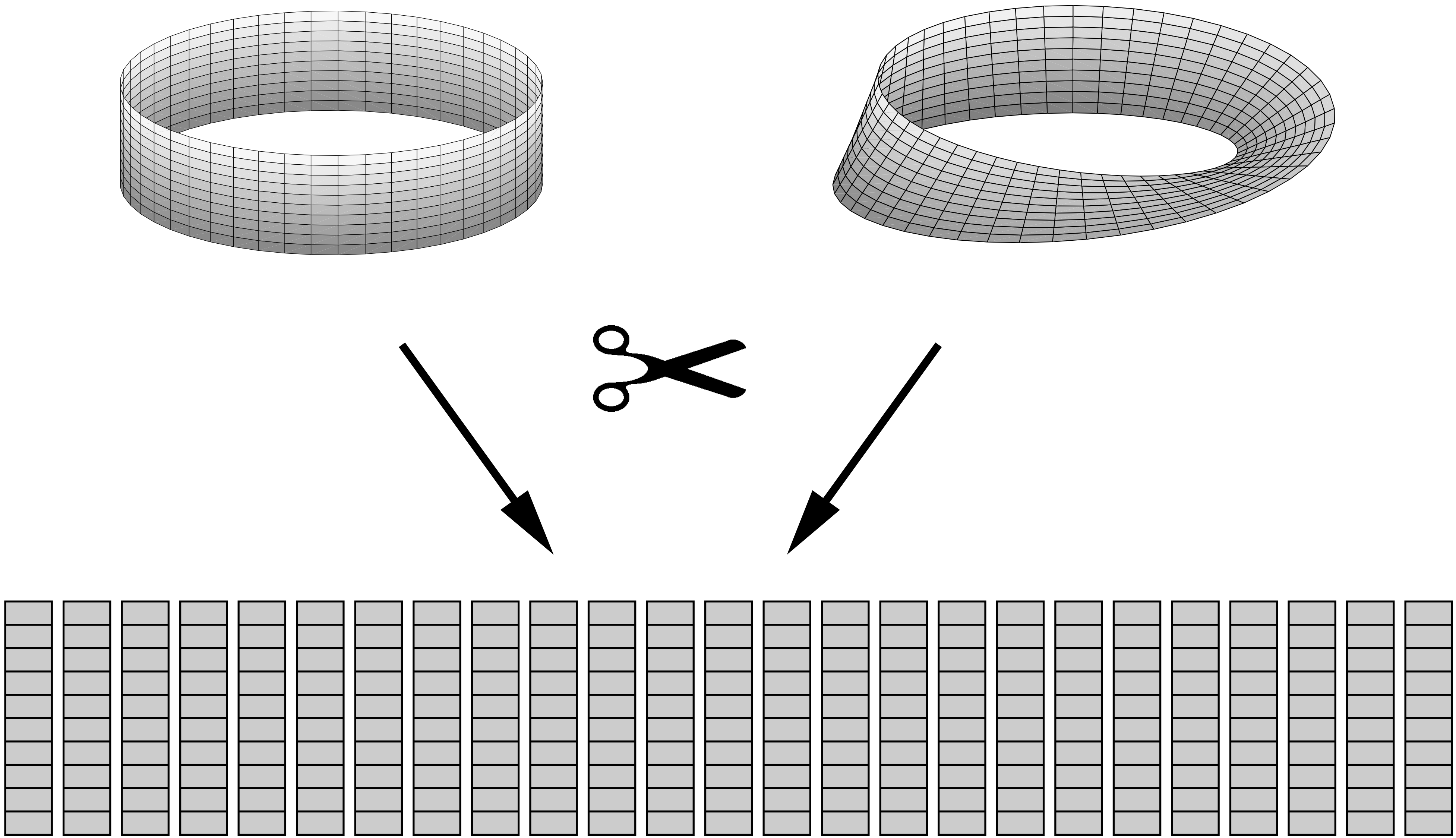


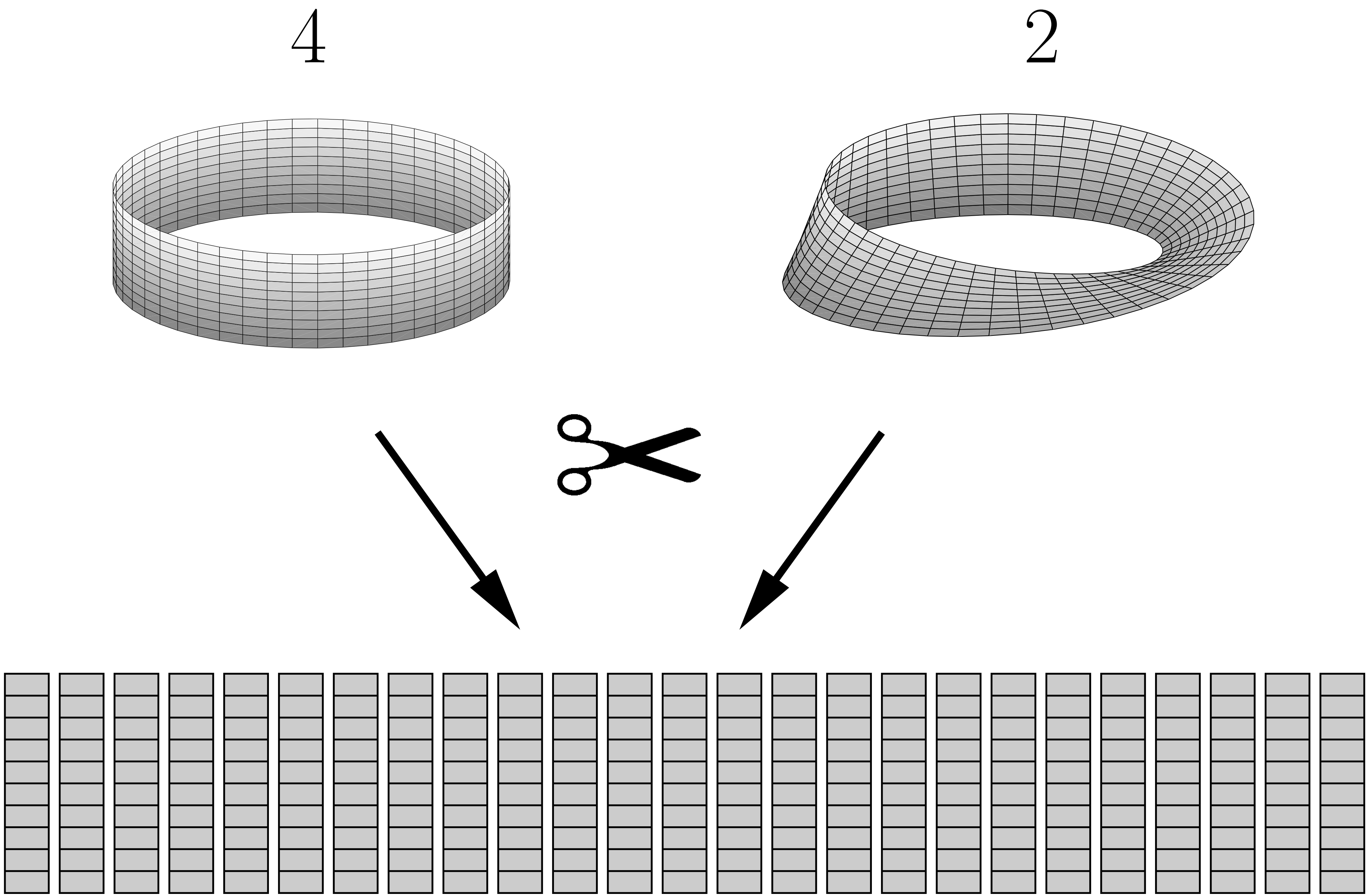


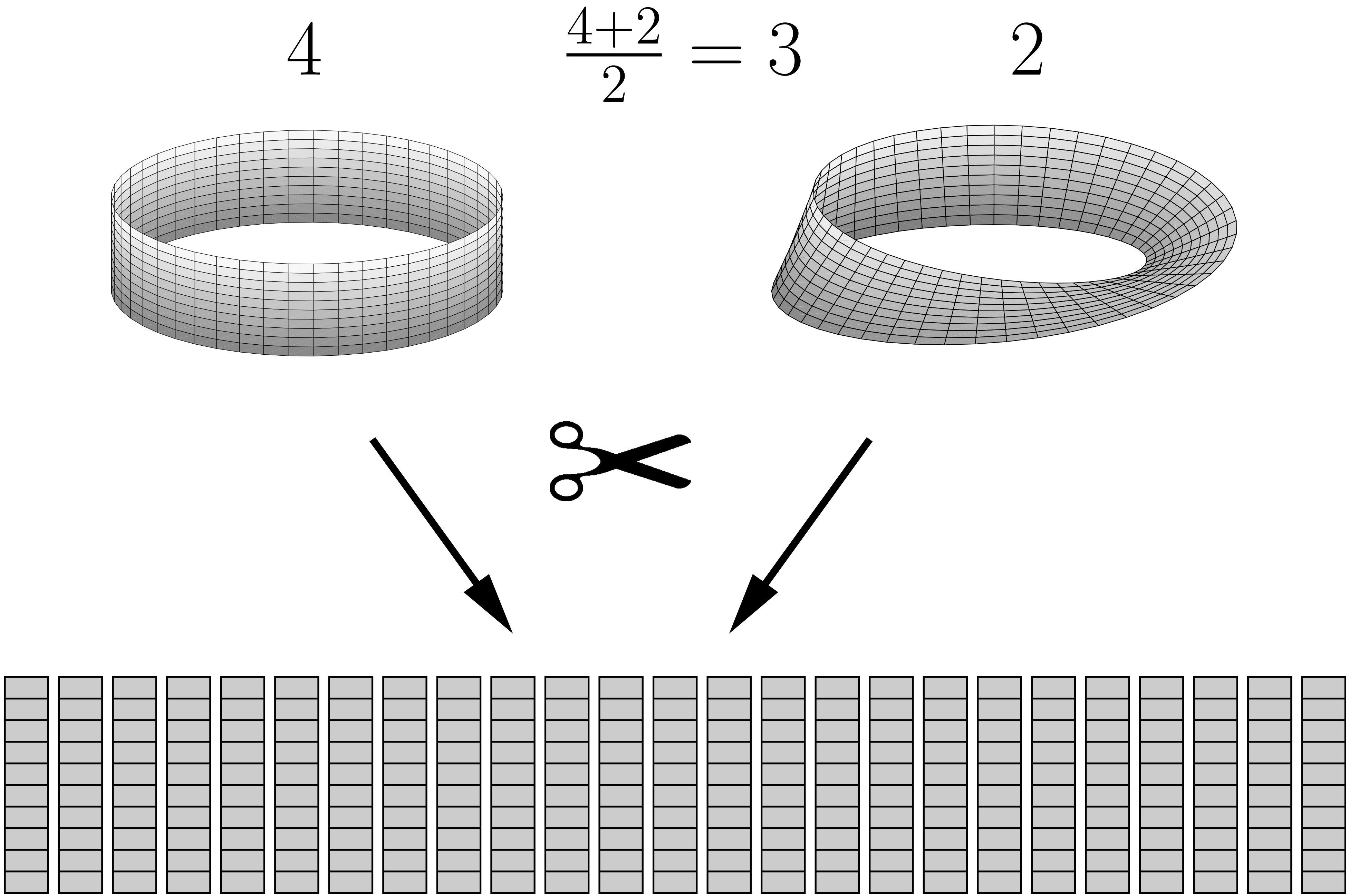


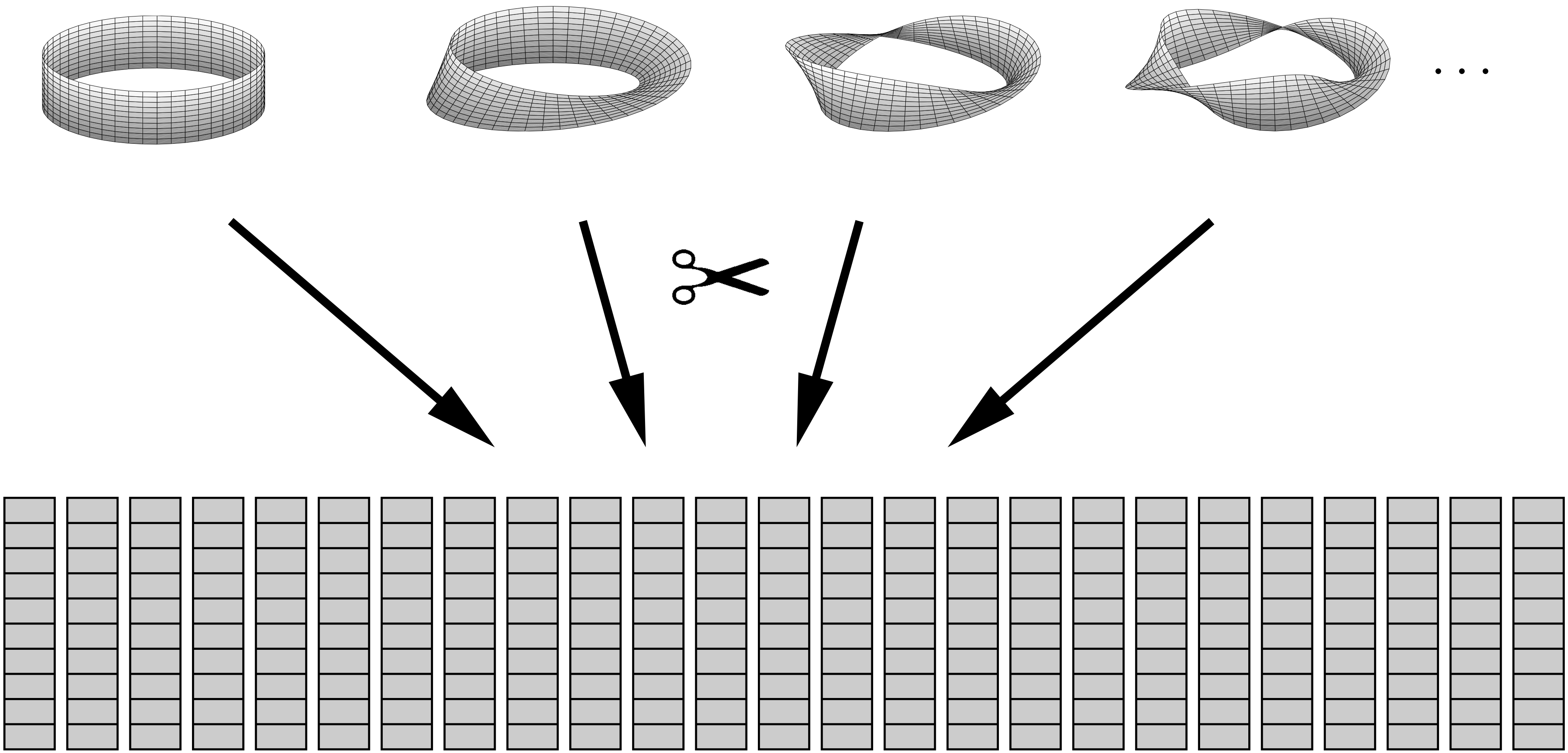


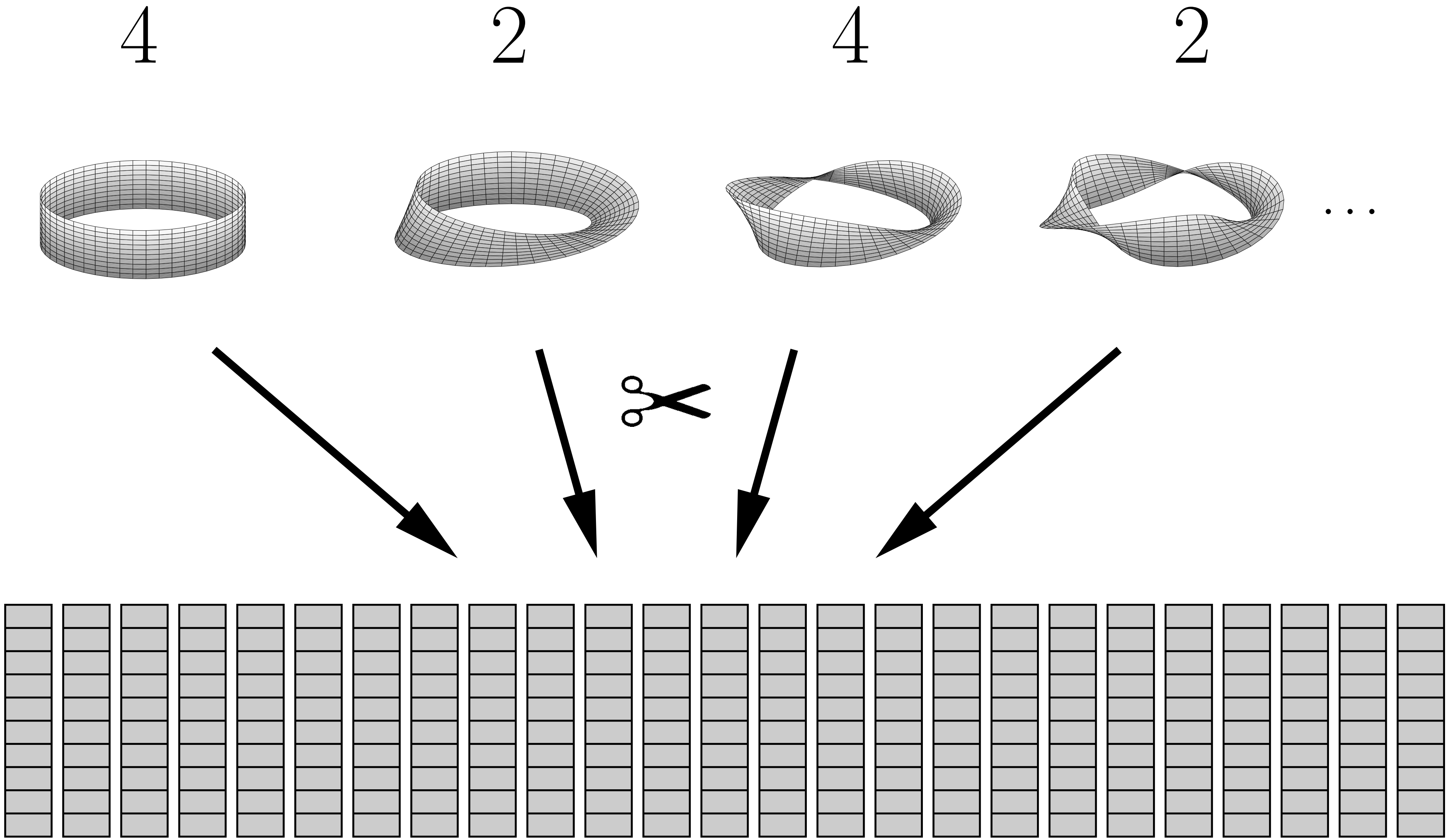





4
2


4
$\frac{4+2}{2} = 3$
2




4
2
4
2
...

The permanent of a matrix

Determinant vs. Permanent of a Matrix

Consider the matrix $\boldsymbol{\theta} = \begin{pmatrix} \theta_{11} & \theta_{12} & \theta_{13} \\ \theta_{21} & \theta_{22} & \theta_{23} \\ \theta_{31} & \theta_{32} & \theta_{33} \end{pmatrix}$.

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The determinant of $\boldsymbol{\theta}$:

$$\begin{aligned} \det(\boldsymbol{\theta}) = &+\theta_{11}\theta_{22}\theta_{33} + \theta_{12}\theta_{23}\theta_{31} + \theta_{13}\theta_{21}\theta_{32} \\ &- \theta_{11}\theta_{23}\theta_{32} - \theta_{12}\theta_{21}\theta_{33} - \theta_{13}\theta_{22}\theta_{31}. \end{aligned}$$

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Determinant vs. Permanent of a Matrix

The determinant of an $n \times n$-matrix $\boldsymbol{\theta}$

$$\det(\boldsymbol{\theta}) = \sum_{\sigma} \operatorname{sgn}(\sigma) \prod_{i \in [n]} \theta_{i,\sigma(i)}.$$

where the sum is over all $n!$ permutations of the set $[n] \triangleq \{1, \ldots, n\}$.

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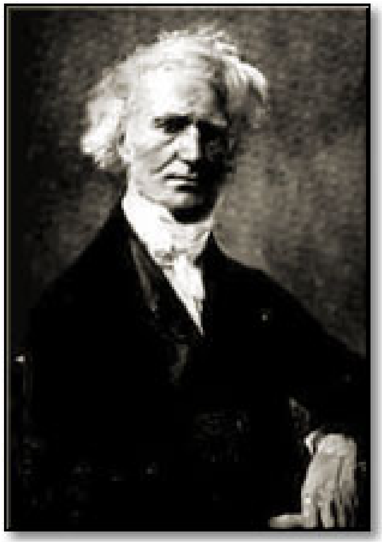
The permanent turns up in a variety of contexts, especially in combinatorial problems, statistical physics (partition function), ...

Historical Remarks

In 1812, Binet and Cauchy **independently** introduced functions that are nowadays called permanents.



G. P. M. Binet, "Mémoire sur un système de formules analytiques, et leur application à des considrations géométriques," Journal de l'École Polytechnique, Paris 9, pp. 280–302, 1812.

L. A. Cauchy, "Mémoire sur les fonctions qui ne peuvent obtenir que deux valeurs égales et de signes contraires par suite des transpositions opérées entre les variables qu'elles renferment," Journal de l'École Polytechnique, Paris 10, pp. 29–112, 1812.

Exactly Computing the Permanent

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- Complexity class [Valiant, 1979]:

#P ("sharp P" or "number P"),

where #P is the set of the counting problems associated with the decision problems in the set NP. (Note that even the computation of the permanent of zero-one matrices is #P-complete.)

Estimating the Permanent

More efficient algorithms are possible if one does not want to compute the permanent of a matrix exactly.

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- For a matrix that contains only non-negative entries:

  $\rightarrow$ "constructive interference of terms in the summation."

Estimating the Permanent

FROM NOW ON: we focus on the case where all entries of the matrix are non-negative, i.e.

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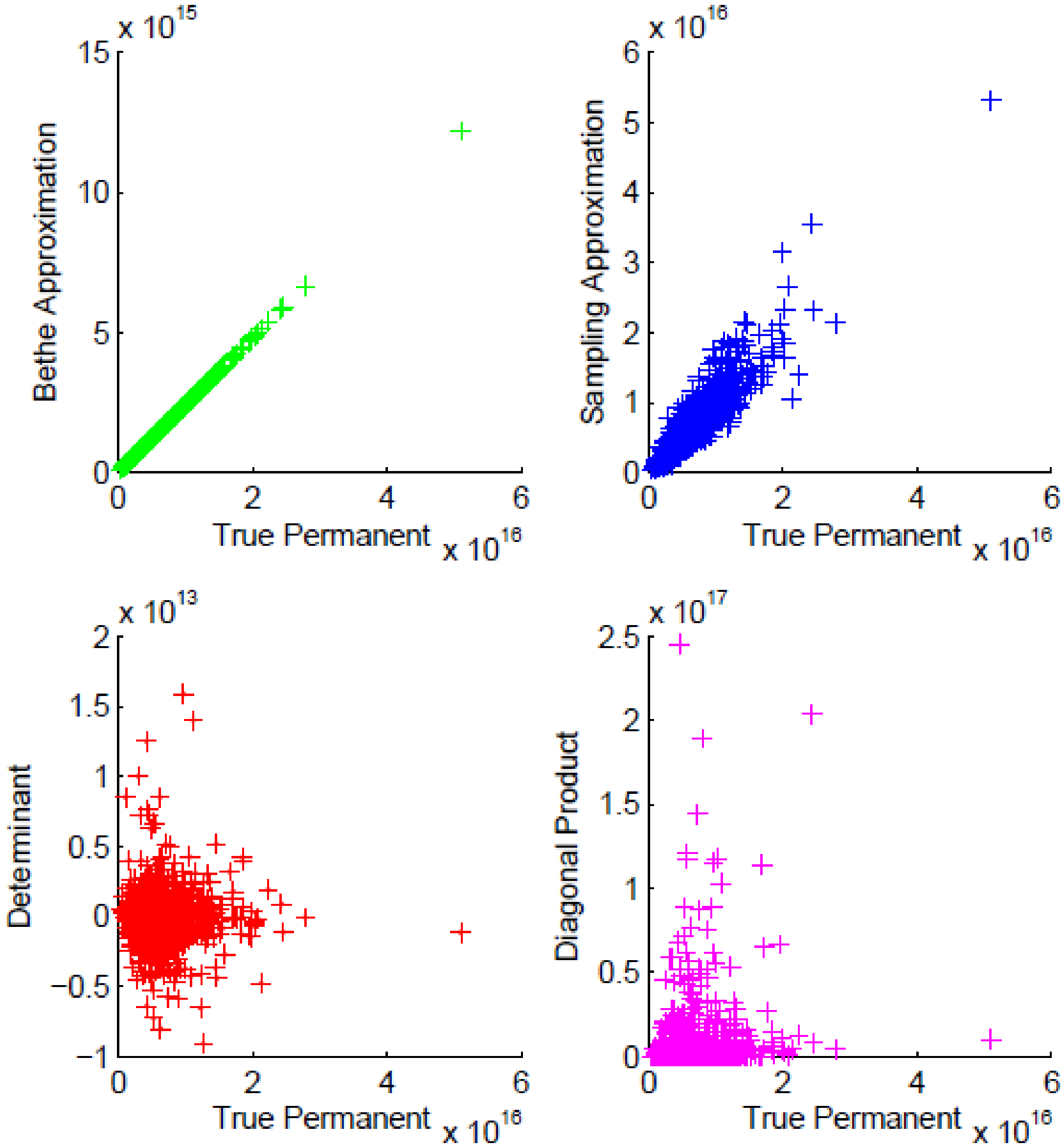
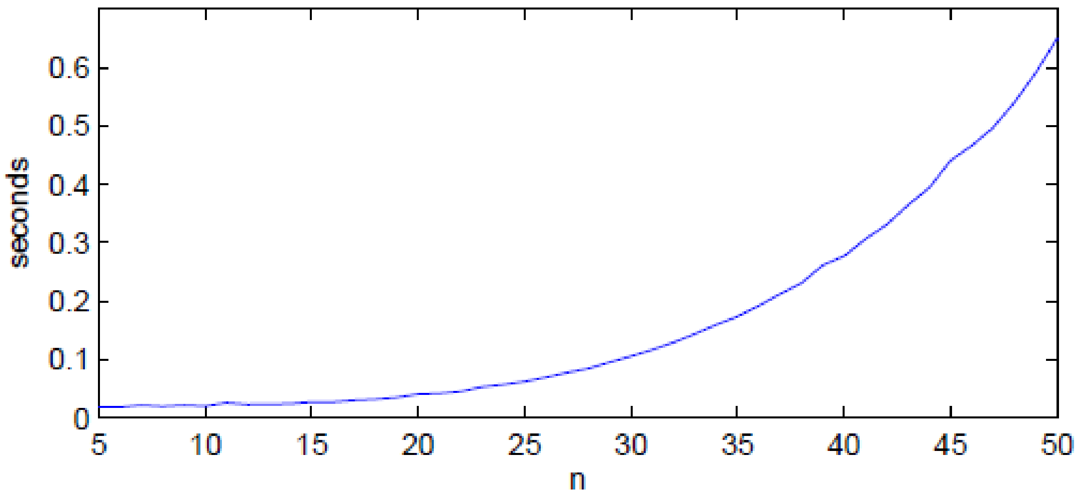
- Bethe-approximation-based / sum-product-algorithm-based methods: [Chertkov et al., 2008], [Huang and Jebara, 2009], ...

Estimating the Permanent

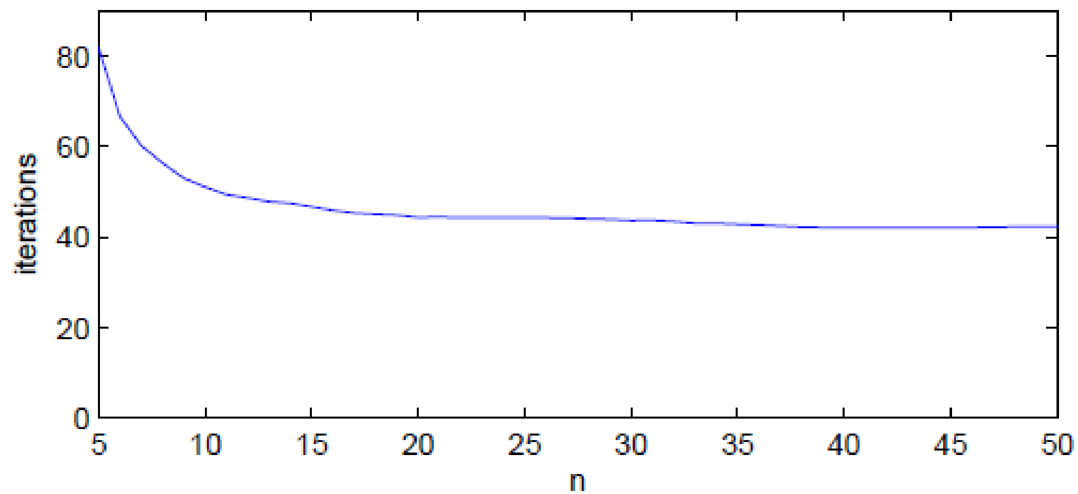


From [Huang/Jebara, 2009].

Estimating the Permanent



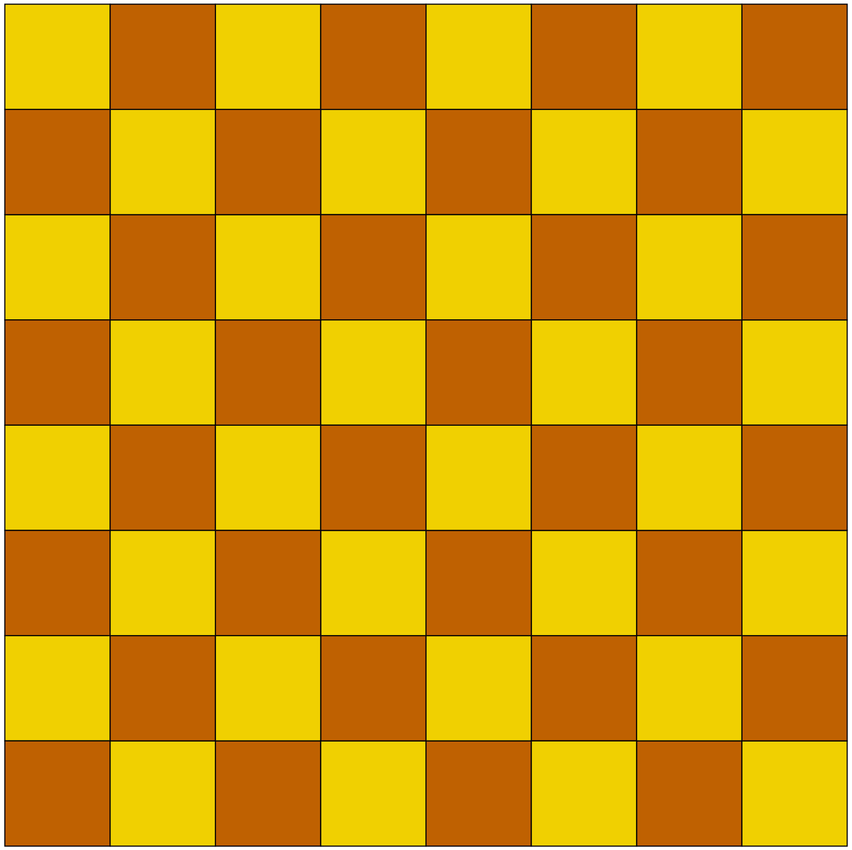
(a) Running time



(b) Iterations

From [Huang/Jebara, 2009].

Valid Rook Configs. and Permanents



Number of valid rook configurations

$$= \operatorname{perm}\begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix}$$

$$= \sum_{\sigma} \prod_{i \in [8]} \theta_{i,\sigma(i)}$$

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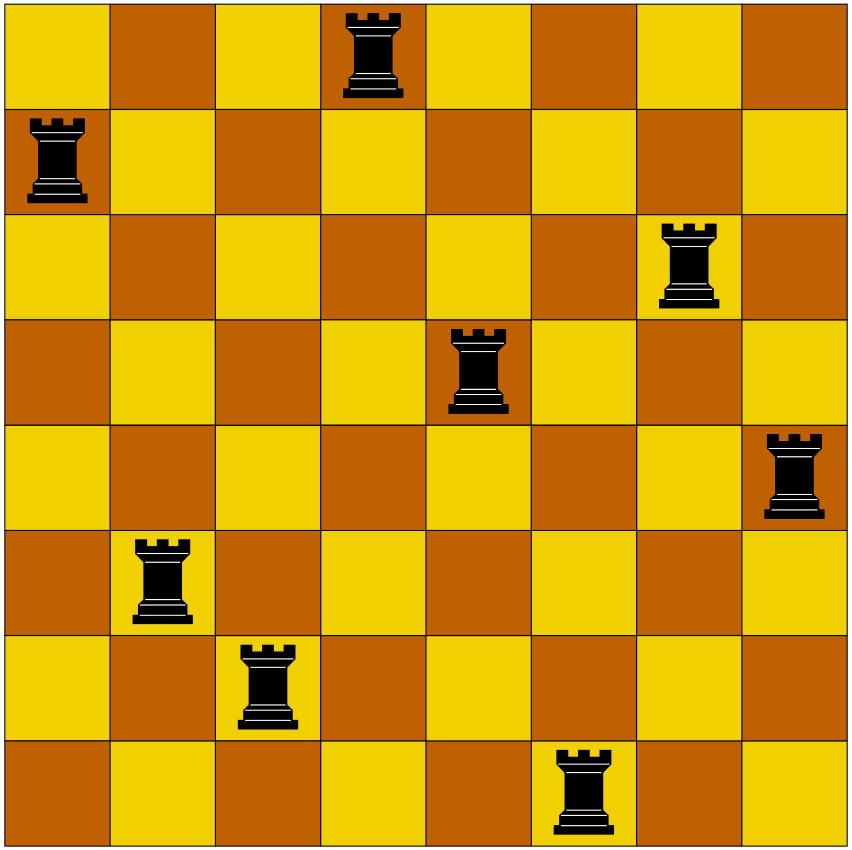

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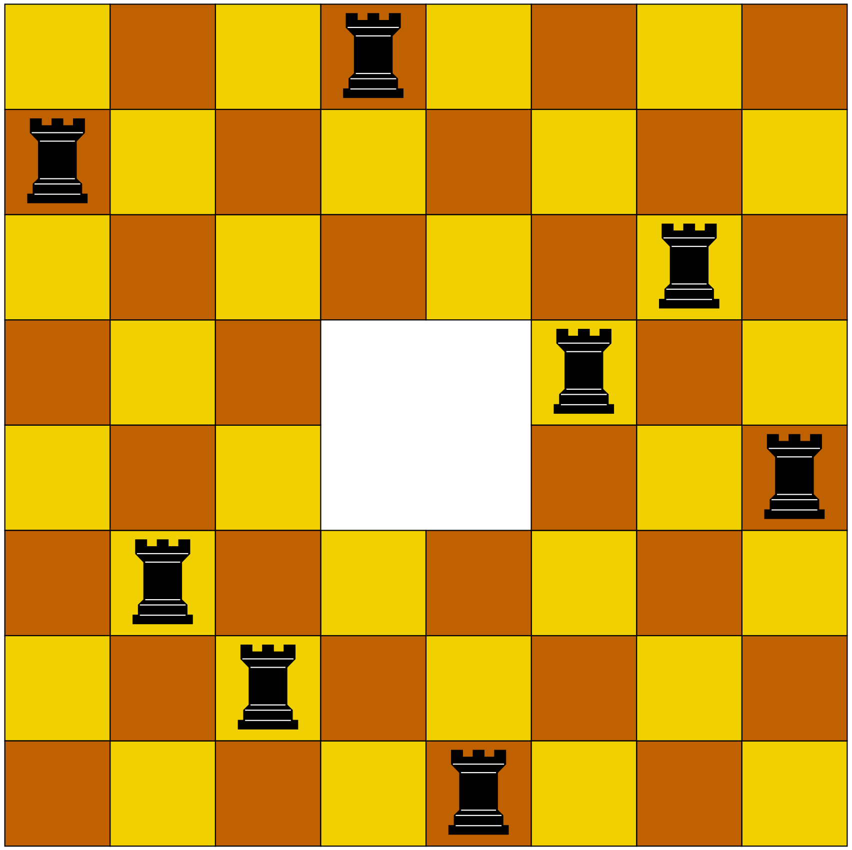
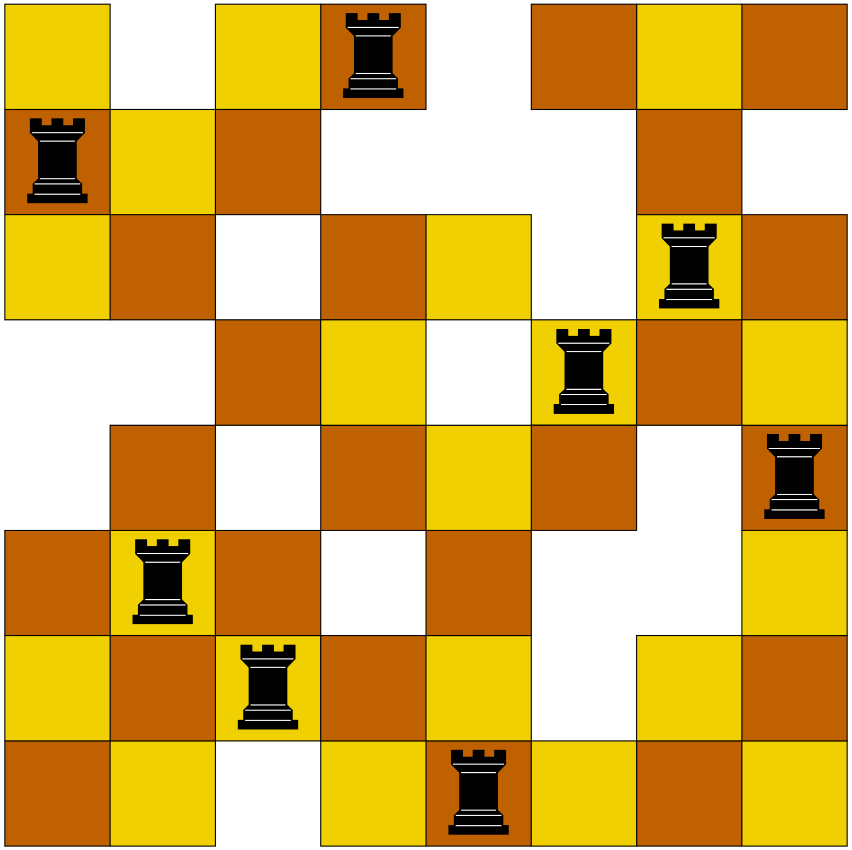


Number of valid rook configurations

$$
= \operatorname{perm}\begin{pmatrix}
1 & 1 & 1 & {\color{red}1} & 1 & 1 & 1 & 1 \\
{\color{red}1} & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 & {\color{red}1} & 1 \\
1 & 1 & 1 & 0 & 0 & {\color{red}1} & 1 & 1 \\
1 & 1 & 1 & 0 & 0 & 1 & 1 & {\color{red}1} \\
1 & {\color{red}1} & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & {\color{red}1} & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & {\color{red}1} & 1 & 1 & 1
\end{pmatrix}
$$

$$
= \sum_{\sigma} {\color{red}\prod_{i \in [8]} \theta_{i,\sigma(i)}}
$$

Valid Rook Configs. and Permanents

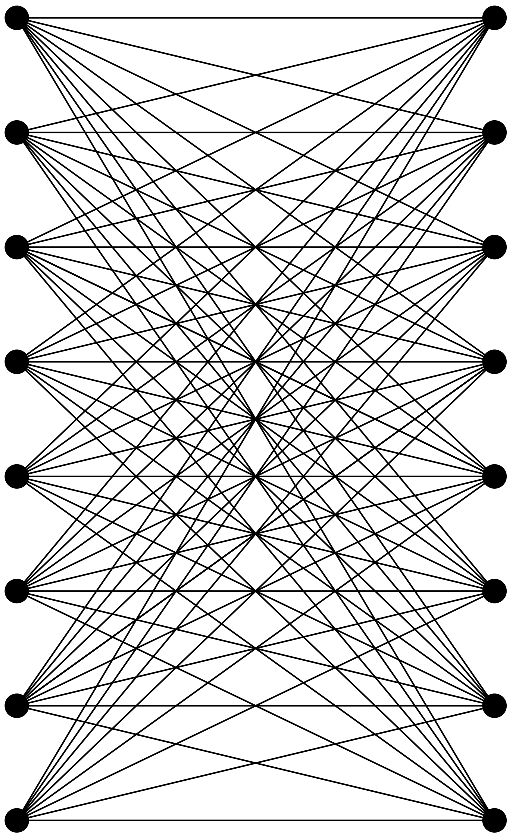


Number of valid rook configurations

$$= \operatorname{perm}\begin{pmatrix} 1 & 0 & 1 & 1 & 0 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 & 1 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 & 1 & 0 & 0 & 1 \\ 1 & 1 & 1 & 1 & 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 & 1 & 1 & 1 & 1 \end{pmatrix}$$

$$= \sum_{\sigma} \prod_{i \in [8]} \theta_{i,\sigma(i)}$$

Perfect Matchings and Permanents



Number of perfect matchings

$$= \mathrm{perm}\begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix}$$

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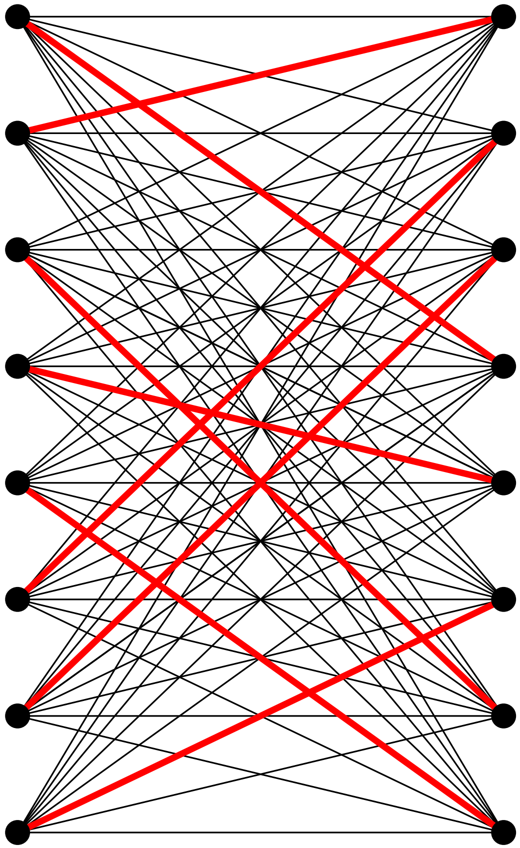
Perfect Matchings and Permanents

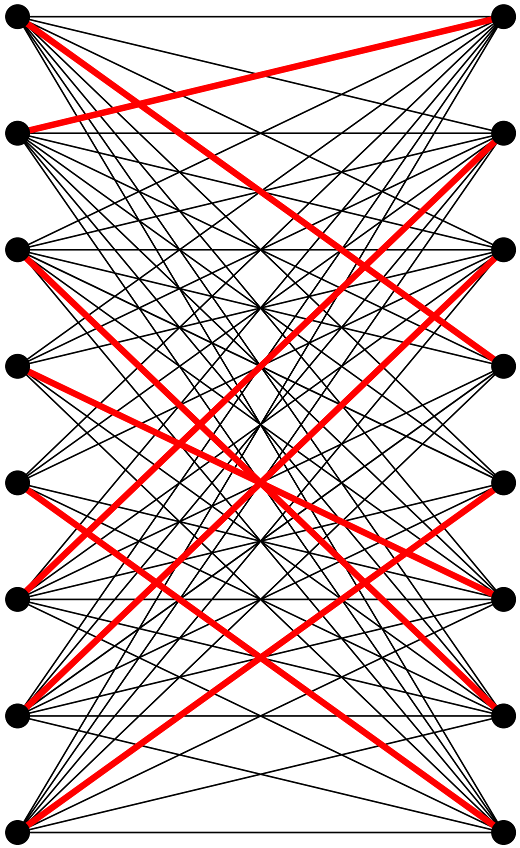


Number of perfect matchings

$$= \operatorname{perm}\begin{pmatrix} 1 & 1 & 1 & \color{red}{\mathbf{1}} & 1 & 1 & 1 & 1 \\ \color{red}{\mathbf{1}} & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & \color{red}{\mathbf{1}} & 1 \\ 1 & 1 & 1 & 1 & \color{red}{\mathbf{1}} & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & \color{red}{\mathbf{1}} \\ 1 & \color{red}{\mathbf{1}} & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & \color{red}{\mathbf{1}} & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & \color{red}{\mathbf{1}} & 1 & 1 \end{pmatrix}$$

$$= \sum_{\sigma} \prod_{i \in [8]} \theta_{i,\sigma(i)}$$

Perfect Matchings and Permanents



Number of perfect matchings

$$= \mathrm{perm}\begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix}$$

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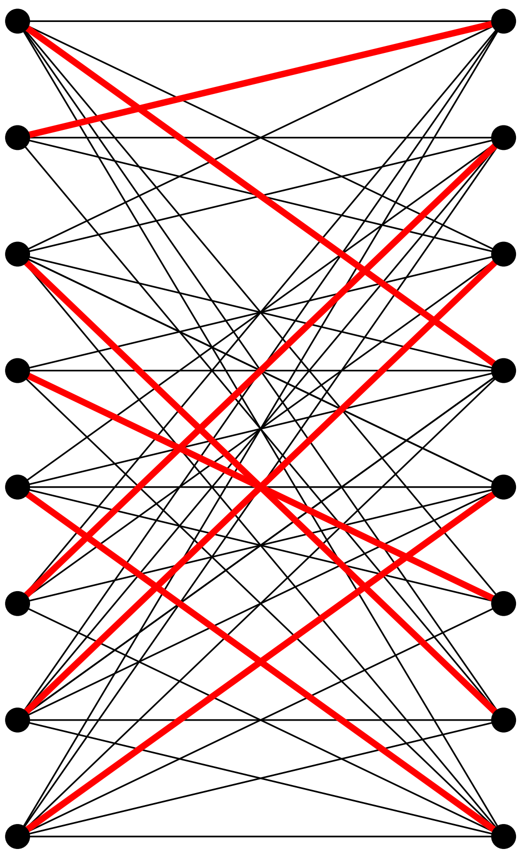
Perfect Matchings and Permanents



Number of perfect matchings

$$= \mathrm{perm}\begin{pmatrix} 1 & 0 & 1 & 1 & 0 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 & 1 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 & 1 & 0 & 0 & 1 \\ 1 & 1 & 1 & 1 & 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 & 1 & 1 & 1 & 1 \end{pmatrix}$$

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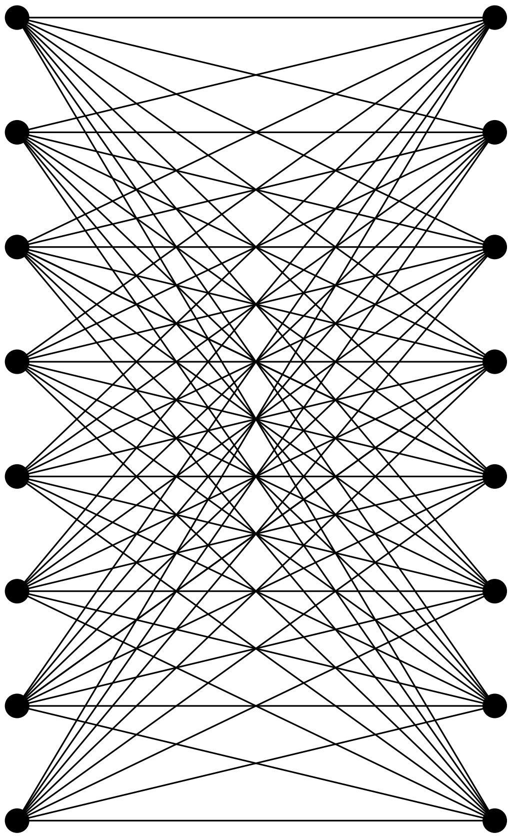
Perfect Matchings and Permanents



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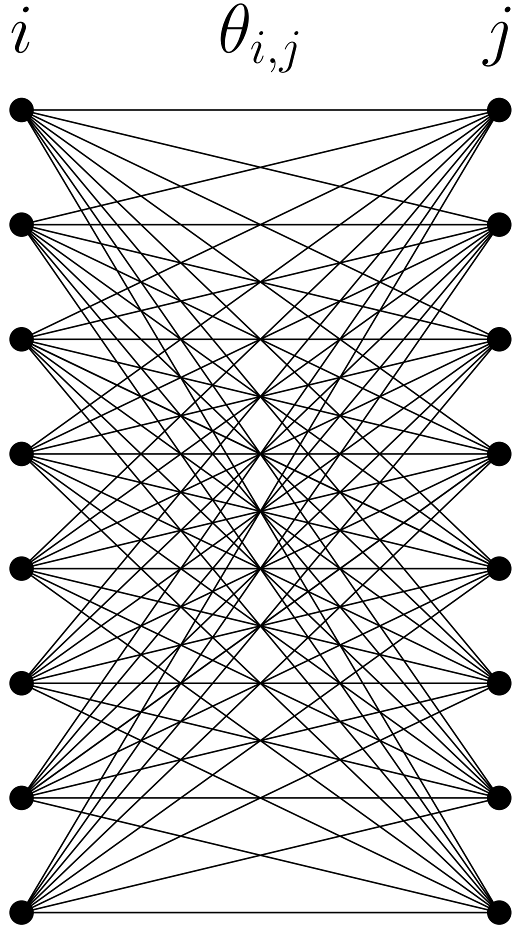
Perfect Matchings and Permanents



Total sum of weighted perf. matchings

$$= \mathrm{perm}\begin{pmatrix} \theta_{11} & \theta_{12} & \theta_{13} & \theta_{14} & \theta_{15} & \theta_{16} & \theta_{17} & \theta_{18} \\ \theta_{21} & \theta_{22} & \theta_{23} & \theta_{24} & \theta_{25} & \theta_{26} & \theta_{27} & \theta_{28} \\ \theta_{31} & \theta_{32} & \theta_{33} & \theta_{34} & \theta_{35} & \theta_{36} & \theta_{37} & \theta_{38} \\ \theta_{41} & \theta_{42} & \theta_{43} & \theta_{44} & \theta_{45} & \theta_{46} & \theta_{47} & \theta_{48} \\ \theta_{51} & \theta_{52} & \theta_{53} & \theta_{54} & \theta_{55} & \theta_{56} & \theta_{57} & \theta_{58} \\ \theta_{61} & \theta_{62} & \theta_{63} & \theta_{64} & \theta_{65} & \theta_{66} & \theta_{67} & \theta_{68} \\ \theta_{71} & \theta_{72} & \theta_{73} & \theta_{74} & \theta_{75} & \theta_{76} & \theta_{77} & \theta_{78} \\ \theta_{81} & \theta_{82} & \theta_{83} & \theta_{84} & \theta_{85} & \theta_{86} & \theta_{87} & \theta_{88} \end{pmatrix}$$

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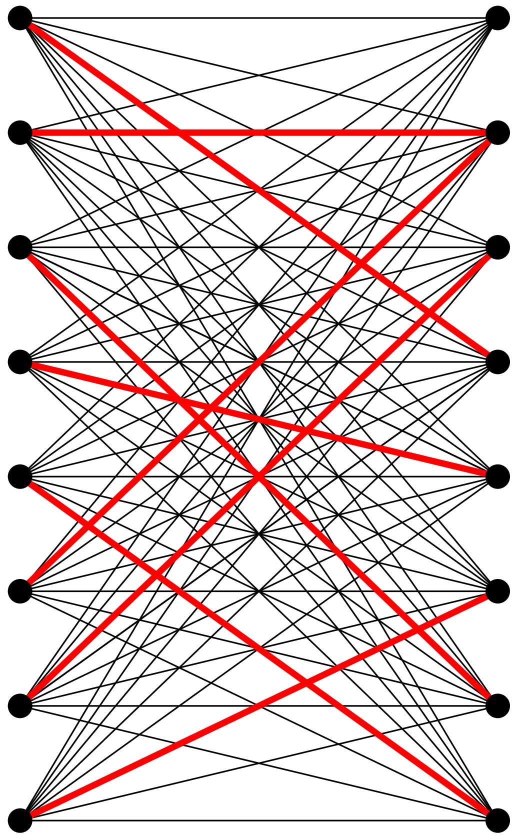
Perfect Matchings and Permanents



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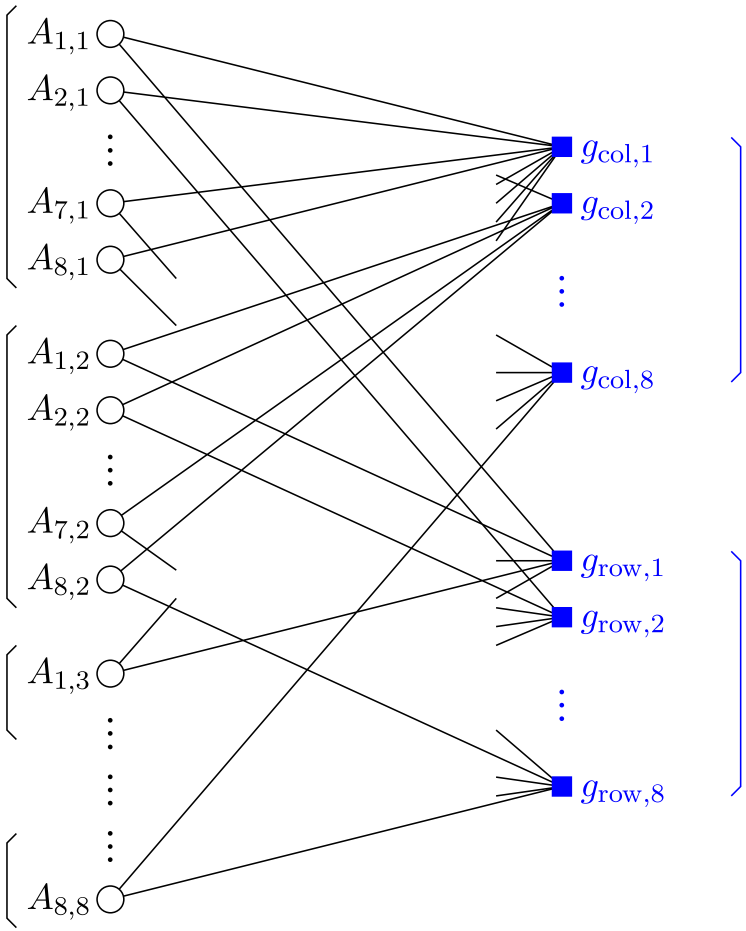
$$= \sum_{\sigma} \prod_{i \in [8]} \theta_{i,\sigma(i)}$$

Graphical Model for Permanent



(function nodes are suitably defined based on $\boldsymbol{\theta}$)

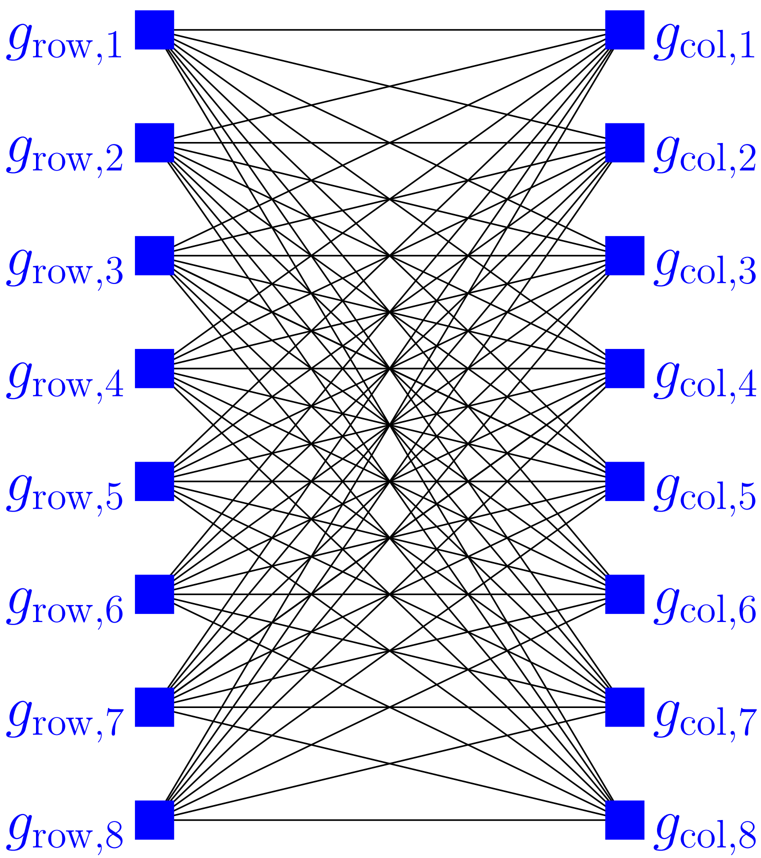
Global function:

$$g(a_{1,1}, \ldots, a_{8,8}) = \prod_j g_{\mathrm{col},j}(a_{1,j}, \ldots, a_{8,j}) \times \prod_i g_{\mathrm{row},i}(a_{i,1}, \ldots, a_{i,8})$$

Permanent:

$$\mathrm{perm}(\boldsymbol{\theta}) = Z = \sum_{a_{1,1},\ldots,a_{8,8}} g(a_{1,1}, \ldots, a_{8,8})$$

Graphical Model for Permanent



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(variable nodes have been omitted)

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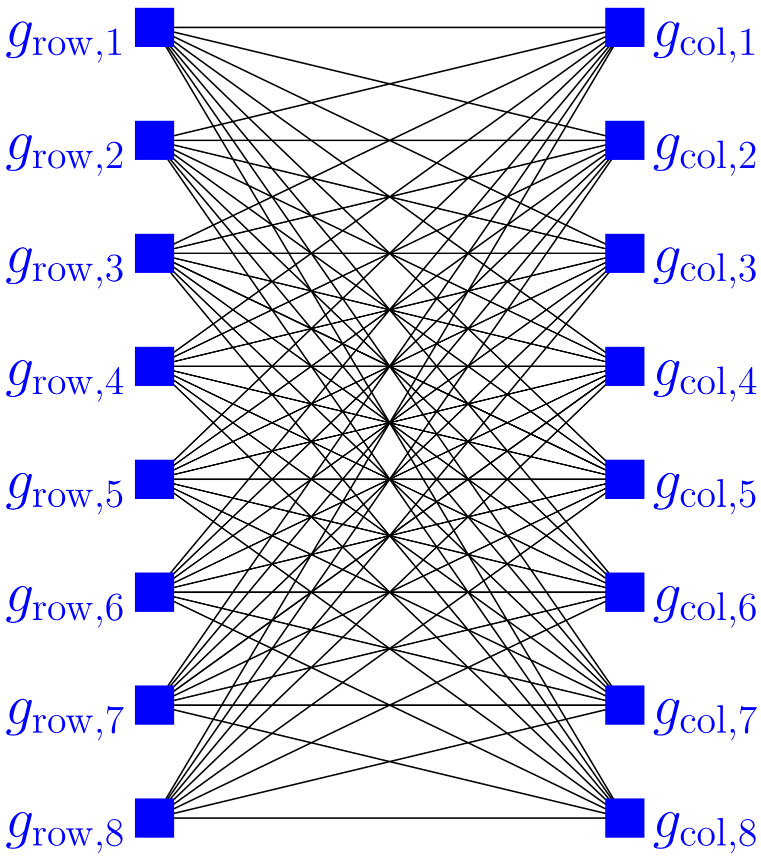
Graphical Model for Permanent



(function nodes are suitably defined based on $\boldsymbol{\theta}$)

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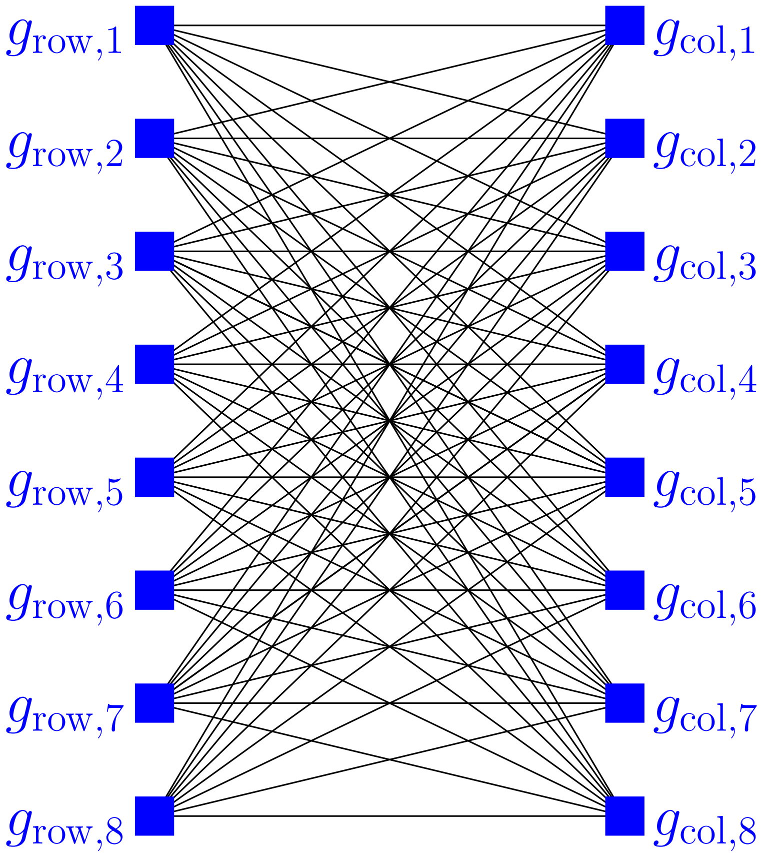
- Many short cycles.
- The vertex degrees are high.

Graphical Model for Permanent



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- ↯ Many short cycles.
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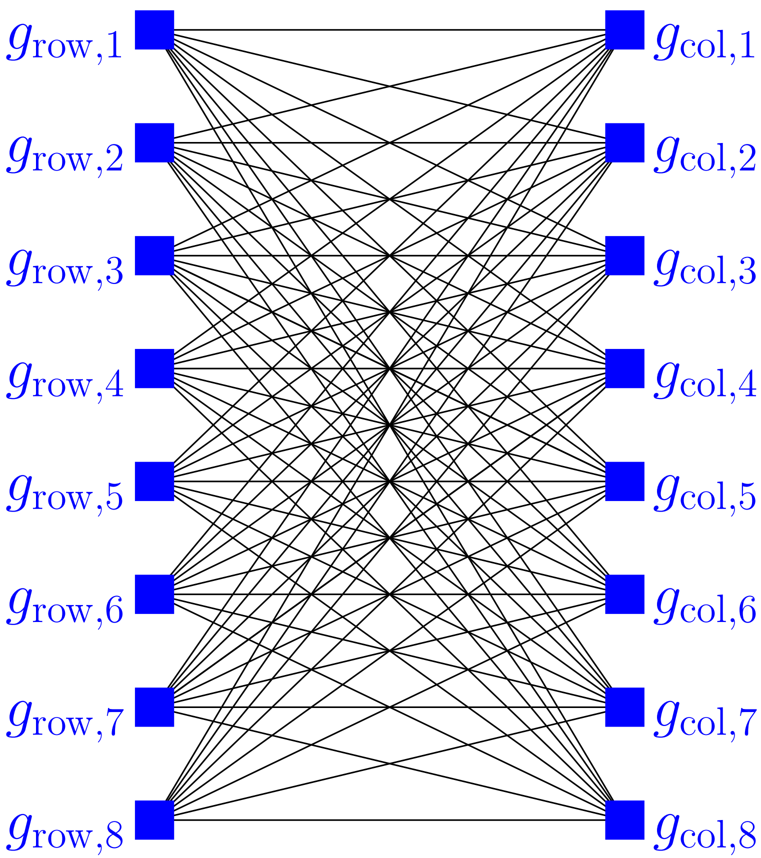
Both facts might suggest that the application of the sum-product algorithm to this factor graph is rather problematic.

Graphical Model for Permanent



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However, luckily this is not the case.

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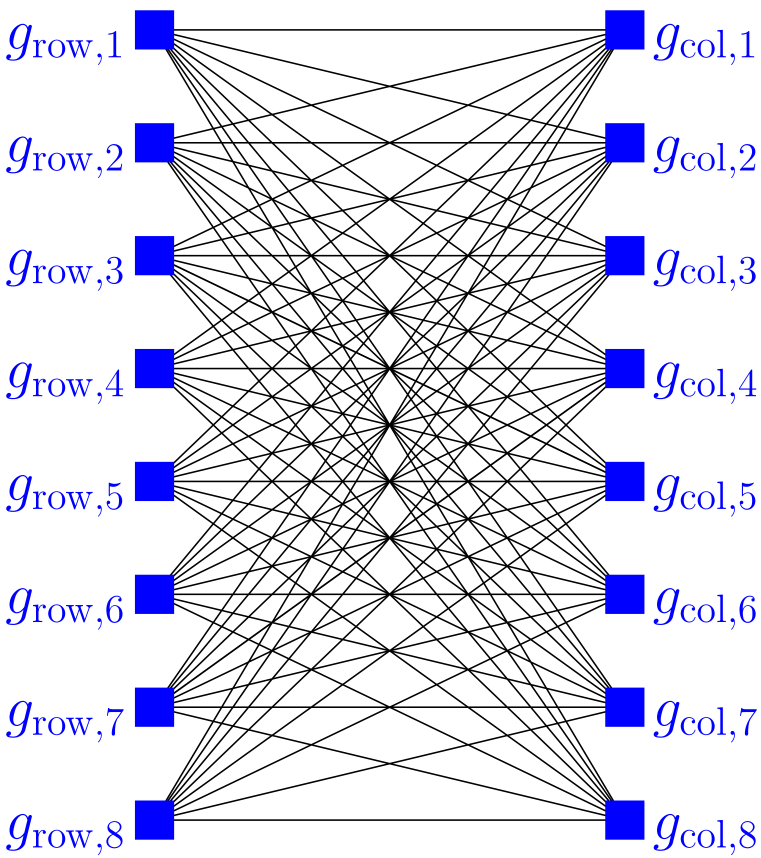

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Both facts might suggest that the application of the sum-product algorithm to this factor graph is rather problematic.

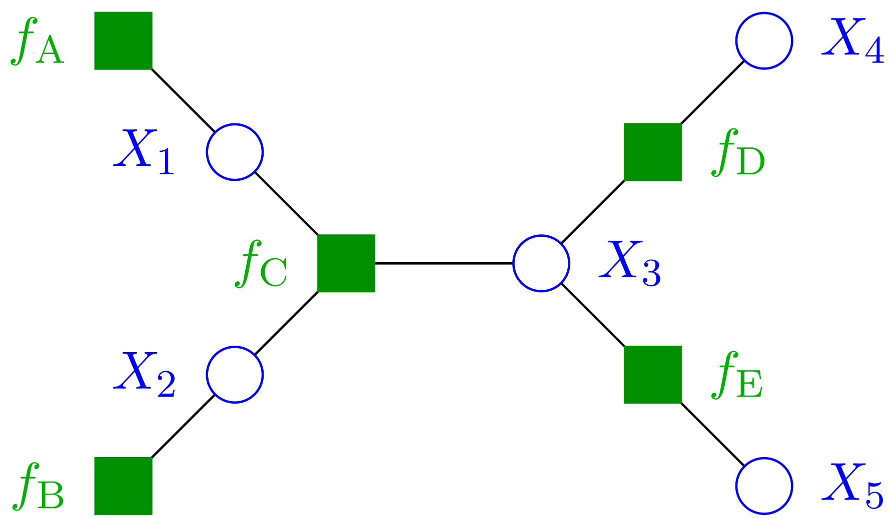
However, luckily this is not the case.

For an SPA suitability assessment, the overall cycle structure and the types of functions nodes are at least as important.

Factor graphs and the sum-product algorithm

The Sum-Product Algorithm

Let us consider the following factor graph (which is a tree).



The global function is

$$\begin{aligned} f(x_1, x_2, x_3, x_4, x_5) \\ &= f_{\mathrm{A}}(x_1) \cdot f_{\mathrm{B}}(x_2) \cdot f_{\mathrm{C}}(x_1, x_2, x_3) \cdot f_{\mathrm{D}}(x_3, x_4) \cdot f_{\mathrm{E}}(x_3, x_5). \end{aligned}$$

The Sum-Product Algorithm

The global function is

$$f(x_1, x_2, x_3, x_4, x_5) = f_{\mathrm{A}}(x_1) \cdot f_{\mathrm{B}}(x_2) \cdot f_{\mathrm{C}}(x_1, x_2, x_3) \cdot f_{\mathrm{D}}(x_3, x_4) \cdot f_{\mathrm{E}}(x_3, x_5).$$

The Sum-Product Algorithm

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Very often one wants to calculate marginal functions. E.g.

$$\begin{aligned} \eta_{X_1}(x_1) &= \sum_{x_2, x_3, x_4, x_5} f(x_1, x_2, x_3, x_4, x_5) \\ &= \sum_{x_2, x_3, x_4, x_5} f_{\mathrm{A}}(x_1) \cdot f_{\mathrm{B}}(x_2) \cdot f_{\mathrm{C}}(x_1, x_2, x_3) \cdot f_{\mathrm{D}}(x_3, x_4) \cdot f_{\mathrm{E}}(x_3, x_5). \end{aligned}$$

The Sum-Product Algorithm

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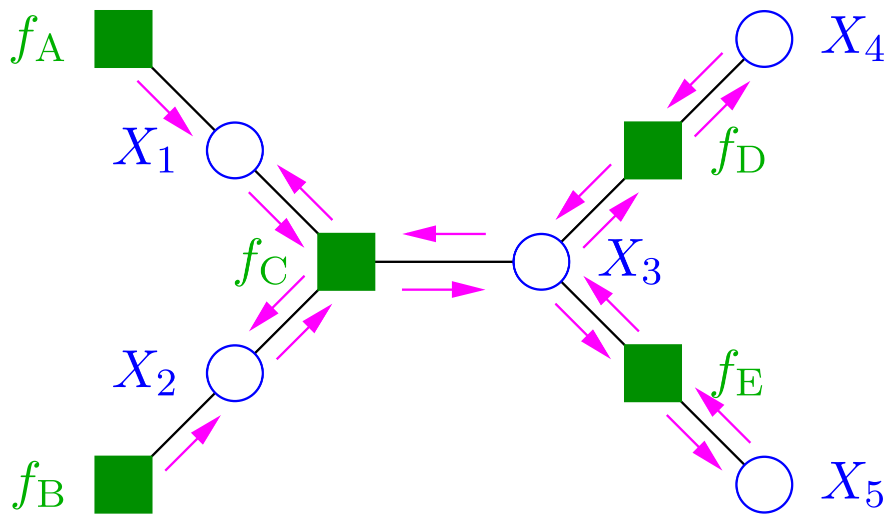
$$\begin{aligned} \eta_{X_3}(x_3) &= \sum_{x_1, x_2, x_4, x_5} f(x_1, x_2, x_3, x_4, x_5) \\ &= \sum_{x_1, x_2, x_4, x_5} f_{\mathrm{A}}(x_1) \cdot f_{\mathrm{B}}(x_2) \cdot f_{\mathrm{C}}(x_1, x_2, x_3) \cdot f_{\mathrm{D}}(x_3, x_4) \cdot f_{\mathrm{E}}(x_3, x_5). \end{aligned}$$

etc.

The Sum-Product Algorithm

The figure shows the messages that are necessary for calculating $\eta_{X_1}(x_1)$, $\eta_{X_2}(x_2)$, $\eta_{X_3}(x_3)$, $\eta_{X_4}(x_4)$, and $\eta_{X_5}(x_5)$.



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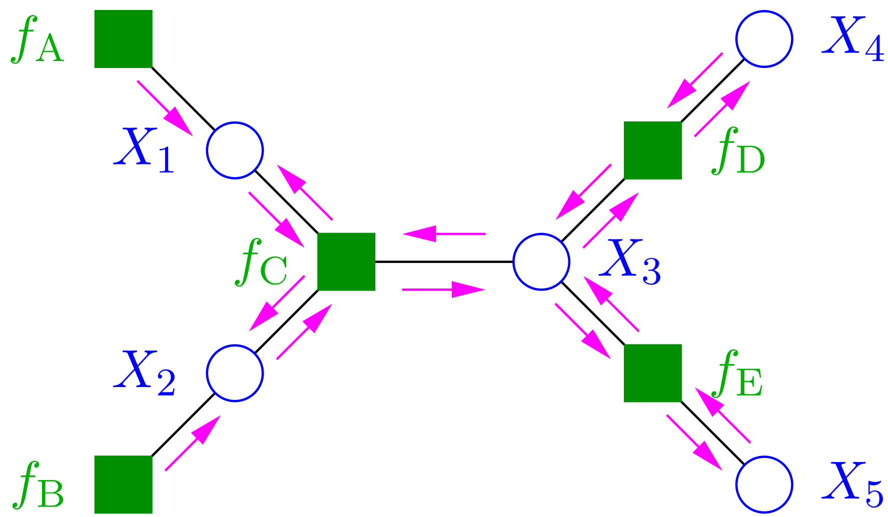

- **Edges:** Messages are sent along edges.

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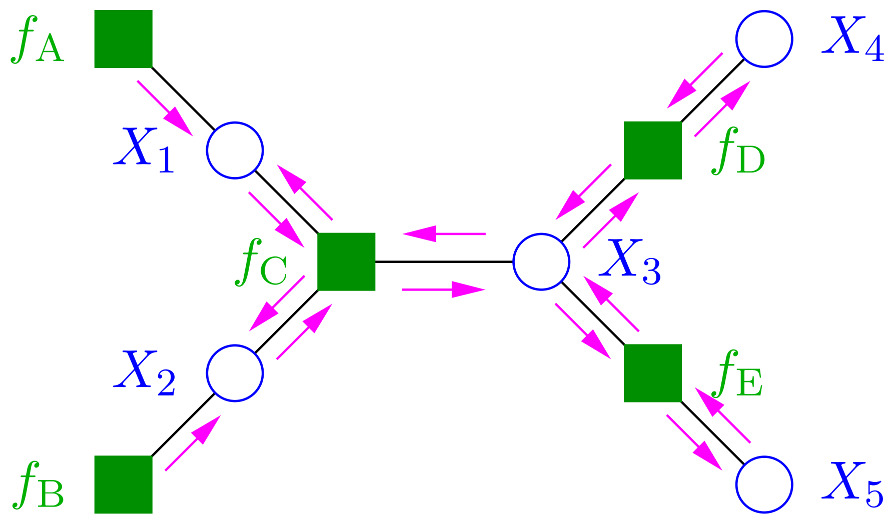

- Edges: Messages are sent along edges.
- Processing: Taking products and doing summations is done at the vertices.

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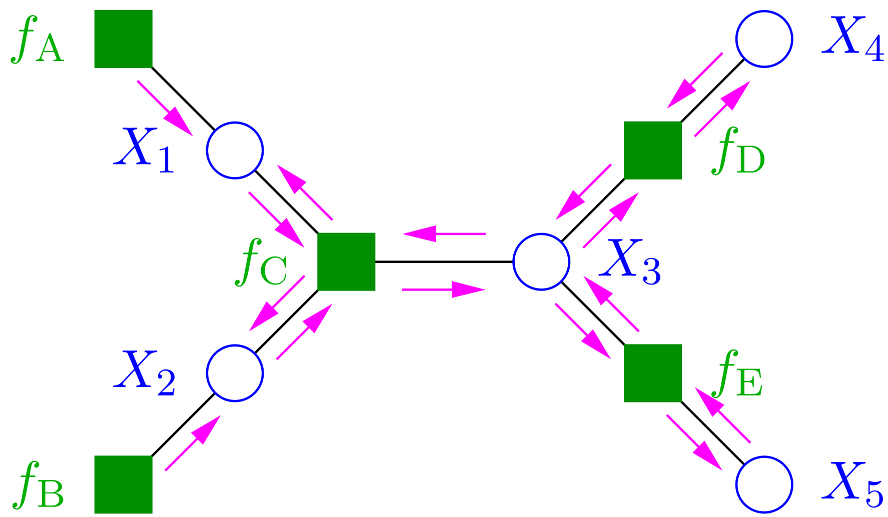
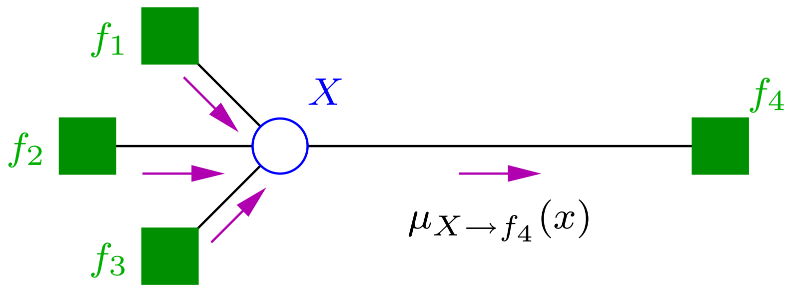


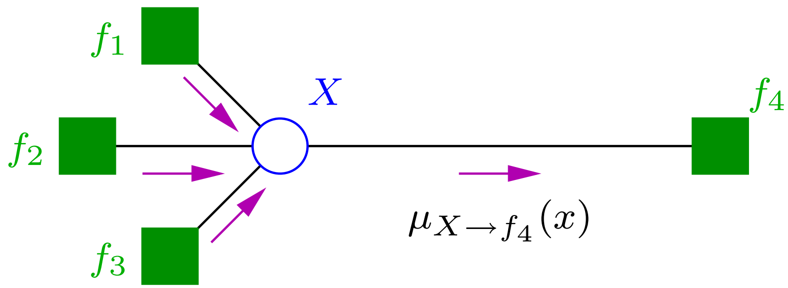
- **Edges:** Messages are sent along edges.
- **Processing:** Taking products and doing summations is done at the vertices.
- **Reuse of messages:** We see that messages can be “reused” in the sense that many partial calculations are the same; so it suffices to perform them only once.

The Sum-Product Algorithm



$$\mu_{X \to f_4}(x) = \mu_{f_1 \to X}(x) \cdot \mu_{f_2 \to X}(x) \cdot \mu_{f_3 \to X}(x)$$

The Sum-Product Algorithm



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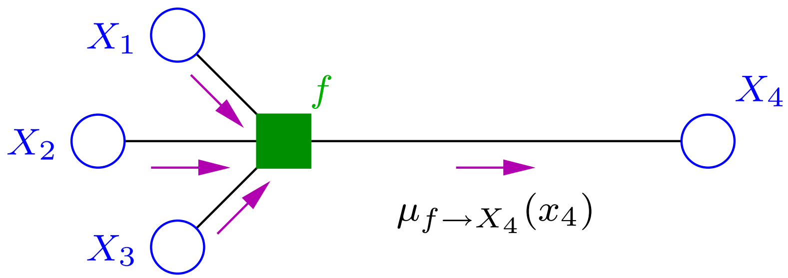
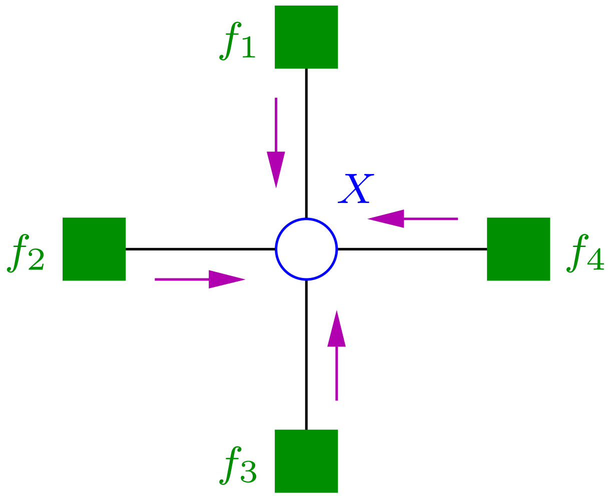


$$\mu_{f \to X_4}(x_4) = \sum_{x_1} \sum_{x_2} \sum_{x_3} f(x_1, x_2, x_3, x_4) \cdot \mu_{X_1 \to f}(x_1) \cdot \mu_{X_2 \to f}(x_2) \cdot \mu_{X_3 \to f}(x_3)$$

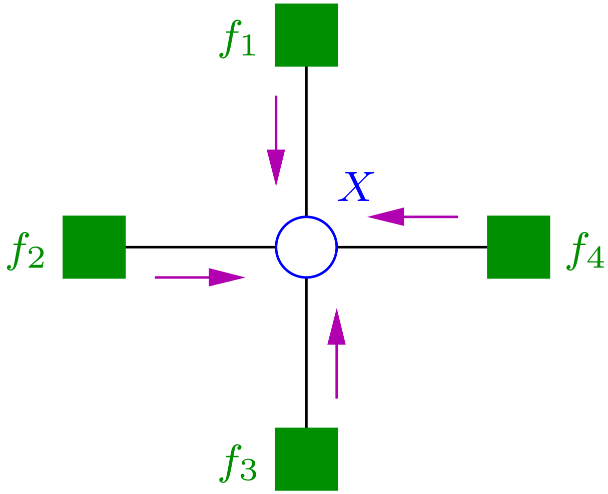
The Sum-Product Algorithm



Computation of marginal at variable node:

$$\eta_X(x) = \mu_{f_1\to X}(x) \cdot \mu_{f_2\to X}(x) \cdot \mu_{f_3\to X}(x) \cdot \mu_{f_4\to X}(x)$$

The Sum-Product Algorithm



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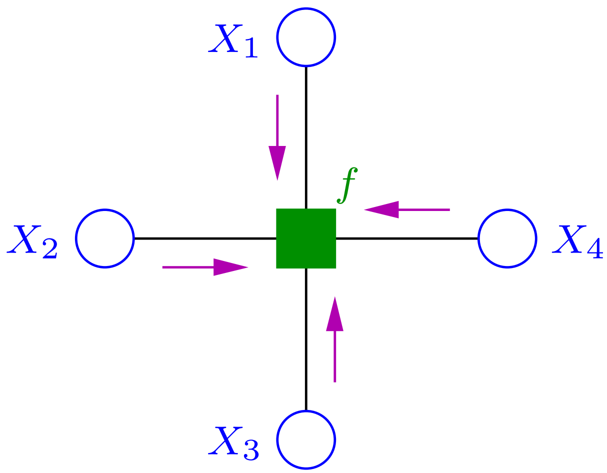

Computation of marginal at function node:

$$\eta_f(x_1, x_2, x_3, x_4) = f(x_1, x_2, x_3, x_4) \cdot \mu_{X_1 \to f}(x_1) \cdot \mu_{X_2 \to f}(x_2) \cdot \mu_{X_3 \to f}(x_3) \cdot \mu_{X_4 \to f}(x_4)$$

The Sum-Product Algorithm

- Factor graph without cycles: in this case it is obvious what messages have to be calculated when.

$\Rightarrow$ Mode of operation 1

The Sum-Product Algorithm

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  $\Rightarrow$ Mode of operation 1

- Factor graph with cycles: one has to decide what update schedule to take.

  $\Rightarrow$ Mode of operation 2

Comments on the Sum-Product Algorithm

- If the factor graph has no cycles then it is obvious what messages have to be calculated when.
- If the factor graphs has cycles one has to decide what update schedule to take.
- Depending on the underlying semi-ring one gets different versions of the summary-product algorithm.
  - For $\langle \mathbb{R}, +, \cdot \rangle$ one gets the sum-product algorithm. (This is the case discussed above.)
  - For $\langle \mathbb{R}^+, \max, \cdot \rangle$ one gets the max-product algorithm.
  - For $\langle \mathbb{R}, \min, + \rangle$ one gets the min-sum algorithm.
  - etc.

Partition function (total sum)

Partition Function

$$Z = \sum_{x_1, x_2, x_3, x_4, x_5} f(x_1, x_2, x_3, x_4, x_5)$$

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Recall:

$$\eta_{X_1}(x_1) = \sum_{x_2, x_3, x_4, x_5} f(x_1, x_2, x_3, x_4, x_5)$$

$$\eta_{X_2}(x_2) = \sum_{x_1, x_3, x_4, x_5} f(x_1, x_2, x_3, x_4, x_5)$$

$$\vdots \qquad \qquad \vdots$$

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$$\vdots \qquad \qquad \vdots$$

Define:

$$Z_{X_1} = \sum_{x_1} \eta_{X_1}(x_1)$$

$$Z_{X_2} = \sum_{x_2} \eta_{X_2}(x_2)$$

$$\vdots \qquad \qquad \vdots$$

Partition Function

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Recall:

$$\eta_{X_1}(x_1) = \sum_{x_2,x_3,x_4,x_5} f(x_1, x_2, x_3, x_4, x_5)$$

$$\eta_{X_2}(x_2) = \sum_{x_1,x_3,x_4,x_5} f(x_1, x_2, x_3, x_4, x_5)$$

$$\vdots \qquad \vdots$$

Define:

$$Z_{X_1} = \sum_{x_1} \eta_{X_1}(x_1) = Z$$

$$Z_{X_2} = \sum_{x_2} \eta_{X_2}(x_2) = Z$$

$$\vdots \qquad \vdots$$

Partition Function

$$Z = \sum_{x_1, x_2, x_3, x_4, x_5} f(x_1, x_2, x_3, x_4, x_5)$$

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Recall:

$$\begin{array}{ccc} \vdots & & \vdots \\ \eta_{f_C}(x_1, x_2, x_3) & = & \sum_{x_4,x_5} f(x_1, x_2, x_3, x_4, x_5) \\ \vdots & & \vdots \end{array}$$

Partition Function

$$Z = \sum_{x_1,x_2,x_3,x_4,x_5} f(x_1, x_2, x_3, x_4, x_5)$$

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$$\vdots \qquad \vdots$$

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$$\vdots \qquad \vdots$$

Define:

$$\vdots \qquad \vdots$$

$$Z_{f_C} = \sum_{x_1,x_2,x_3} \eta_{f_C}(x_1, x_2, x_3)$$

$$\vdots \qquad \vdots$$

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$$\vdots \qquad\qquad \vdots$$

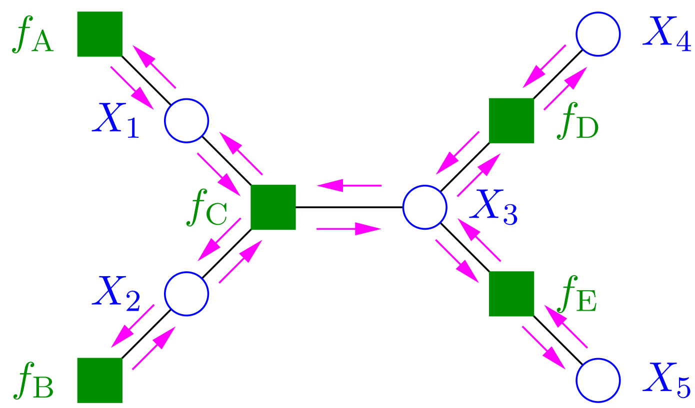
Define:

$$\vdots \qquad\qquad \vdots$$

$$Z_{f_C} = \sum_{x_1,x_2,x_3} \eta_{f_C}(x_1, x_2, x_3) = Z$$

$$\vdots \qquad\qquad \vdots$$

Partition Function



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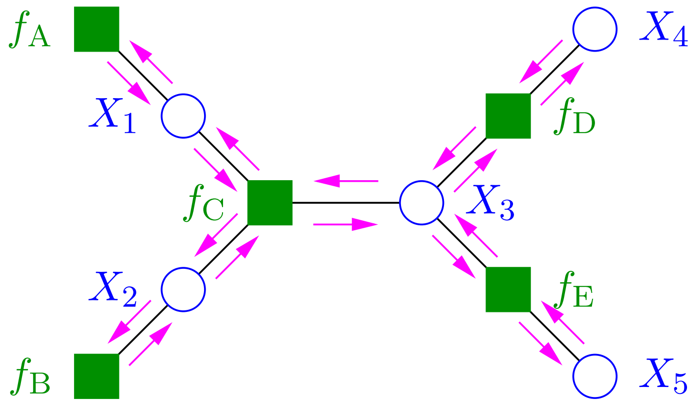

$$Z = Z_{X_1} = Z_{X_2} = Z_{X_3} = Z_{X_4} = Z_{X_5} = Z_{f_A} = Z_{f_B} = Z_{f_C} = Z_{f_D} = Z_{f_E}$$

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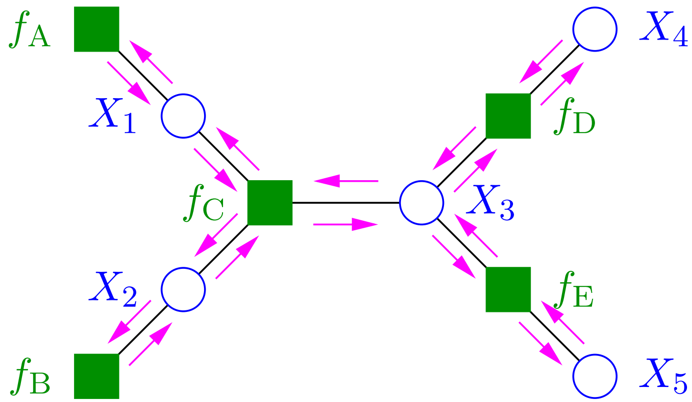

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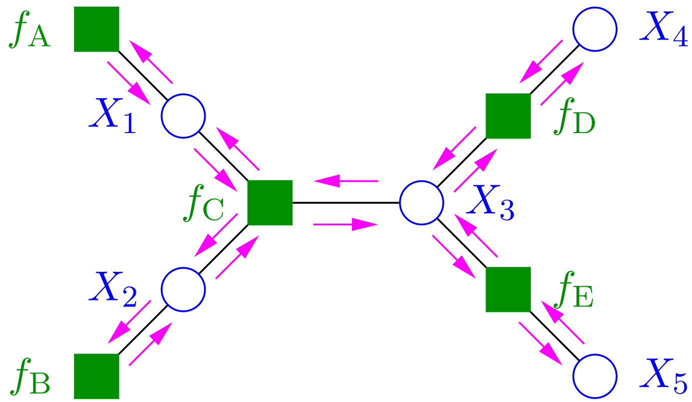
Claim:

$$Z = \frac{Z_{f_{\mathrm{A}}} \cdot Z_{f_{\mathrm{B}}} \cdot Z_{f_{\mathrm{C}}} \cdot Z_{f_{\mathrm{D}}} \cdot Z_{f_{\mathrm{E}}} \cdot Z_{X_1} \cdot Z_{X_2} \cdot Z_{X_3} \cdot Z_{X_4} \cdot Z_{X_5}}{Z_{X_1}^2 \cdot Z_{X_2}^2 \cdot Z_{X_3}^3 \cdot Z_{X_4}^1 \cdot Z_{X_5}^1}$$

(Note: exponents in denominator equal variable node degrees.)

Partition Function



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Claim:

$$Z = \frac{Z^{\#\text{vertices}}}{Z^{\#\text{edges}}} = \frac{Z_{f_\mathrm{A}} \cdot Z_{f_\mathrm{B}} \cdot Z_{f_\mathrm{C}} \cdot Z_{f_\mathrm{D}} \cdot Z_{f_\mathrm{E}} \cdot Z_{X_1} \cdot Z_{X_2} \cdot Z_{X_3} \cdot Z_{X_4} \cdot Z_{X_5}}{Z_{X_1}^2 \cdot Z_{X_2}^2 \cdot Z_{X_3}^3 \cdot Z_{X_4}^1 \cdot Z_{X_5}^1}$$

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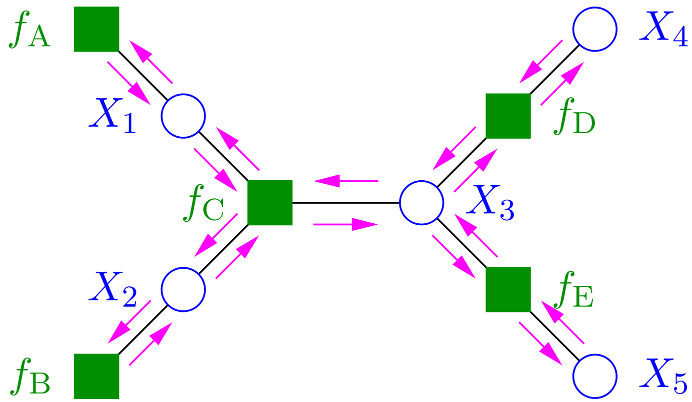

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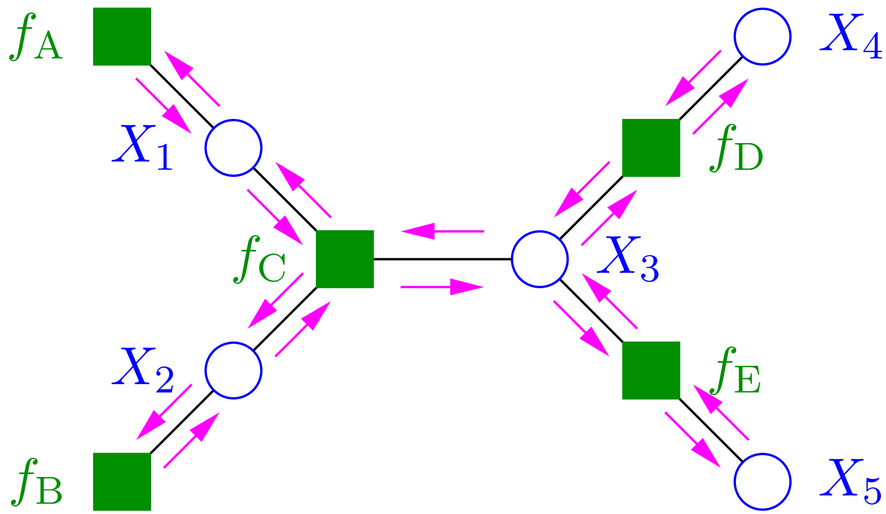
(Here we used the fact that for a graph with one component and no cycles it holds that

$\#$vertices $= \#$edges $+ 1$.)

Partition Function



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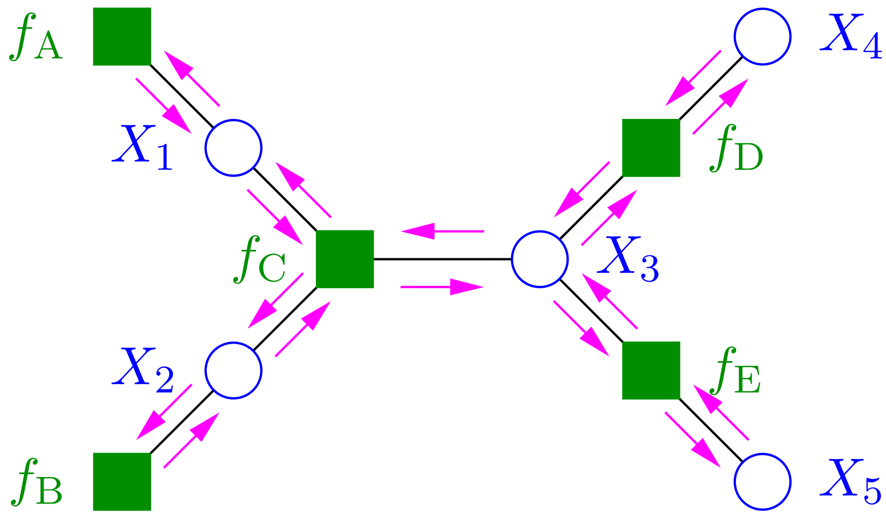

$$Z = \frac{\prod_f Z_f \cdot \prod_X Z_X}{\prod_X Z_X^{\deg(\mathrm{X})}}$$

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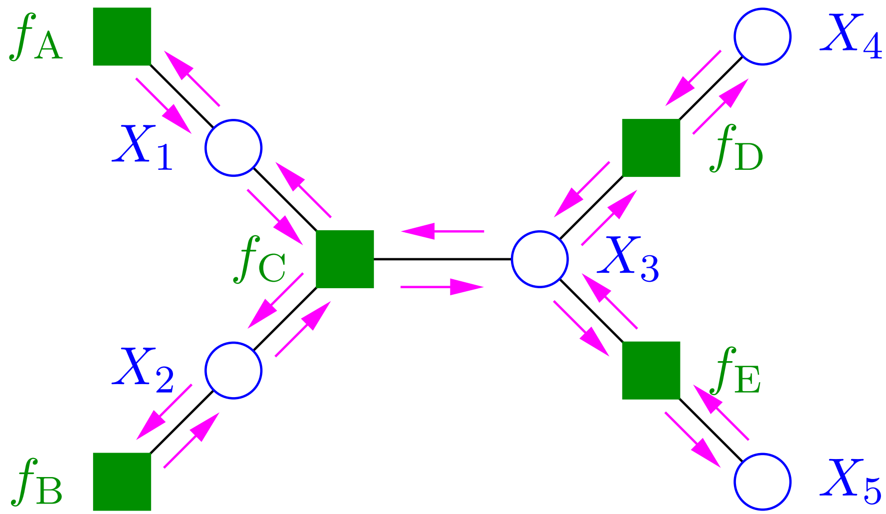

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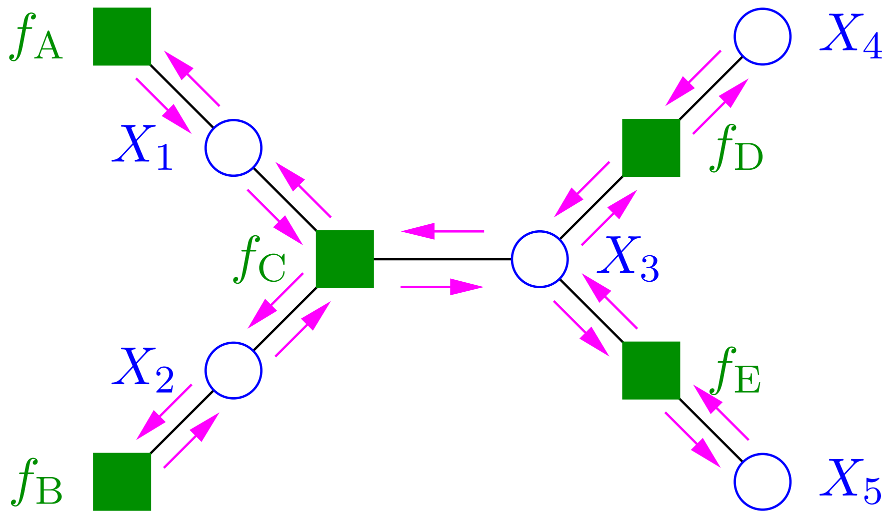
Bethe approximation:

Use the above type of expression also when factor graph has cycles.

Partition Function



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$$\to Z'_{\mathrm{Bethe}}$$

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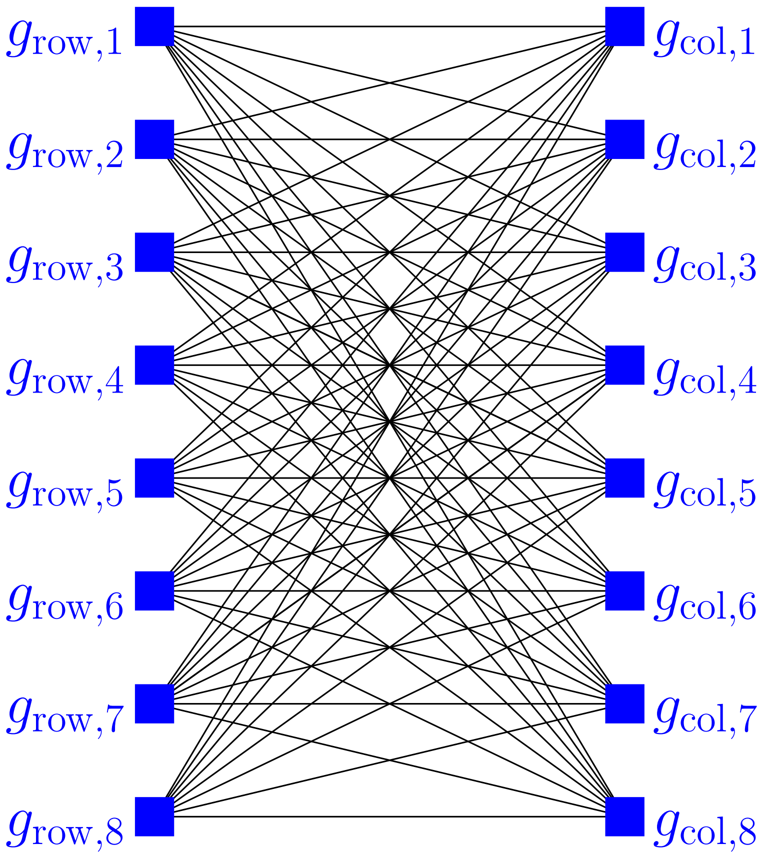
  Therefore, we call Z'_{Bethe} a (local) Bethe partition function only if we are at a fixed point of the SPA.

- Factor graph with cycles: the SPA can have multiple fixed points. We define the Bethe partition function to be

$$Z_{\mathrm{Bethe}} \triangleq \max_{\text{fixed points of SPA}} Z'_{\mathrm{Bethe}}.$$

Graphical Model for Permanent



(function nodes are suitably defined based on $\boldsymbol{\theta}$)

(variable nodes have been omitted)

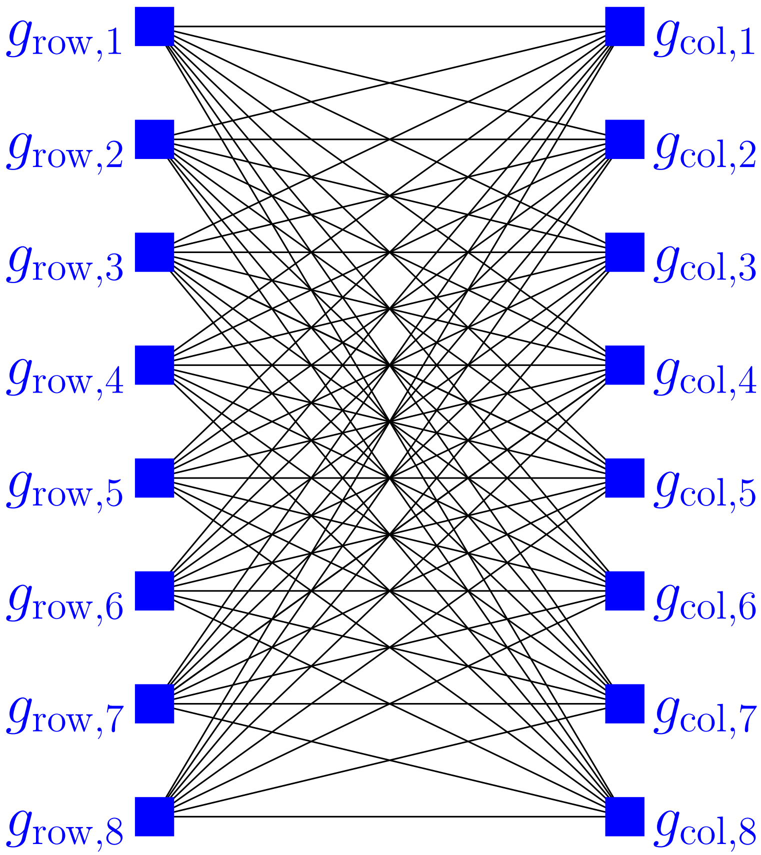
Global function:

$$g(a_{1,1}, \ldots, a_{8,8}) = \prod_j g_{\text{col},j}(a_{1,j}, \ldots, a_{8,j}) \times \prod_i g_{\text{row},i}(a_{i,1}, \ldots, x_{i,8})$$

Permanent:

$$\text{perm}(\boldsymbol{\theta}) = Z = \sum_{a_{1,1},\ldots,a_{8,8}} g(a_{1,1}, \ldots, a_{8,8})$$

Graphical Model for Permanent



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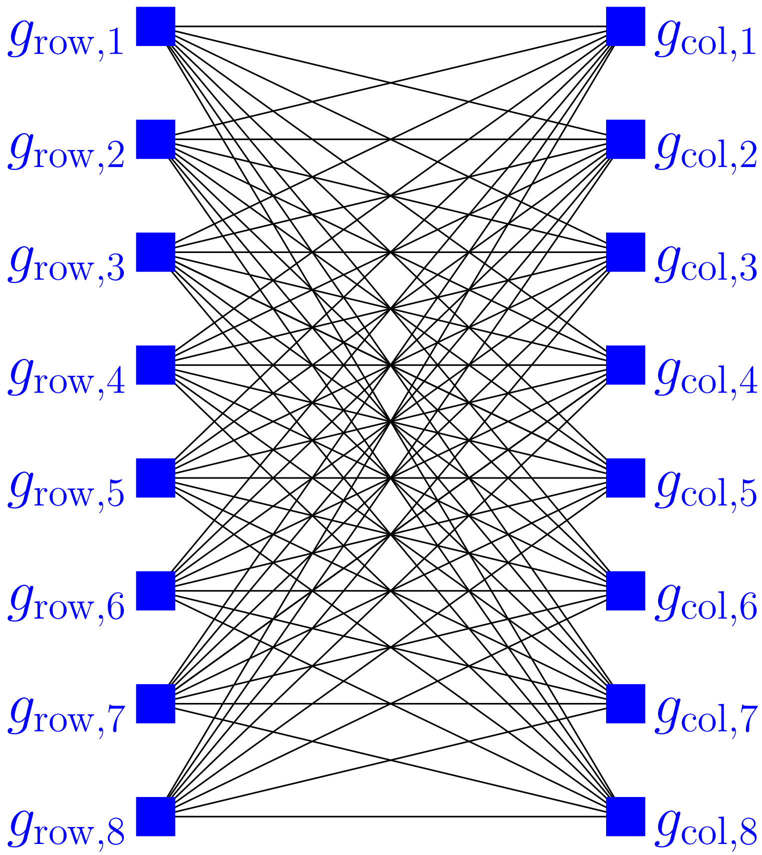

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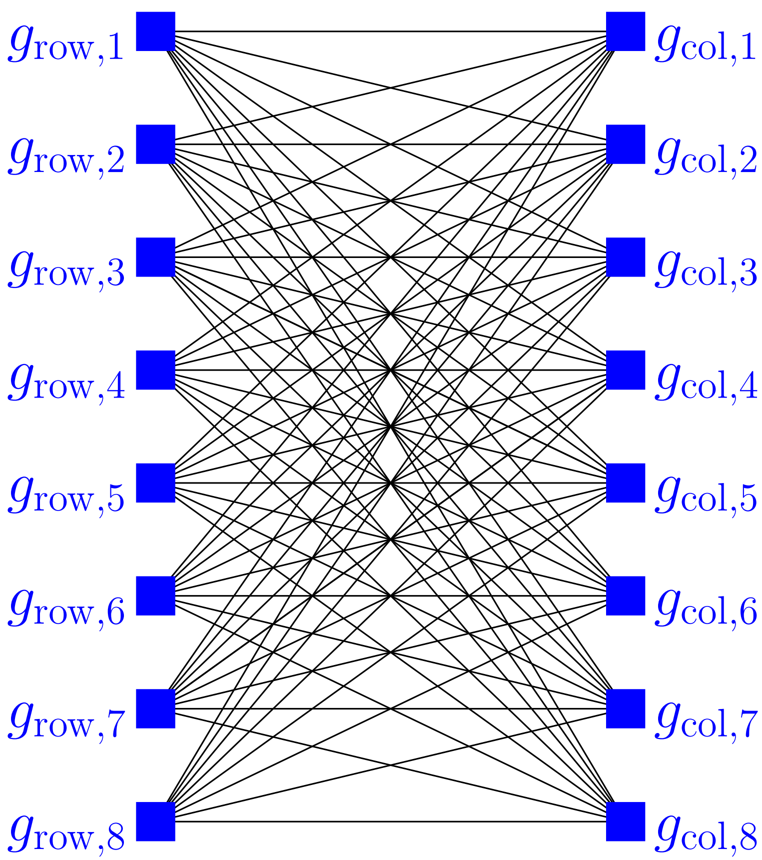
However, the SPA is a locally operating algorithm and so has its limitations in the conclusions that it can reach.

Graphical Model for Permanent



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This locality of the SPA turns out to be well-captured by so-called finite graph covers, especially at fixed points of the SPA.

A combinatorial interpretation of the Bethe permanent

Reminder:
Kronecker Product of two Matrices

- Consider a matrix $\boldsymbol{\theta}$ of size $n \times n$.
- Consider a matrix $\mathbf{B}$ of size $M \times M$.
- The Kronecker product of $\boldsymbol{\theta}$ and $\mathbf{B}$ is defined to be

$$\boldsymbol{\theta} = \begin{pmatrix} \theta_{1,1} & \cdots & \theta_{1,n} \\ \vdots & & \vdots \\ \theta_{n,1} & \cdots & \theta_{n,n} \end{pmatrix} \quad \longrightarrow \quad \boldsymbol{\theta} \otimes \mathbf{B} \triangleq \begin{pmatrix} \theta_{1,1}\mathbf{B} & \cdots & \theta_{1,n}\mathbf{B} \\ \vdots & & \vdots \\ \theta_{n,1}\mathbf{B} & \cdots & \theta_{n,n}\mathbf{B} \end{pmatrix}.$$

- Clearly, $\boldsymbol{\theta} \otimes \mathbf{B}$ has size $(nM) \times (nM)$.

$\mathbf{P}$-lifting of a Matrix

$$\boldsymbol{\theta} = \begin{pmatrix} \theta_{1,1} & \cdots & \theta_{1,n} \\ \vdots & & \vdots \\ \theta_{n,1} & \cdots & \theta_{n,n} \end{pmatrix} \quad \underset{\text{of } \boldsymbol{\theta}}{\xrightarrow{\mathbf{P}\text{-lifting}}} \quad \boldsymbol{\theta}^{\uparrow \mathbf{P}} \triangleq \begin{pmatrix} \theta_{1,1}\mathbf{P}^{(1,1)} & \cdots & \theta_{1,n}\mathbf{P}^{(1,n)} \\ \vdots & & \vdots \\ \theta_{n,1}\mathbf{P}^{(n,1)} & \cdots & \theta_{n,n}\mathbf{P}^{(n,n)} \end{pmatrix}.$$

P-lifting of a Matrix

- Consider the non-negative matrix $\boldsymbol{\theta}$ of size $n \times n$.
- Let $\mathcal{P}_{M \times M}$ be the set of all permutation matrices of size $M \times M$.
- For every positive integer M, we define Ψ_M be the set

$$\Psi_M \triangleq \left\{ \mathbf{P} = \left\{ \mathbf{P}^{(i,j)} \right\}_{(i,j) \in [n]^2} \;\middle|\; \mathbf{P}^{(i,j)} \in \mathcal{P}_{M \times M} \right\}.$$

- For $\mathbf{P} \in \Psi_M$ we define the $\mathbf{P}$-lifting of $\boldsymbol{\theta}$ to be the following $(nM) \times (nM)$ matrix

$$\boldsymbol{\theta} = \begin{pmatrix} \theta_{1,1} & \cdots & \theta_{1,n} \\ \vdots & & \vdots \\ \theta_{n,1} & \cdots & \theta_{n,n} \end{pmatrix} \quad \xrightarrow[\text{of } \boldsymbol{\theta}]{\mathbf{P}\text{-lifting}} \quad \boldsymbol{\theta}^{\uparrow \mathbf{P}} \triangleq \begin{pmatrix} \theta_{1,1}\mathbf{P}^{(1,1)} & \cdots & \theta_{1,n}\mathbf{P}^{(1,n)} \\ \vdots & & \vdots \\ \theta_{n,1}\mathbf{P}^{(n,1)} & \cdots & \theta_{n,n}\mathbf{P}^{(n,n)} \end{pmatrix}.$$

Degree-M Bethe Permanent

Definition: For any positive integer M, we define the degree-M Bethe permanent of $\boldsymbol{\theta}$ to be

$$\mathrm{perm}_{\mathrm{B},M}(\boldsymbol{\theta}) \triangleq \sqrt[M]{\left\langle \mathrm{perm}\left(\boldsymbol{\theta}^{\uparrow \mathbf{P}}\right) \right\rangle_{\mathbf{P} \in \Psi_M}}.$$

Theorem:

$$\mathrm{perm}_{\mathrm{B}}(\boldsymbol{\theta}) = \limsup_{M \to \infty} \mathrm{perm}_{\mathrm{B},M}(\boldsymbol{\theta}).$$

Special Case: Permanent for $n = 2$

We want to obtain some appreciation why the Bethe permanent of $\boldsymbol{\theta}$ is close to the permanent of $\boldsymbol{\theta}$, and where the differences are.

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In particular,

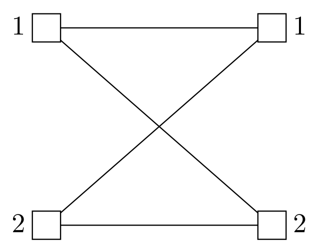
$$\boldsymbol{\theta} = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \qquad \text{with} \qquad \operatorname{perm}(\boldsymbol{\theta}) = 1 \cdot 1 + 1 \cdot 1 = 2.$$

Special Case: Permanent for $n = 2$

Recall that the permanent of a zero/one matrix like

$$\boldsymbol{\theta} = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

equals the number of perfect matchings in the following bipartite graph:



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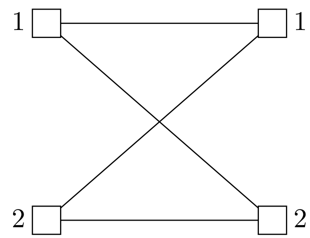
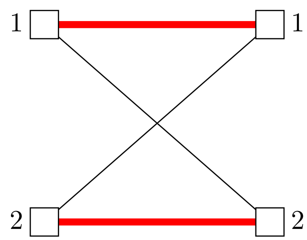
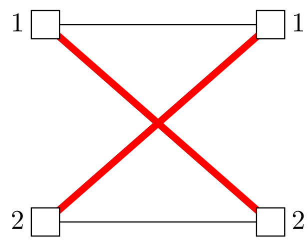


Namely,





Special Case: Degree-M Bethe Permanent for $n = 2$

For this $\boldsymbol{\theta}$, a $\mathbf{P}$-lifting looks like

$$\boldsymbol{\theta}^{\uparrow \mathbf{P}} = \begin{pmatrix} 1 \cdot \mathbf{P}_{1,1} & 1 \cdot \mathbf{P}_{1,2} \\ 1 \cdot \mathbf{P}_{2,1} & 1 \cdot \mathbf{P}_{2,2} \end{pmatrix} = \begin{pmatrix} \mathbf{P}_{1,1} & \mathbf{P}_{1,2} \\ \mathbf{P}_{2,1} & \mathbf{P}_{2,2} \end{pmatrix}.$$

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Applying some row and column permutations, we obtain

$$\operatorname{perm}\left(\boldsymbol{\theta}^{\uparrow\mathbf{P}}\right) = \operatorname{perm}\begin{pmatrix} \mathbf{I} & \mathbf{I} \\ \mathbf{I} & \mathbf{P}_{2,1}^{-1}\mathbf{P}_{2,2}\mathbf{P}_{1,2}^{-1}\mathbf{P}_{1,1} \end{pmatrix}.$$

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Therefore,

$$\mathrm{perm}_{\mathrm{B},M}(\boldsymbol{\theta}) \triangleq \sqrt[M]{\left\langle \mathrm{perm}\begin{pmatrix} \mathbf{I} & \mathbf{I} \\ \mathbf{I} & \mathbf{P}'_{2,2} \end{pmatrix} \right\rangle_{\mathbf{P}'_{2,2} \in \mathcal{P}_{M \times M}}}.$$

Special Case: Degree-2 Bethe Permanent for $n = 2$

For $M = 2$ we have

$$\operatorname{perm}_{\mathrm{B},2}(\boldsymbol{\theta}) \triangleq \sqrt[2]{\left\langle \operatorname{perm}\begin{pmatrix} \mathbf{I} & \mathbf{I} \\ \mathbf{I} & \mathbf{P}'_{2,2} \end{pmatrix} \right\rangle_{\mathbf{P}'_{2,2} \in \mathcal{P}_{2\times 2}}}$$

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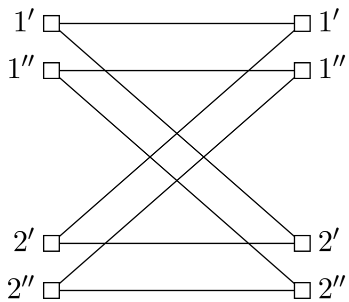
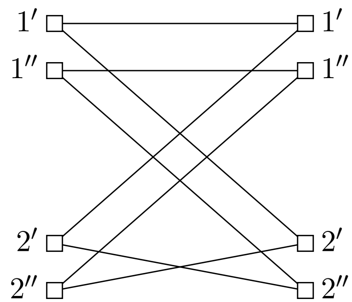
corresponds to computing the average number of perfect matchings in the following 2-covers (and taking the 2nd root):



4



2

Special Case: Degree-2 Bethe Permanent for $n = 2$

For $M = 2$ we have

$$\mathrm{perm}_{\mathrm{B},2}(\boldsymbol{\theta}) = \sqrt[2]{\frac{1}{2!} \cdot (4 + 2)}$$

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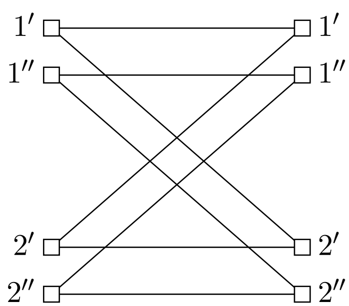

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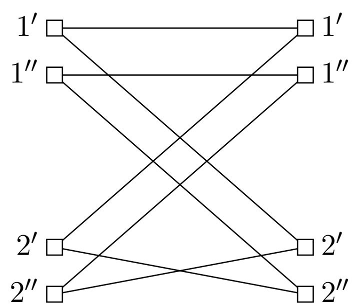

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$$= \sqrt[3]{\frac{1}{2!} \cdot 6} = \sqrt[2]{3} \approx 1.732$$

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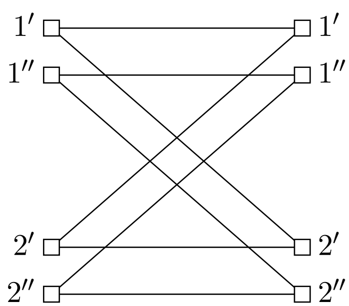

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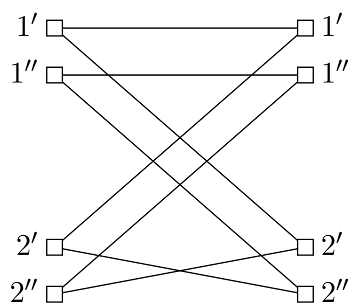

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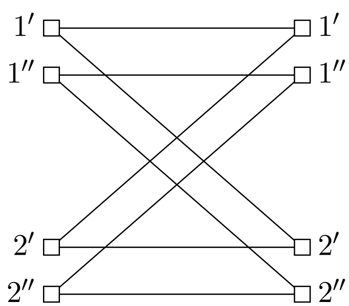

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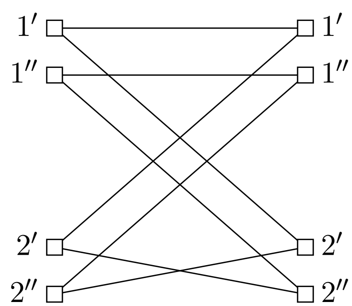
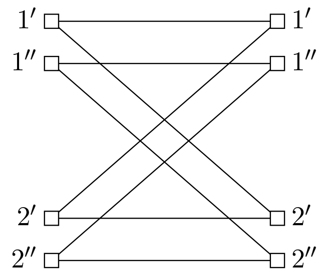


2

Special Case:
Degree-2 Bethe Permanent for $n = 2$

Let us have a closer look at the perfect matchings in the graph



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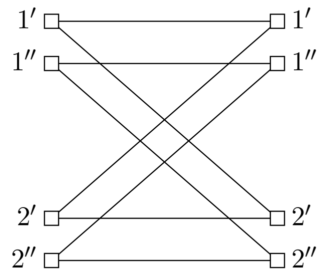
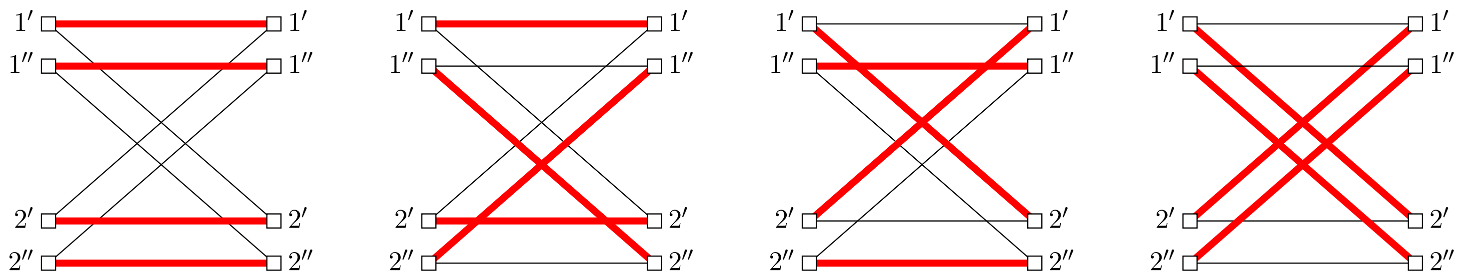


For this graph, the perfect matchings are



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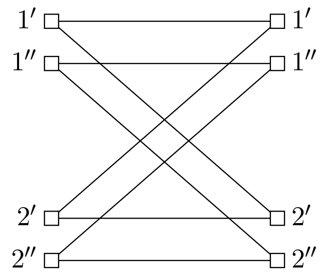

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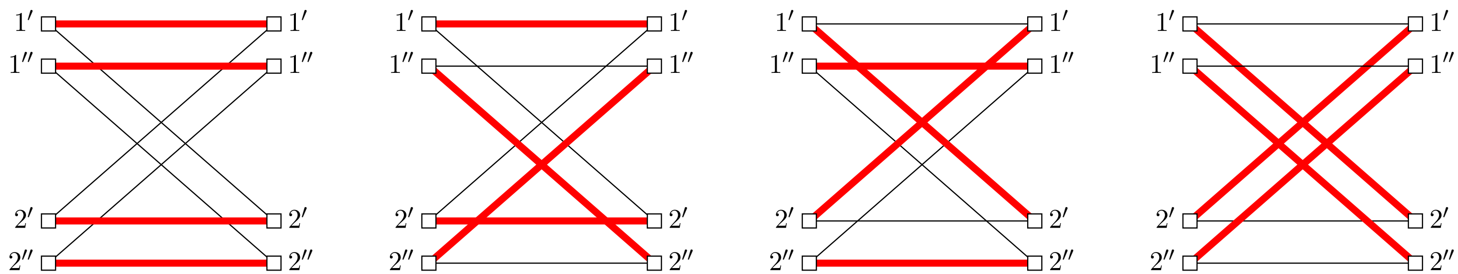

*Because this double cover consists of two **independent copies** of the base graph, the number of perfect matchings is $2^2 = 4$.*

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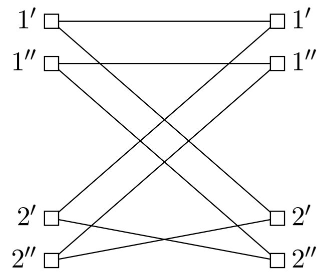

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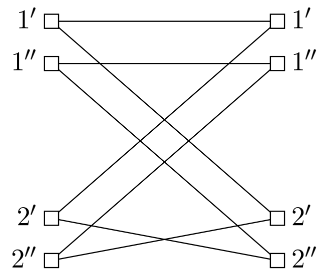

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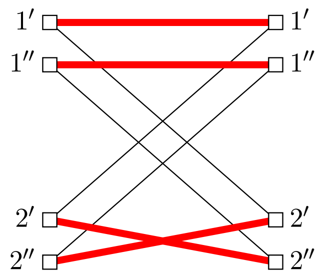

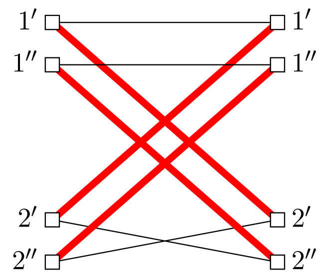

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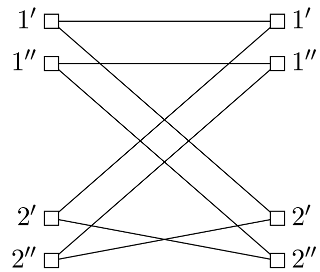

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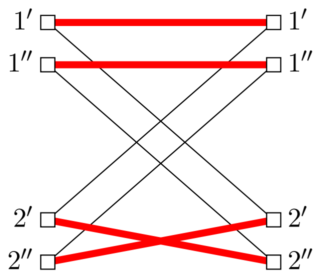
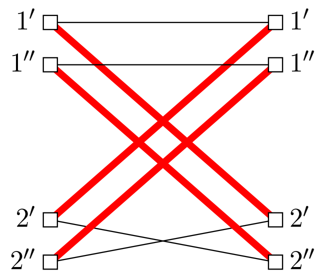




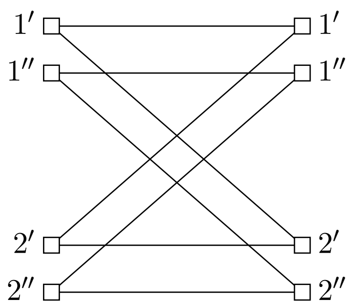
The ***coupling of the cycles*** *causes this graph to have fewer than 2^2 perfect matchings!*

Special Case: Degree-2 Bethe Permanent for $n = 2$

On the other hand, for $M = 2$ we have

$$\begin{aligned} \mathrm{perm}_{\mathrm{B},2}(\boldsymbol{\theta}) &= \sqrt[2]{\frac{1}{2!} \cdot (4+2)} \\ &= \sqrt[3]{\frac{1}{2!} \cdot 6} = \sqrt[2]{3} \approx 1.732 \; < \; \sqrt[2]{4} = 2 = \mathrm{perm}(\boldsymbol{\theta}) \end{aligned}$$

corresponds to computing the average number of perfect matchings in the following 2-covers (and taking the 2nd root):



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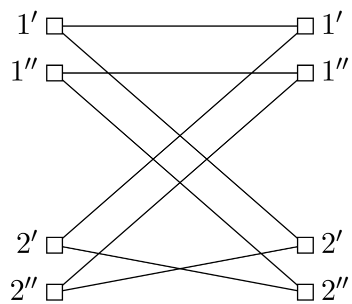


2

Special Case: Degree-M Bethe Permanent for $n = 2$

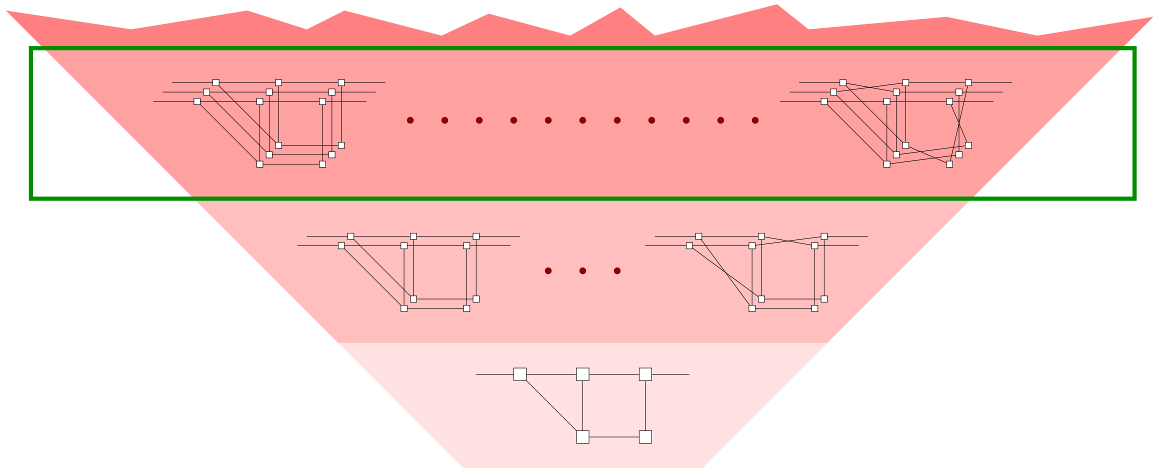
For general M we obtain

$$\mathrm{perm}_{\mathrm{B},M}(\boldsymbol{\theta}) = \sqrt[M]{\zeta_{S_M}} = \sqrt[M]{M+1}.$$

(ζ_{S_M}: cycle index of the symmetric group over M elements.)

A combinatorial interpretation of the Bethe partition function

A Combinatorial Interpretation of the Bethe Partition Function



Definition:

- Let N be a factor graph.
- Let $M \in \mathbb{Z}_{>0}$.

We define the degree-M Bethe partition function to be

$$Z_{\mathrm{B},M}(\mathsf{N}) \triangleq \sqrt[M]{\left\langle Z(\widetilde{\mathsf{N}}) \right\rangle_{\widetilde{\mathsf{N}} \in \widetilde{\mathcal{N}}_M}} .$$

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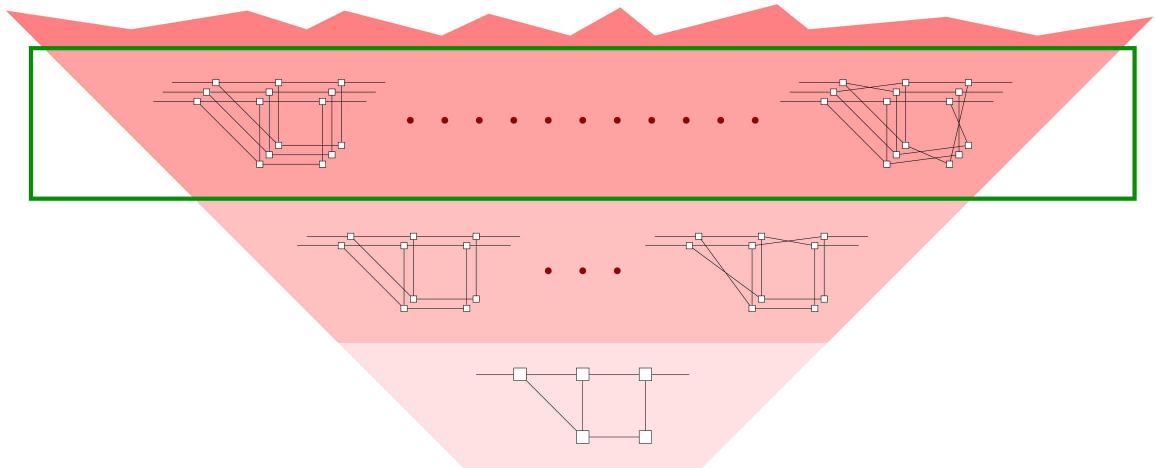

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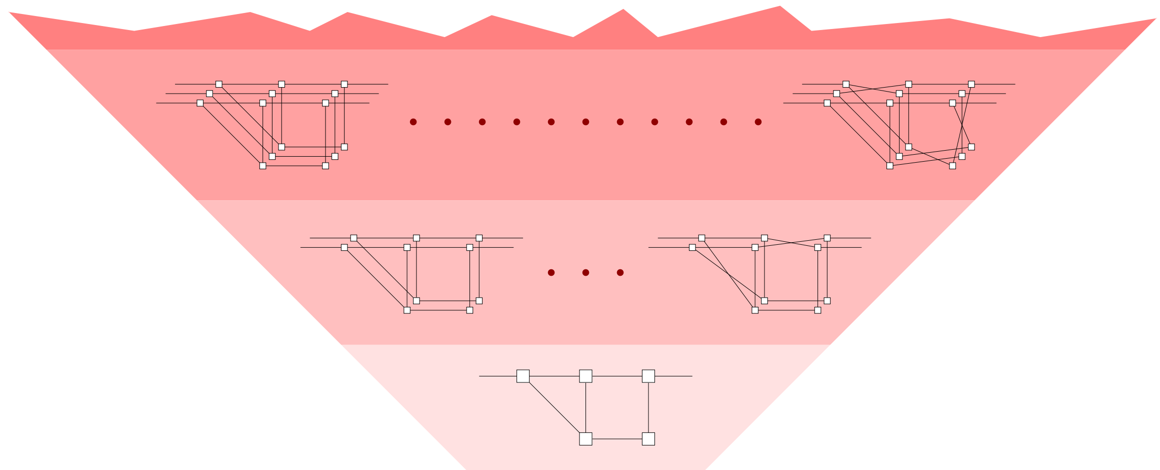
Note that the RHS of the above expression is based on the partition function, and not on the Bethe partition function.

Degree-M Bethe Partition Function

$Z_{\mathrm{B},M}(\mathsf{N})$



Degree-M Bethe Partition Function

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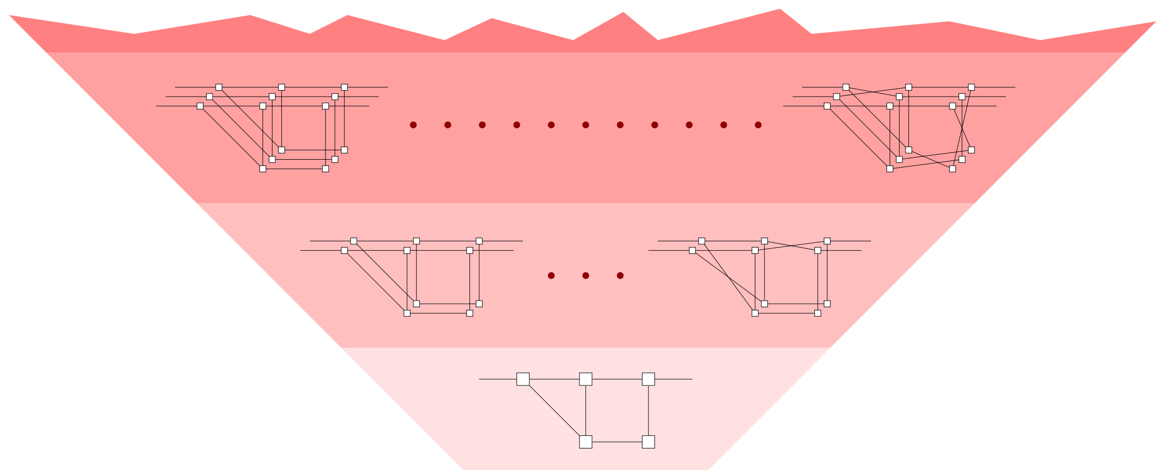

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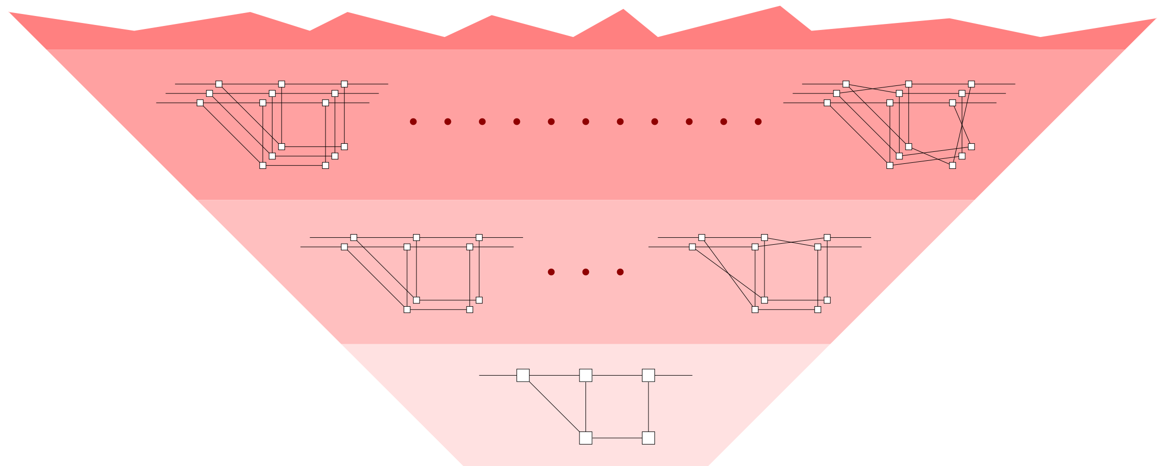

Degree-M Bethe Partition Function

$$Z_{\mathrm{B},M}(\mathsf{N})\Big|_{M\to\infty} = Z_{\mathrm{Bethe}}(\mathsf{N})$$ **(Theorem)**

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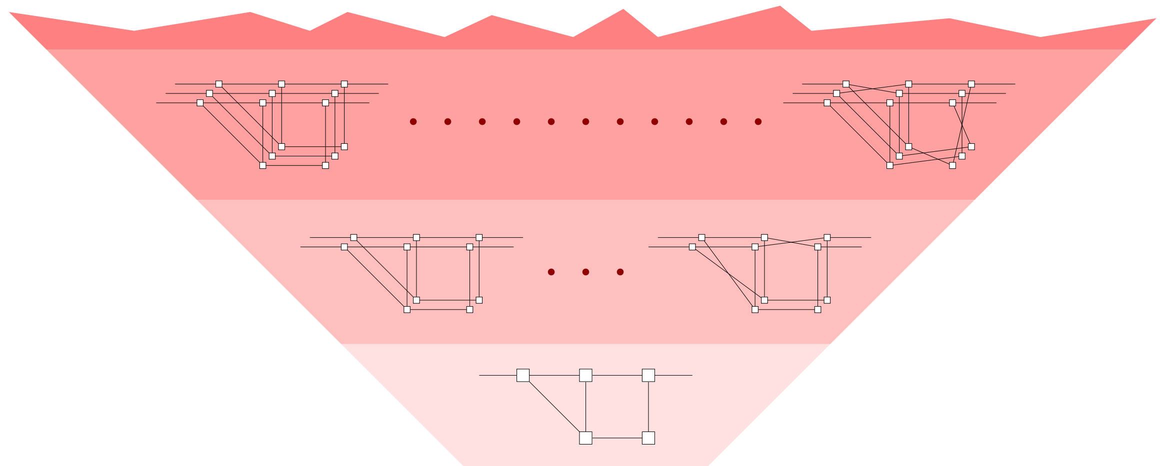

The Gibbs free energy function

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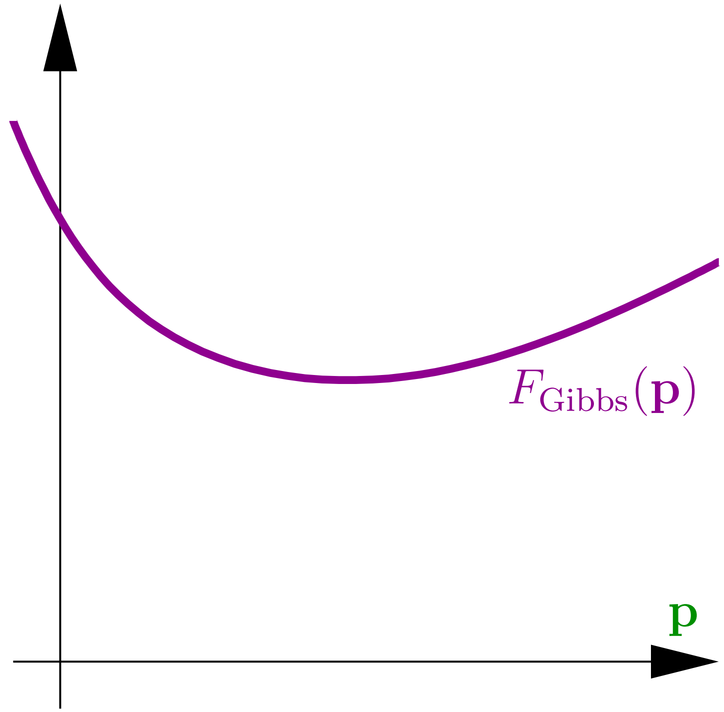
$$F_{\text{Gibbs}}(\mathbf{p}) \triangleq -\sum_{\mathbf{a}} p_{\mathbf{a}} \cdot \log\big(g(\mathbf{a})\big) + \sum_{\mathbf{a}} p_{\mathbf{a}} \cdot \log(p_{\mathbf{a}}).$$



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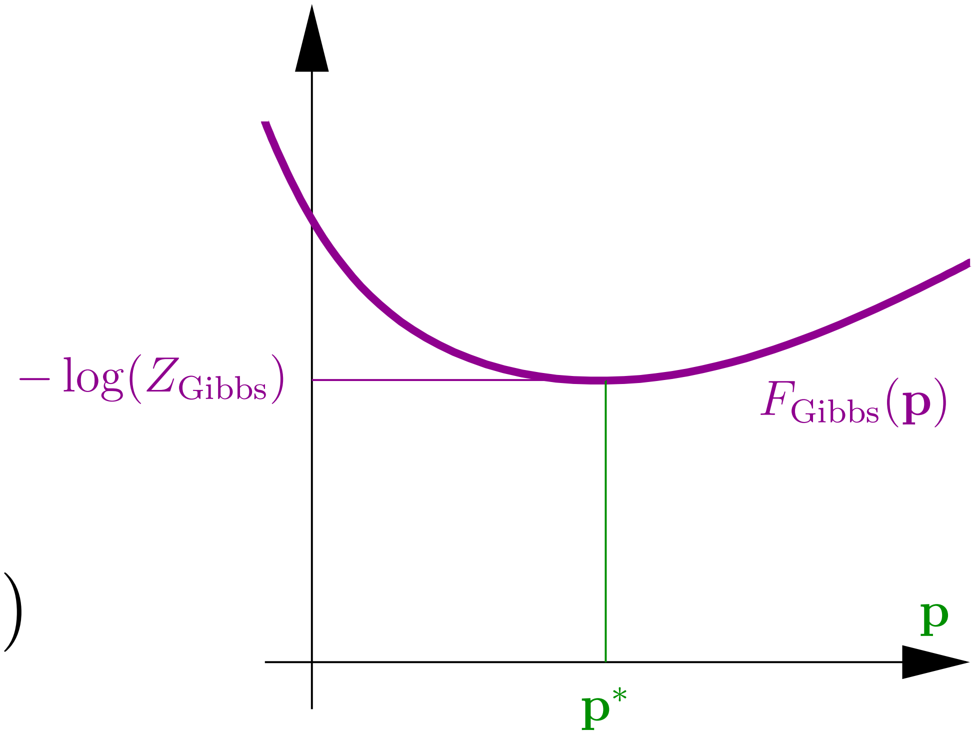

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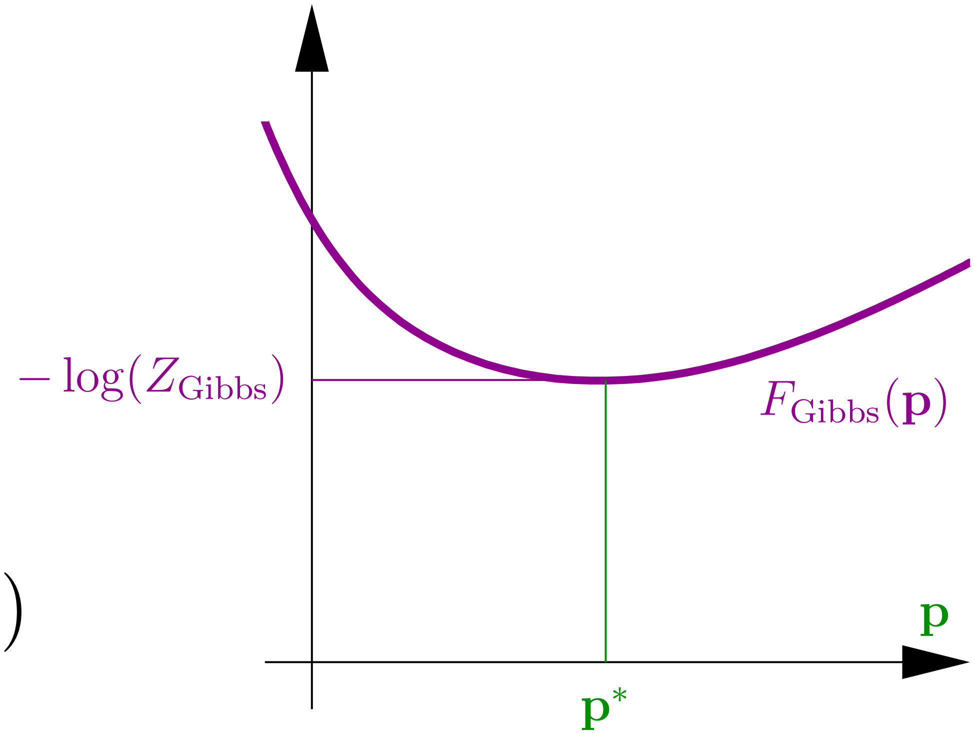

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is defined such that its minimal value is related to the partition function:

$$Z = \exp\left(-\min_{\mathbf{p}} \; F_{\text{Gibbs}}(\mathbf{p})\right).$$

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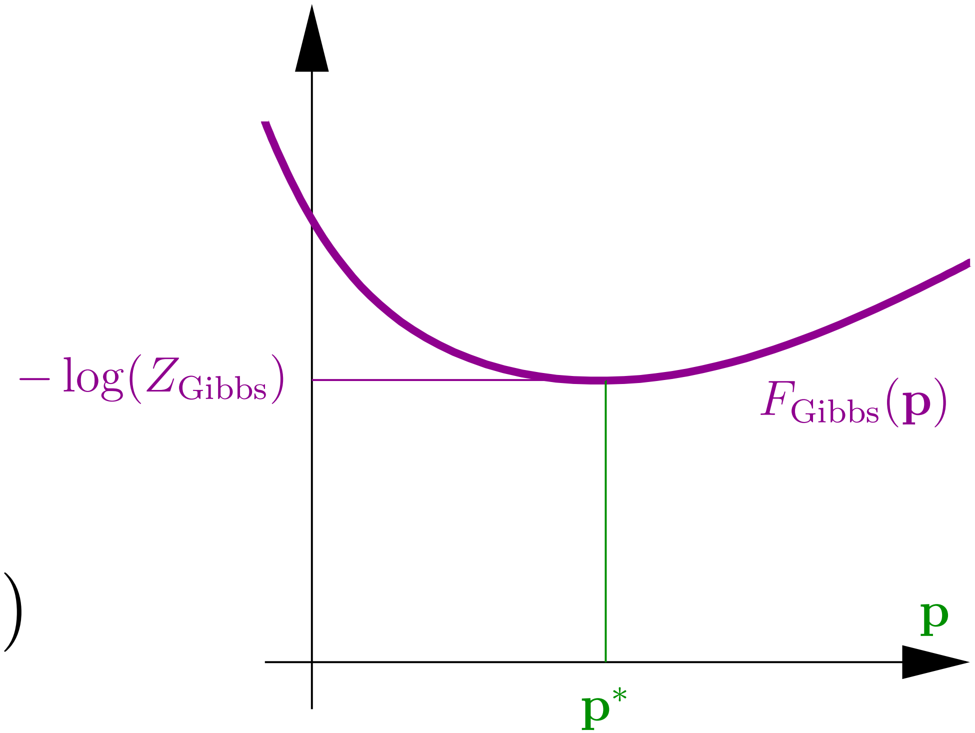

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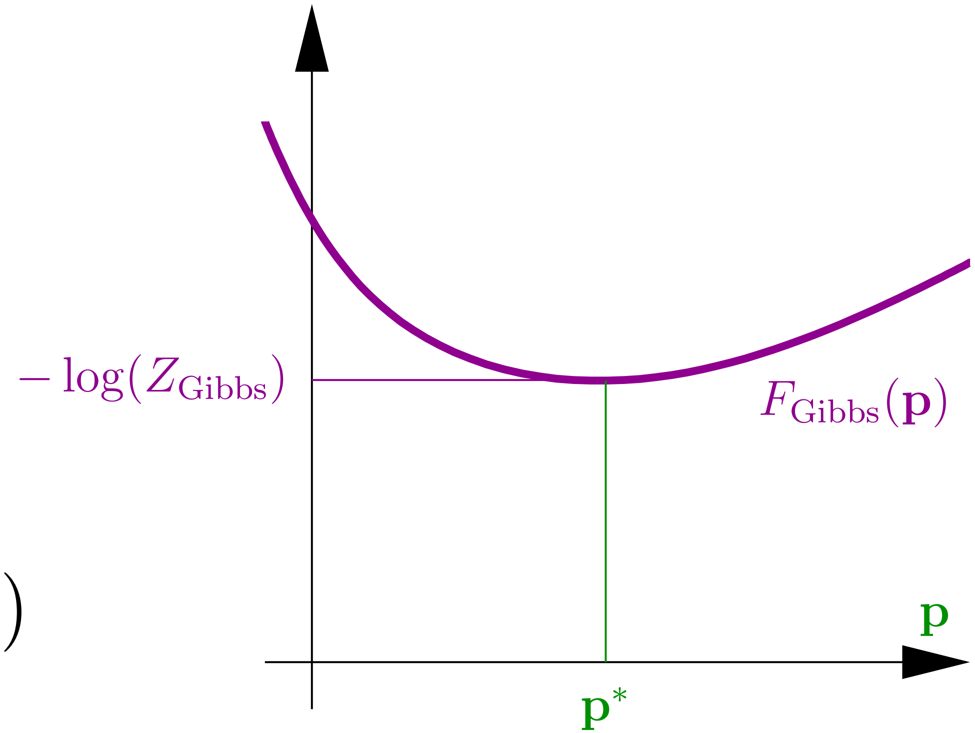

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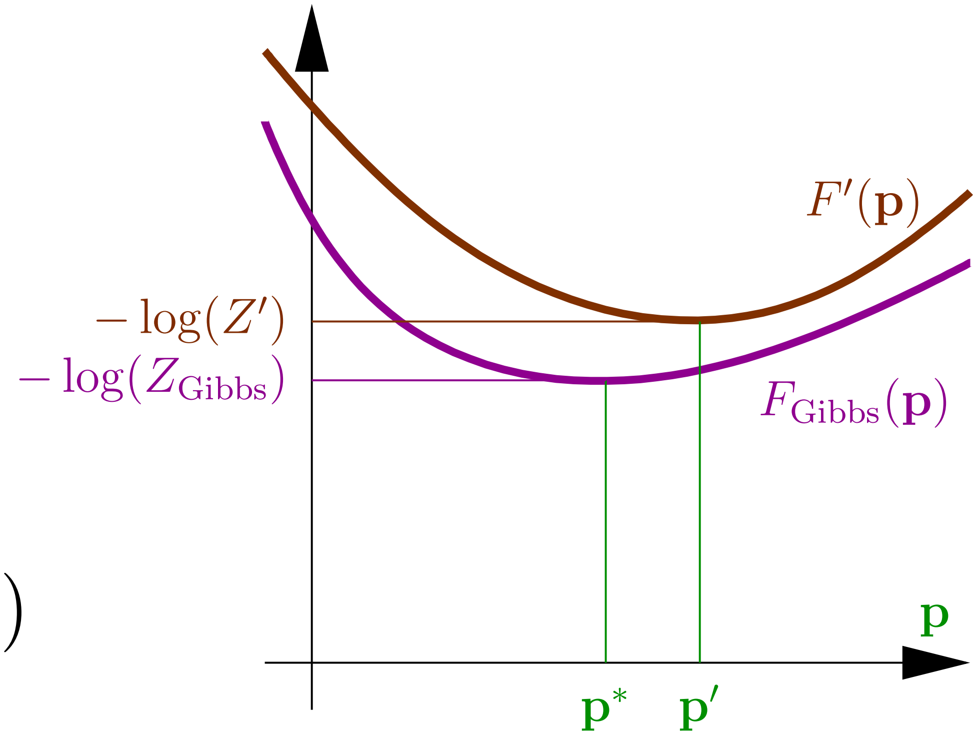
Nice, but it does not yield any computational savings by itself.

Gibbs Free Energy Function



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But it suggests other optimization schemes.

The Bethe approximation

Bethe Approximation

The Bethe approximation to the Gibbs free energy function yields such an alternative optimization scheme.

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This approximation is interesting because of the following theorem:

Theorem (Yedidia/Freeman/Weiss, 2000):
Fixed points of the sum-product algorithm (SPA) correspond to stationary points of the Bethe free energy function.

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Definition: We define the Bethe permanent of $\boldsymbol{\theta}$ to be

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- It is unclear if the sum-product algorithm converges (even to a local minimum of the Bethe free energy).

Bethe Approximation

Luckily, in the case of the permanent approximation problem, the above-mentioned normal factor graph $\mathsf{N}(\boldsymbol{\theta})$ is such that the Bethe free energy function is very well behaved. In particular, one can show that:

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- The sum-product algorithm converges to the minimum of the Bethe free energy. *(More details later.)*

Relationship between Permanent and Bethe Permanent

Theorem (Gurvits, 2011) **Conjecture (Gurvits, 2011)**

$$\mathrm{perm}_{\mathrm{B}}(\boldsymbol{\theta}) \quad \overset{\downarrow}{\leq} \quad \mathrm{perm}(\boldsymbol{\theta}) \quad \overset{\downarrow}{\leq} \quad \sqrt{2}^{\,n} \cdot \mathrm{perm}_{\mathrm{B}}(\boldsymbol{\theta})$$

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This can be rewritten as follows:

Theorem **Conjecture**

$$\frac{1}{n}\log \mathrm{perm}_{\mathrm{B}}(\boldsymbol{\theta}) \overset{\downarrow}{\leq} \frac{1}{n}\log \mathrm{perm}(\boldsymbol{\theta}) \overset{\downarrow}{\leq} \frac{1}{n}\log \mathrm{perm}_{\mathrm{B}}(\boldsymbol{\theta}) + \log(\sqrt{2})$$

Relationship between Permanent and Bethe Permanent

Problem: find large classes of random matrices such that w.h.p.

Theorem (Gurvits, 2011)

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Sum-Product Algorithm Convergence

Theorem: Modulo some minor technical conditions on the initial messages, the sum-product algorithm converges to the (global) minimum of the Bethe free energy function [V., 2010, 2013].

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Comment: the first part of the proof of the above theorem is very similar to the SPA convergence proof in

Bayati and Nair, "*A rigorous proof of the cavity method for counting matchings*," Allerton 2006.

Note that they consider matchings, not perfect matchings. (Although the perfect matching case can be seen as a limiting case of the matching setup, the convergence proof of the SPA is incomplete for that case.)

Other Topics

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Replacing the permanent by the Bethe permanent in various setups:

- Pattern maximum likelihood distribution estimate
- Analysis of pseudo-codewords of LDPC codes
- Kernels in machine learning

Bethe approximation of constraint coding problems:

- Number of two-dimensional weight-constraint arrays

Conclusions

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  Note: One can also give a combinatorial interpretation of the Kikuchi partition function.

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- Inspired by the approaches mentioned in this talk, Mori recently showed that many replica method computations can be simplified and made quite a bit more intuitive.

- With the help of the Bethe permanent, Gurvits recently proved Friedland's "Asymptotic Lower Matching Conjecture" for the monomer-dimer entropy.

- With the help of our reformulation of the Bethe partition function, Ruozzi proves a conjecture by Sudderth, Wainwright, and Willsky that the partition function of attractive graphical models (more precisely, log-supermodular graphical models) is lower bounded by the Bethe partition function.

References (Part 1/2)

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Thank you!