Faster Simulated Annealing Algorithms for Combinatorial Counting

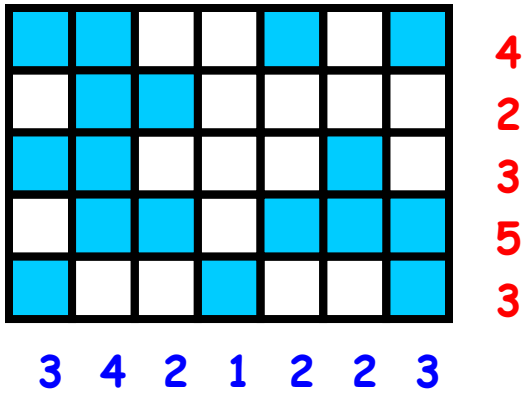
Ivona Bezáková

Rochester Institute of Technology

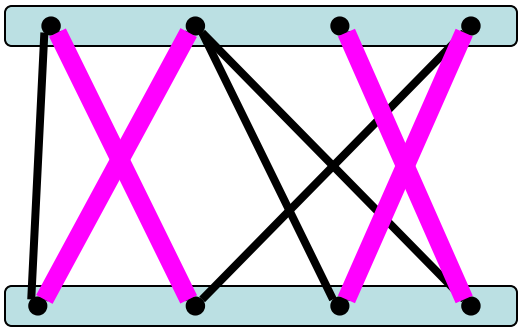
September 22, 2006

Problems

Binary
contingency tables

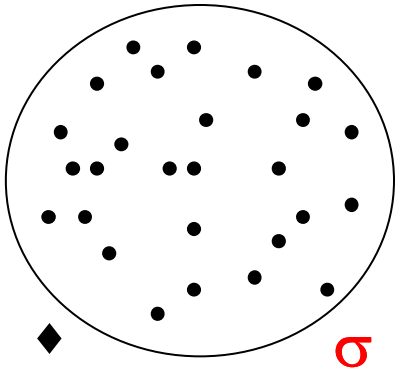


Permanent



Heuristics

Importance sampling



Simulated annealing

Problems

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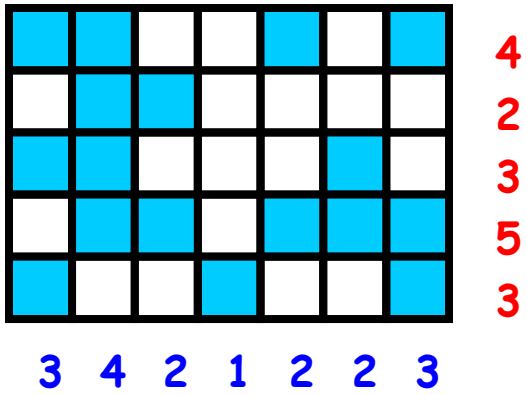

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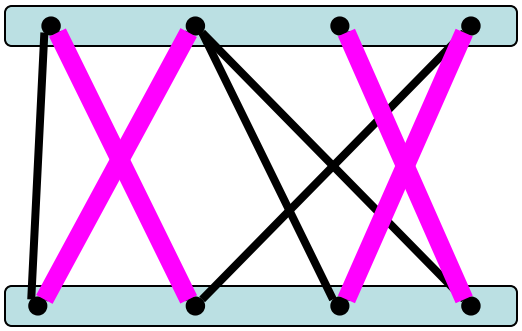

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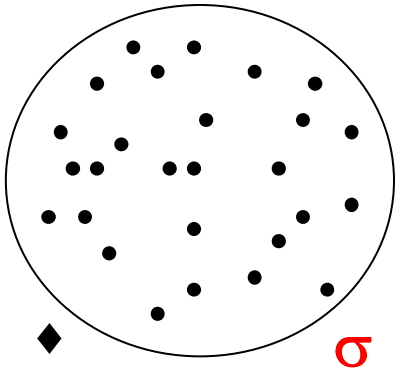
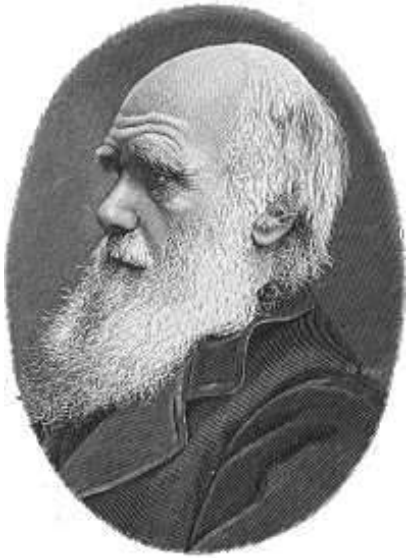
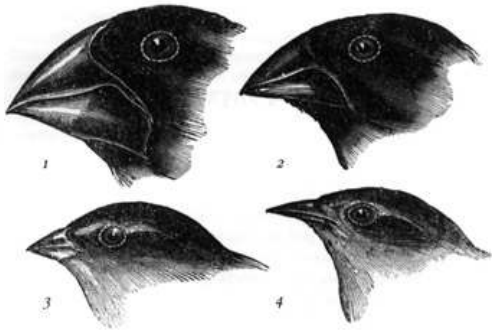


Simulated annealing

Darwin's Finches





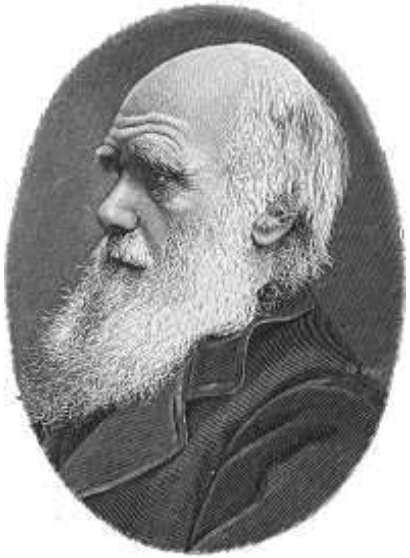
The Voyage of the Beagle

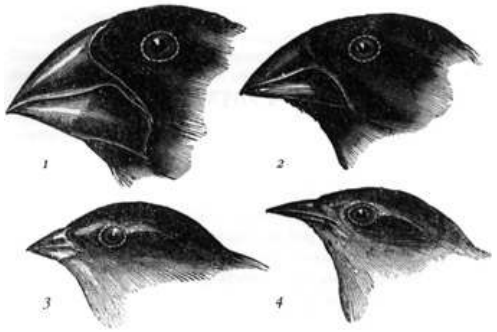
Galápagos archipelago (1835)

Darwin's Finches

Distribution of Darwin's Finches on Visitor Islands

	Santa Cruz	Plaza	Santa Fe	San Cristobal	Espanola	Floreana	Isabela	Fernandina	Santiago	Rabida
Small Ground Finch	●	●	●	●	●	●	●	●	●	●
Medium Ground Finch	●	●	●	●		●	●	●	●	●
Large Ground Finch	●						●	●	●	●
Cactus Ground Finch	●	●	●	●		●	●		●	●
Large Cactus Ground Finch					●					
Sharp-beaked Ground Finch								●	●	
Vegetarian Finch	●			●		●	●	●	●	●
Small Tree Finch	●		●	●		●	●	●	●	●
Medium Tree Finch						●				
Large Tree Finch	●					●	●	●	●	●
Woodpecker Finch	●			●			●		●	
Mangrove Finch							●	●		
Warbler Finch	●		●	●	●	●	●	●	●	●





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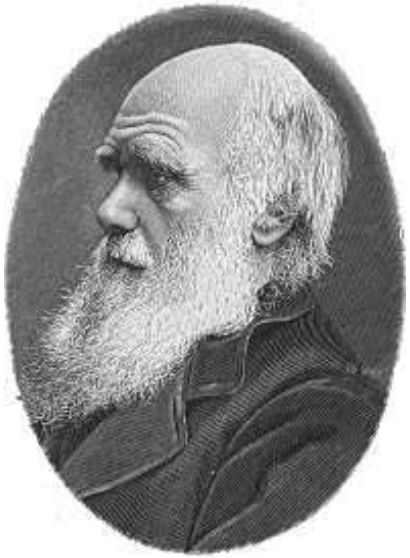

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Vegetarian Finch	●			●		●	●	●	●	●
Small Tree Finch	●		●	●		●	●	●	●	●
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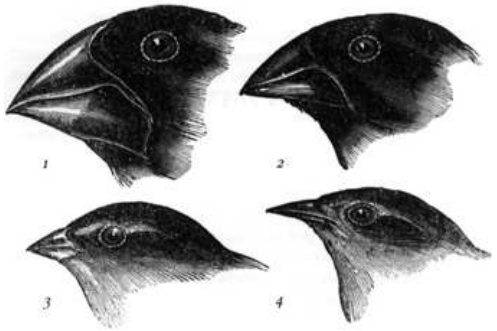
Woodpecker Finch	●			●			●		●	
Mangrove Finch							●	●		
Warbler Finch	●		●	●	●	●	●	●	●	●

8

10



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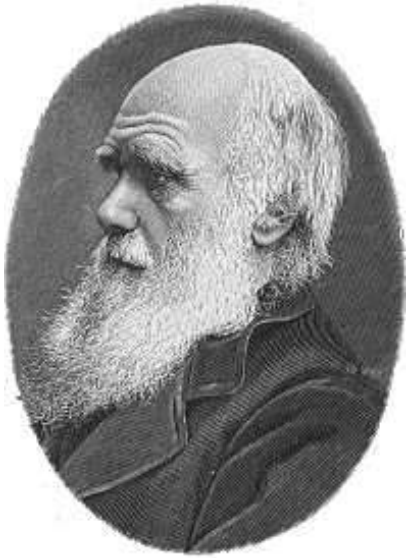
Medium Ground Finch	●	●	●	●		●	●	●	●	●	9
Large Ground Finch	●						●	●	●	●	6
Cactus Ground Finch	●	●	●	●		●	●		●	●	8
Large Cactus Ground Finch					●						2
Sharp-beaked Ground Finch								●	●		3
Vegetarian Finch	●			●		●	●	●	●	●	7
Small Tree Finch	●		●	●		●	●	●	●	●	8
Medium Tree Finch						●					1
Large Tree Finch	●					●	●	●	●	●	6
Woodpecker Finch	●			●			●		●		4
Mangrove Finch							●	●			2
Warbler Finch	●		●	●	●	●	●	●	●	●	10
	9	3	5	7	3	8	10	9	10	8	



chance

OR

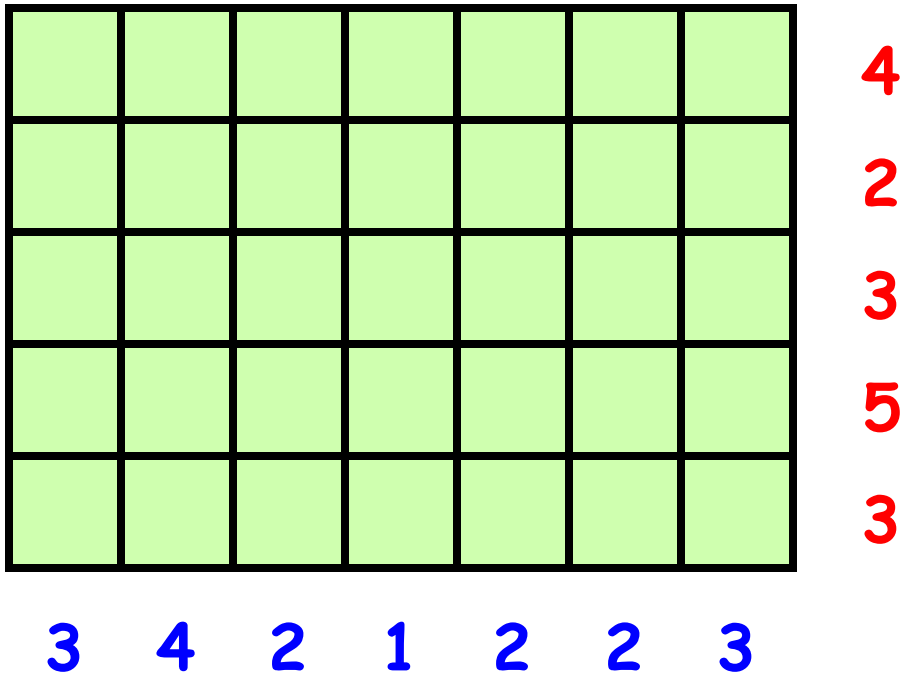
competitive pressures

?

Binary Contingency Tables

Given: marginals (row sums, column sums)

Goal:
- sample tables uniformly at random
- count tables



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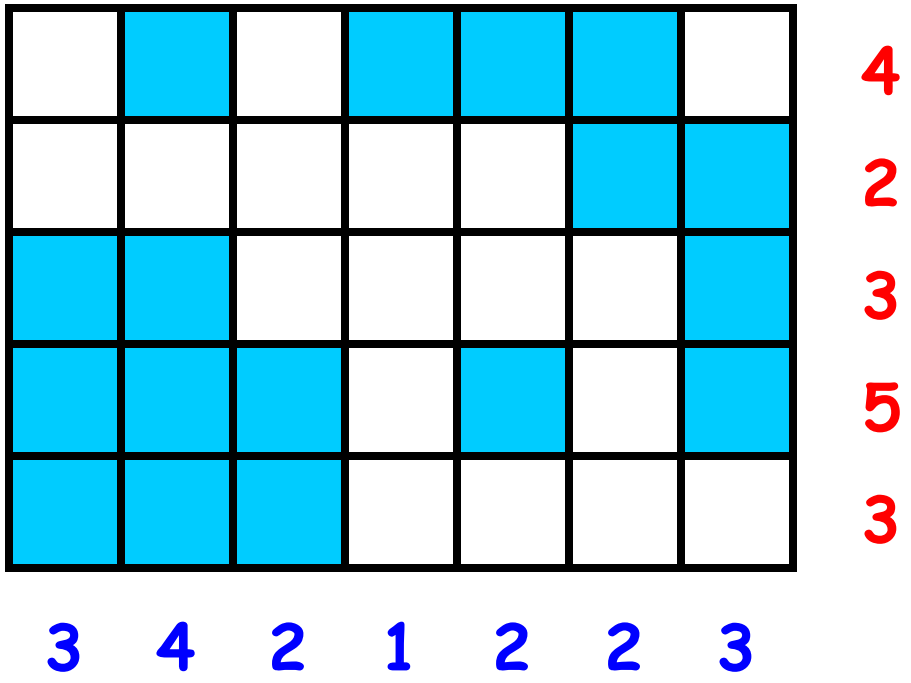

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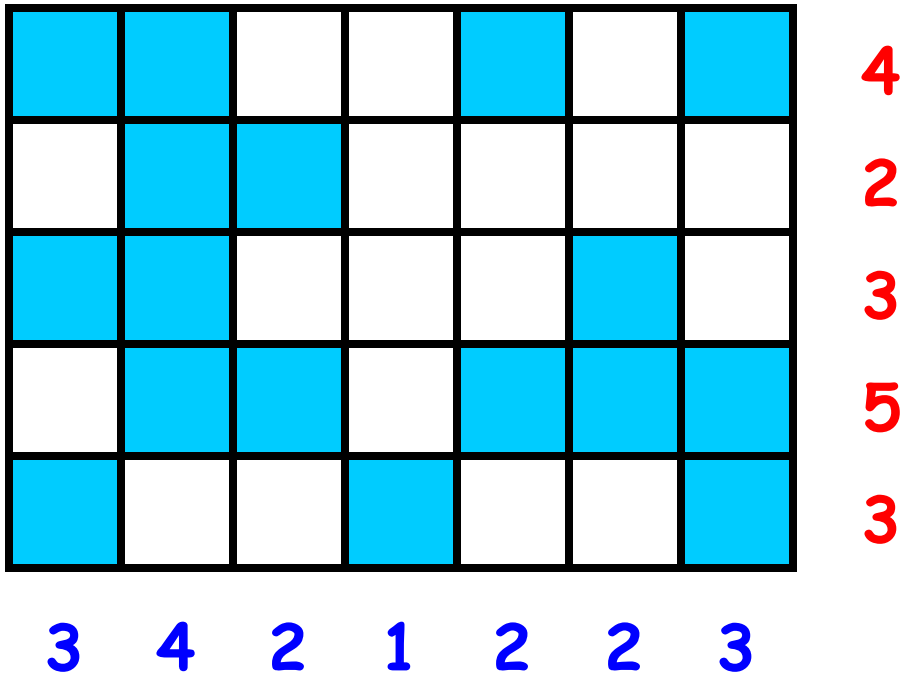

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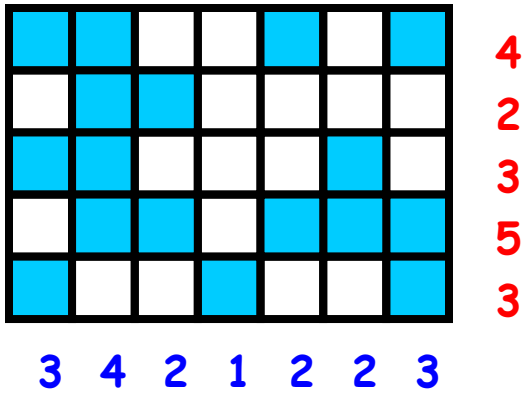
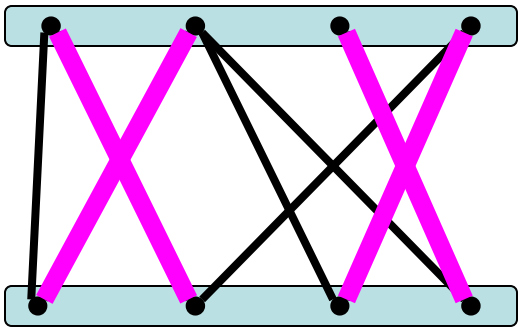


Permanent



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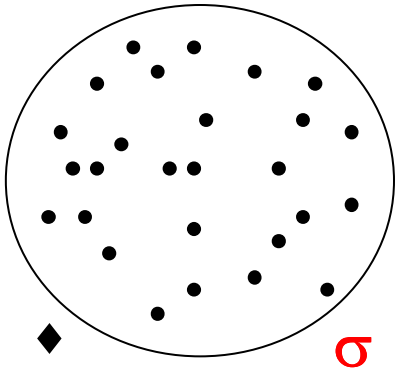

Simulated annealing

Permanent of an n x n matrix A

$$\mathrm{Per}(A) = \sum_{\pi \in S_n} \prod_{i=1}^{n} a_{i,\pi(i)}$$

in 1812:

Augustin-Louis Cauchy

Jacques Binet

$A =$

5	1	0	3	4
2	0	1	4	4
5	7	9	2	2
1	1	6	1	0
3	3	0	8	7

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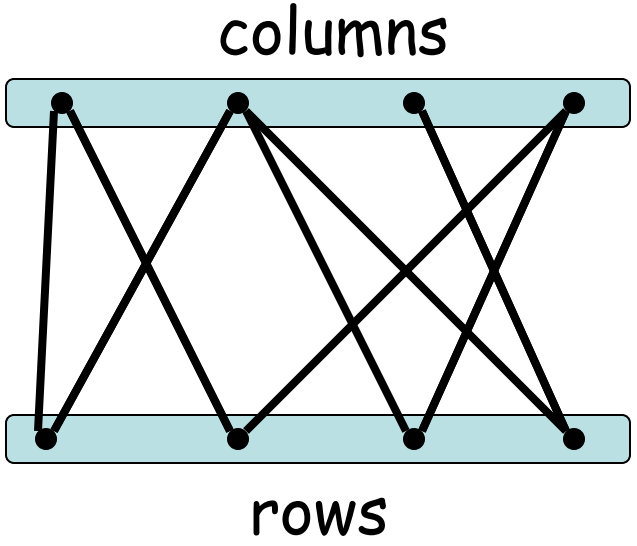

columns

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

rows

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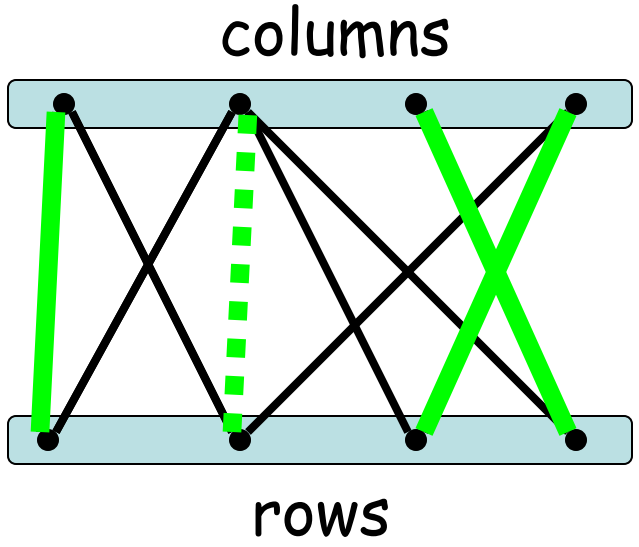

π

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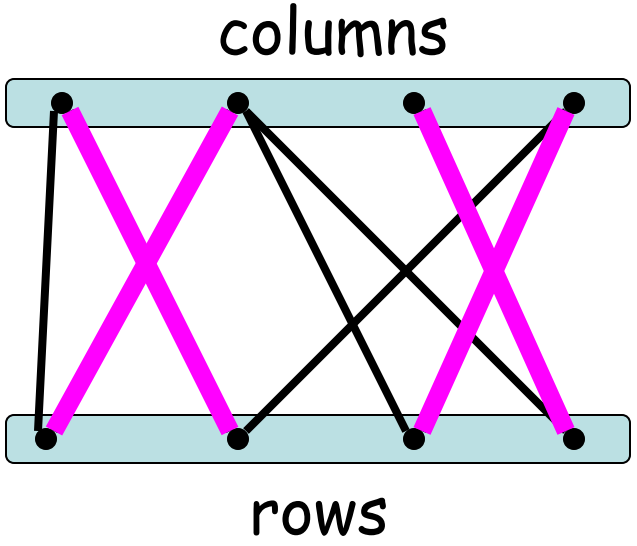

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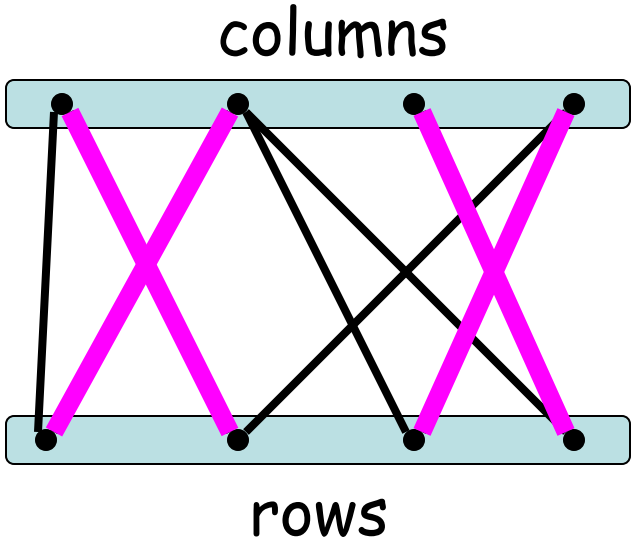
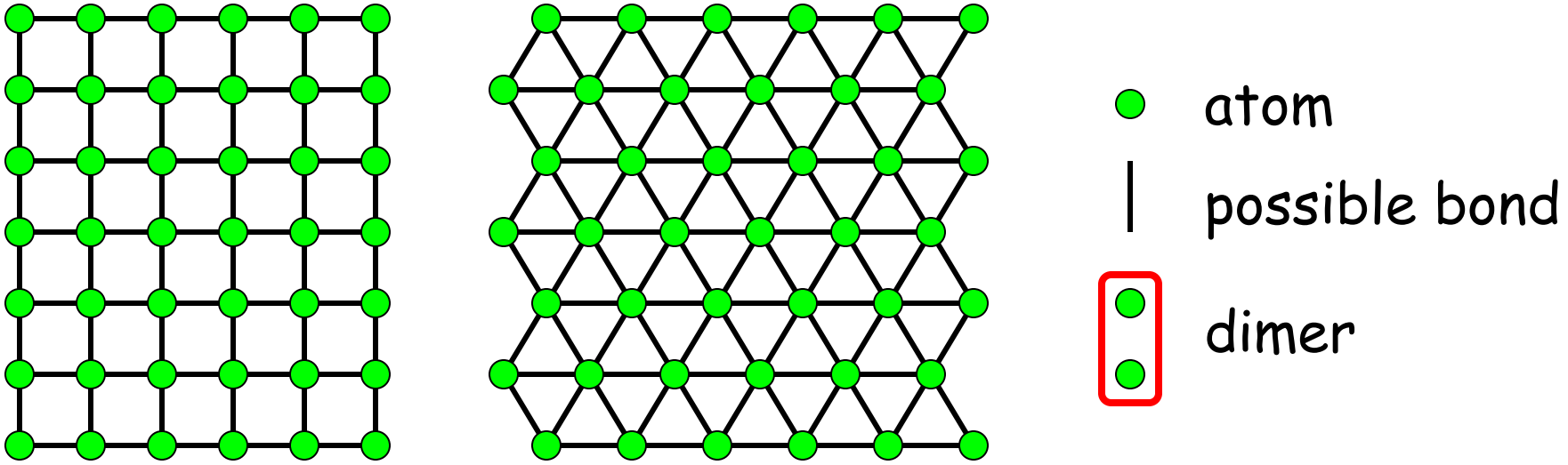


Count perfect matchings of a bipartite graph

Permanent: Counting Perfect Matchings

[Kasteleyn '63] **planar graphs** in polytime

Dimer model



Partition function = permanent (in bipartite case)

- for computation of thermodynamic properties

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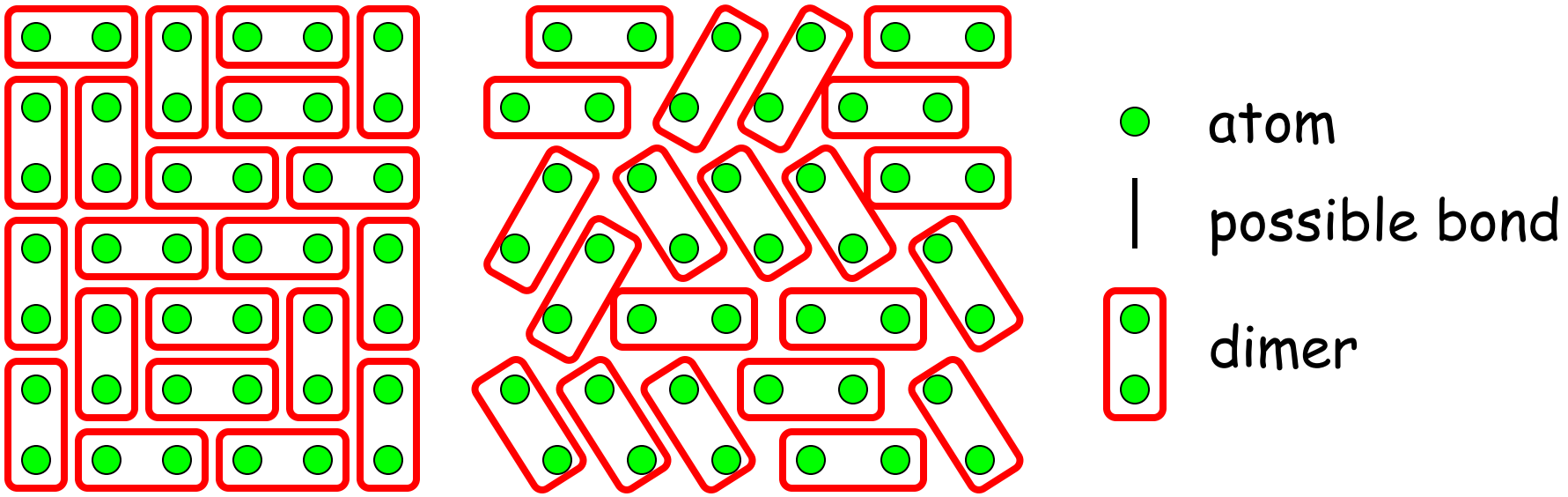

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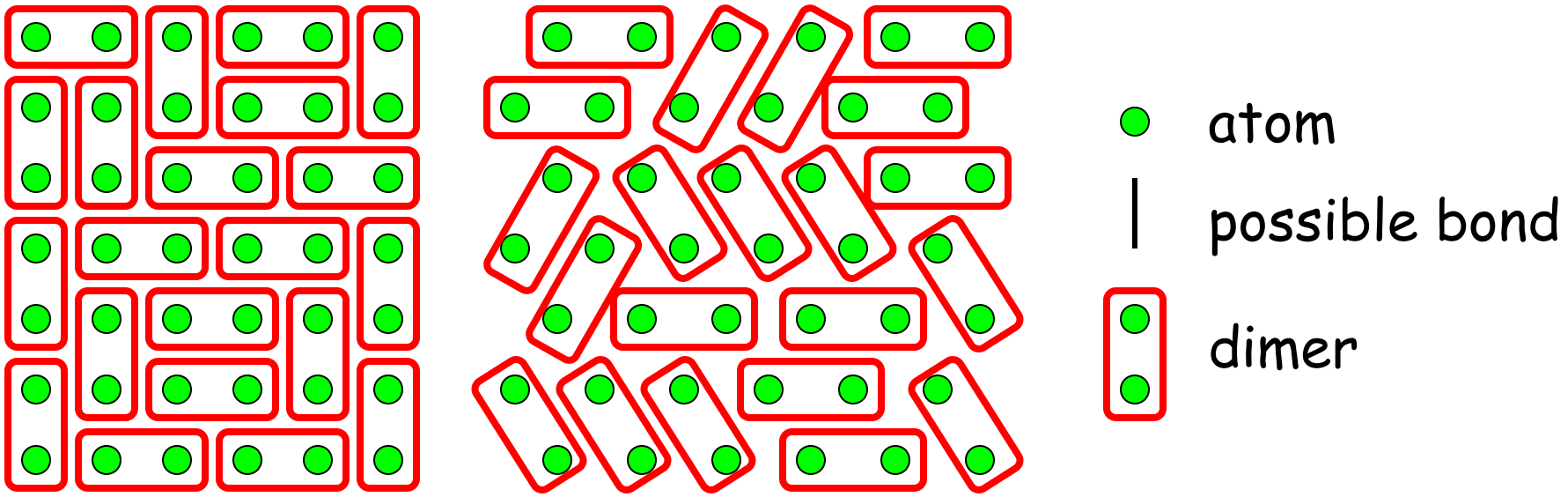
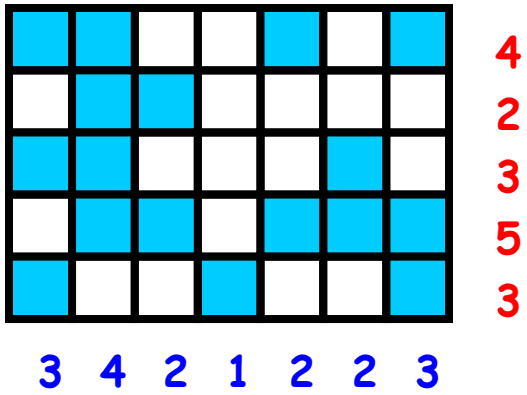


[Valiant '79] **#P-complete** for general (bipartite) graphs

Problems

Binary
contingency tables



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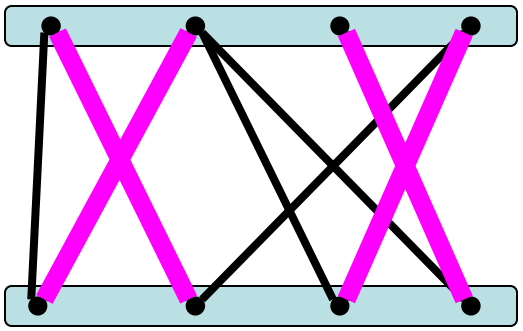

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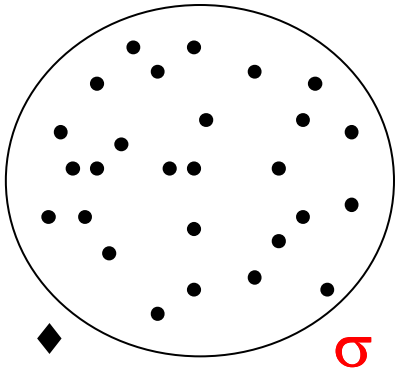
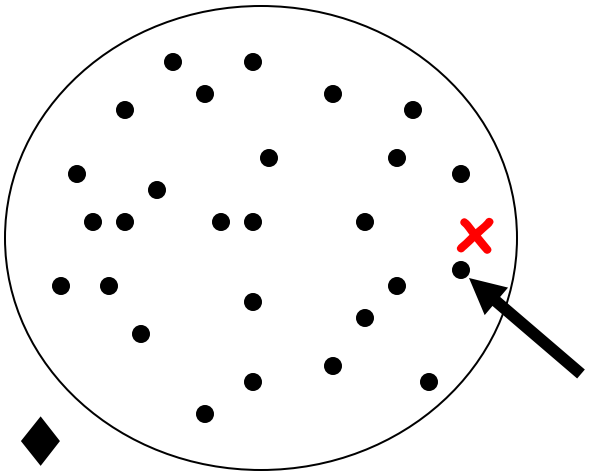


Simulated annealing

Importance Sampling for counting problems



Probability distribution σ
on the points + ♦

with positive probability $\sigma(x)>0$

Random variable

$$\eta(s) = \begin{cases} 1/\sigma(s) & \text{if } s \text{ in the set} \\ 0 & \text{if } s \text{ is } \blacklozenge \end{cases}$$

Unbiased estimator

$$E[\eta] = \sum \sigma(x).1/\sigma(x) = \text{size of the set}$$

Problems

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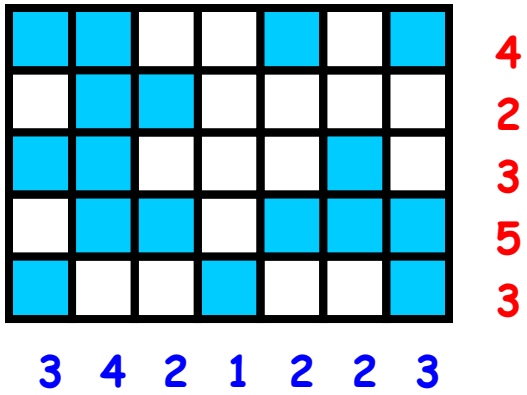

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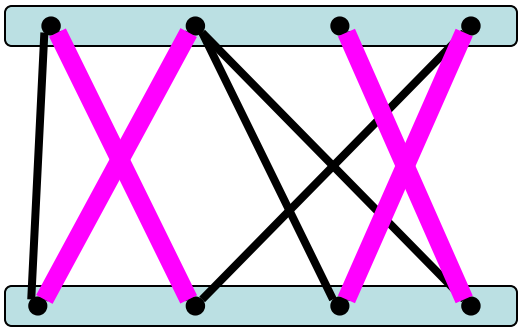

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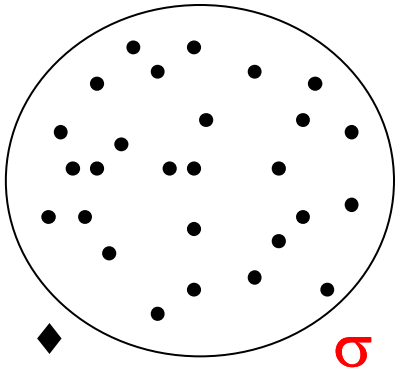


Simulated annealing

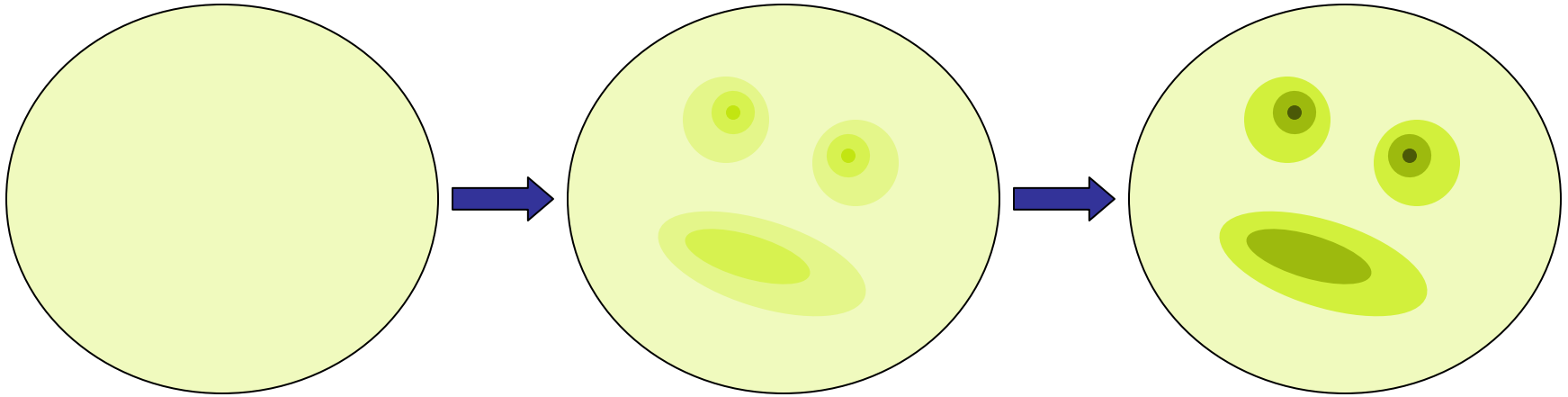
Simulated Annealing

[Kirkpatrick-Gelatt-Vecchi '83]
[Černý '85]

Unordered state → Ordered state

(EASY) (DIFFICULT)

Cooling:



all equivalent differences more and more pronounced

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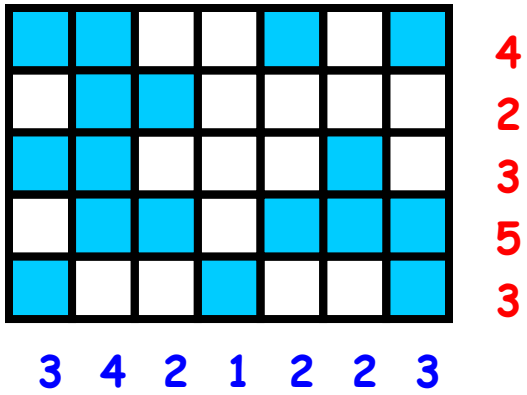

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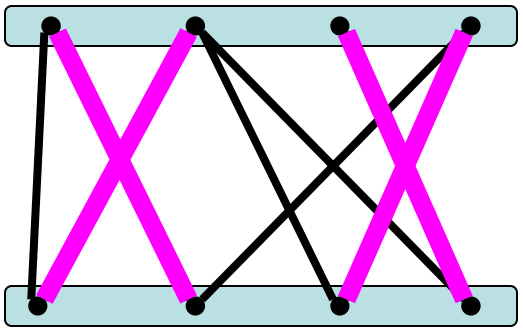

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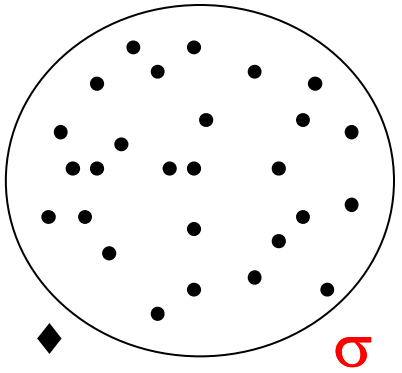

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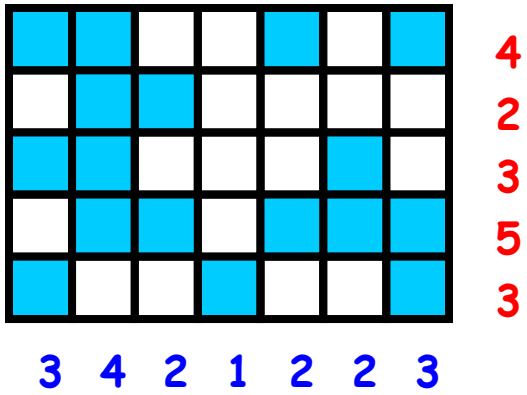

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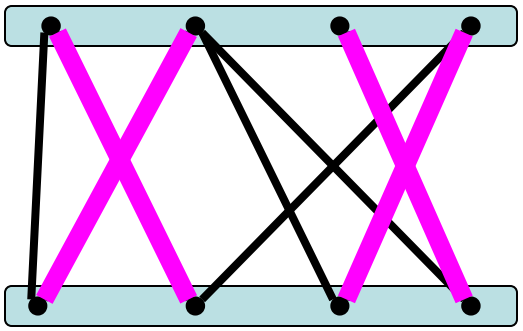

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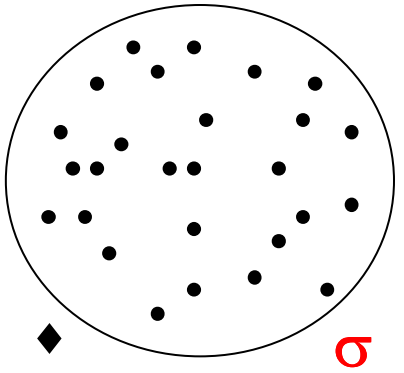

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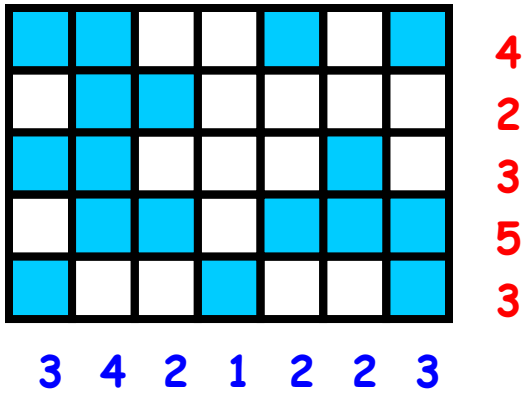

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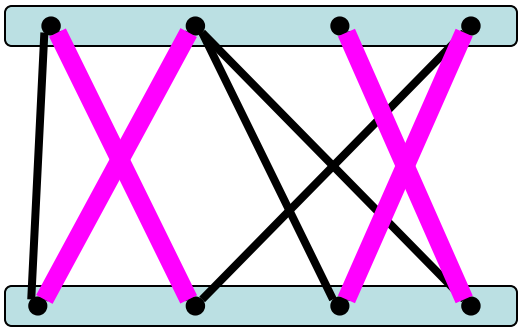

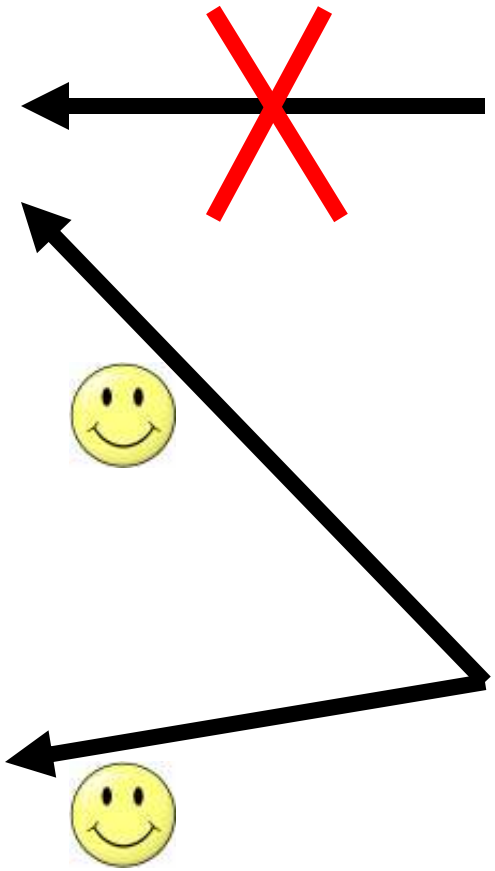

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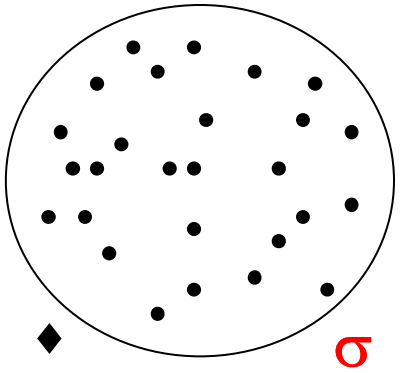

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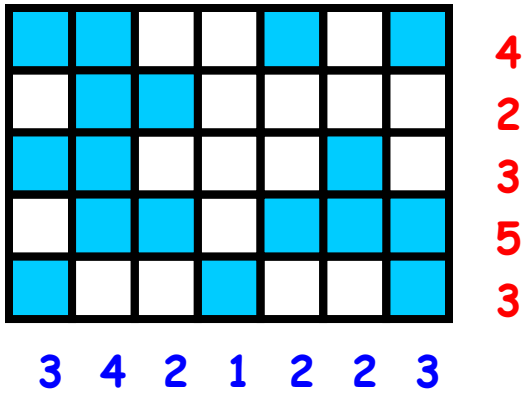

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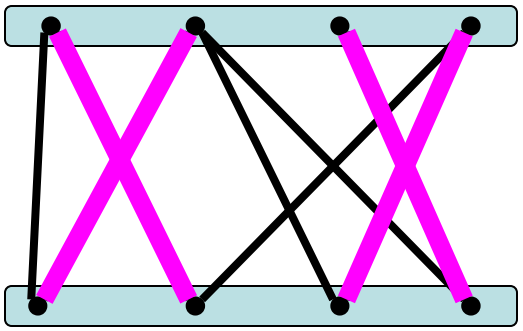

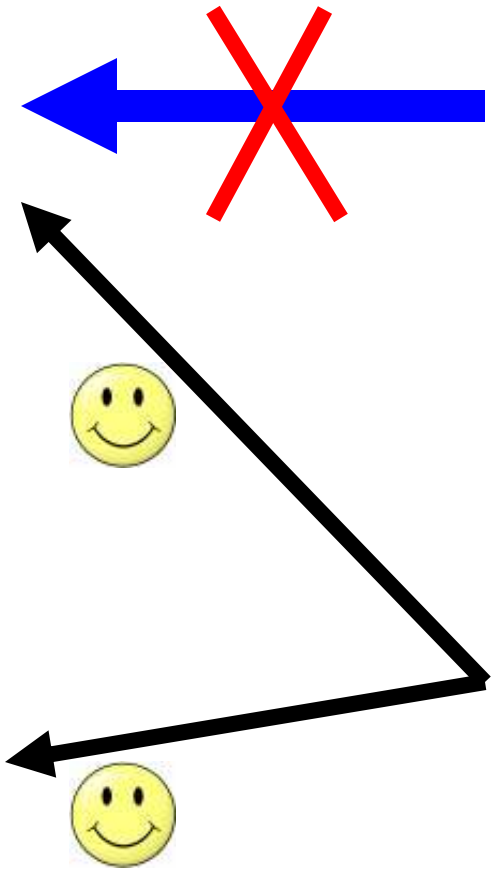

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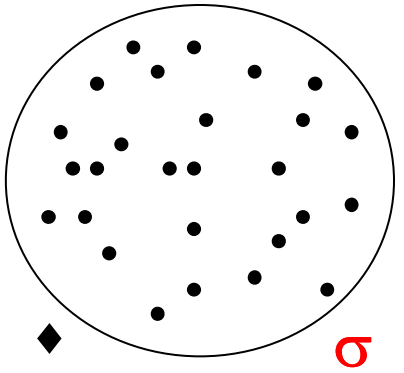

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Sequential Importance Sampling for BCT

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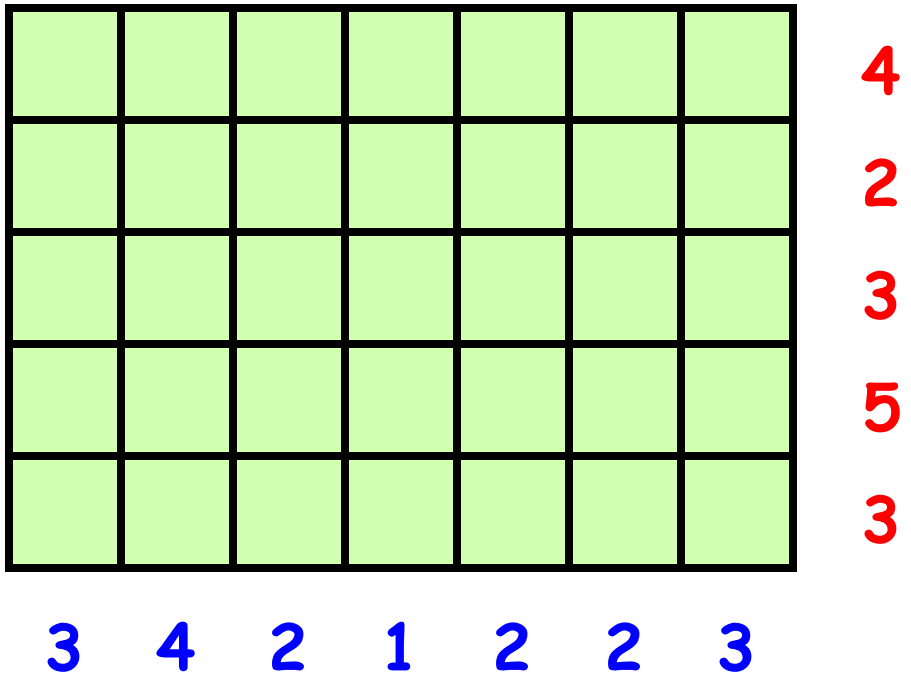

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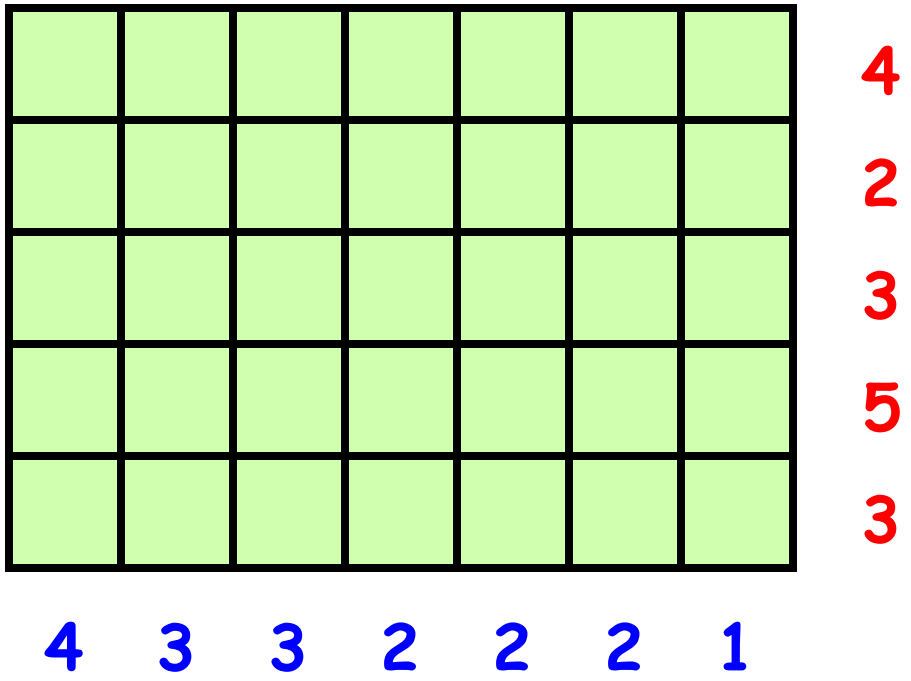

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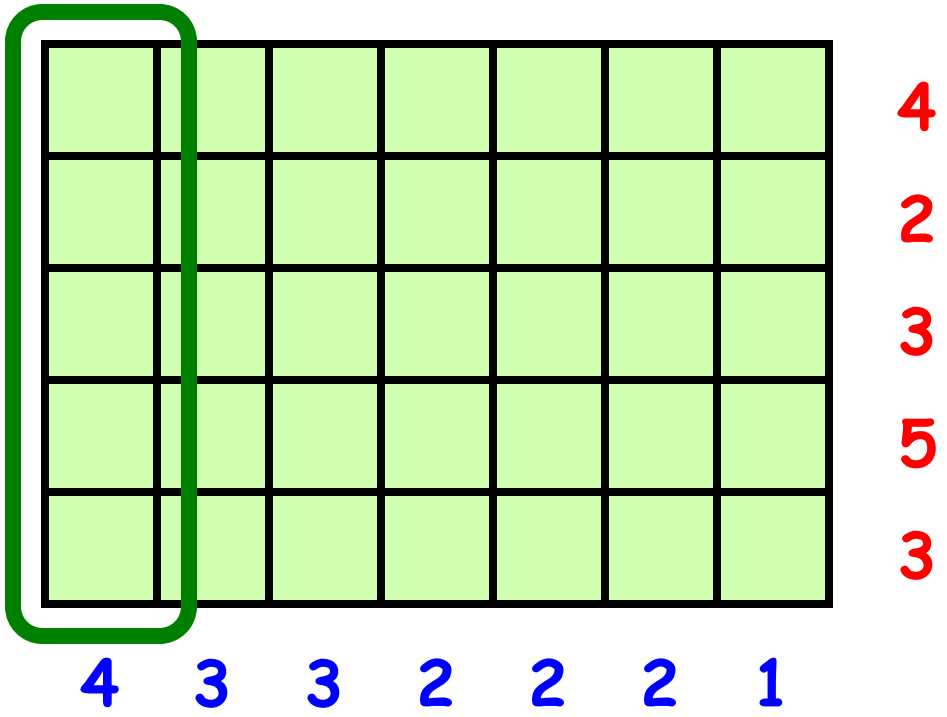

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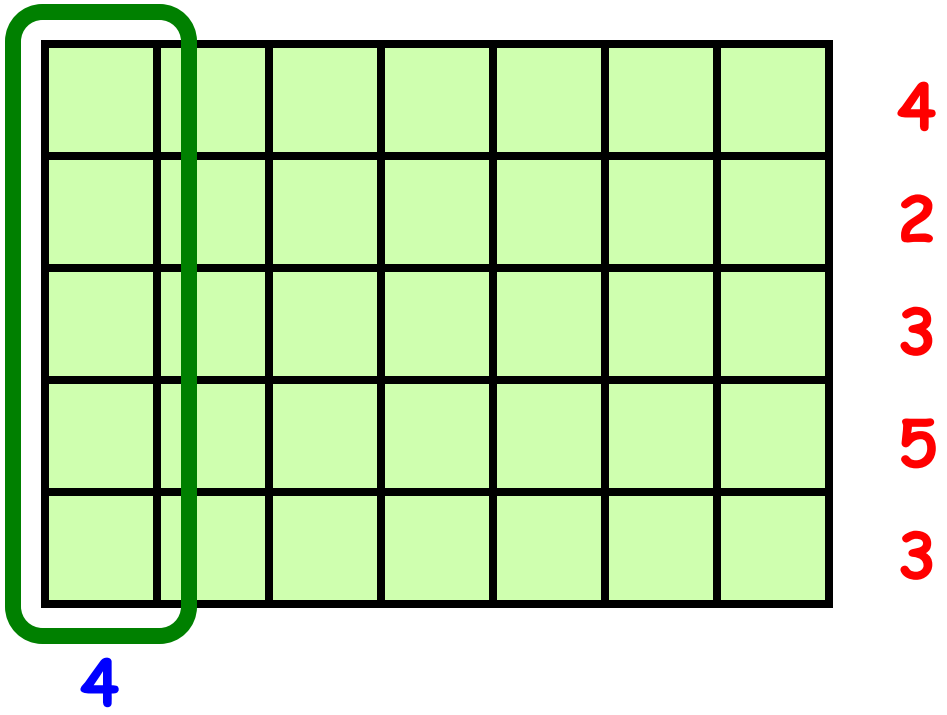

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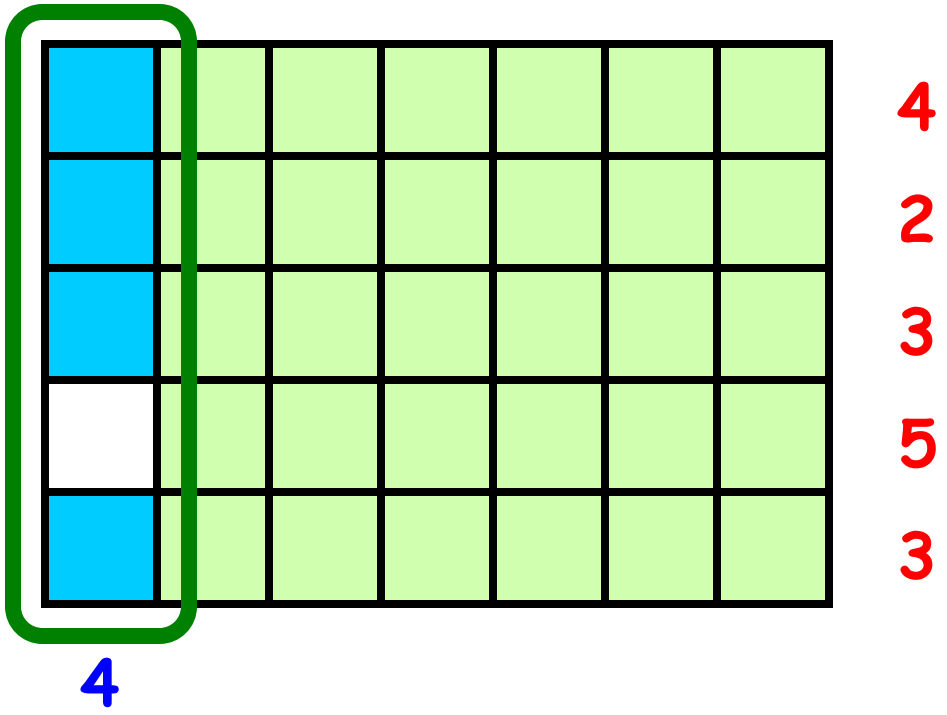

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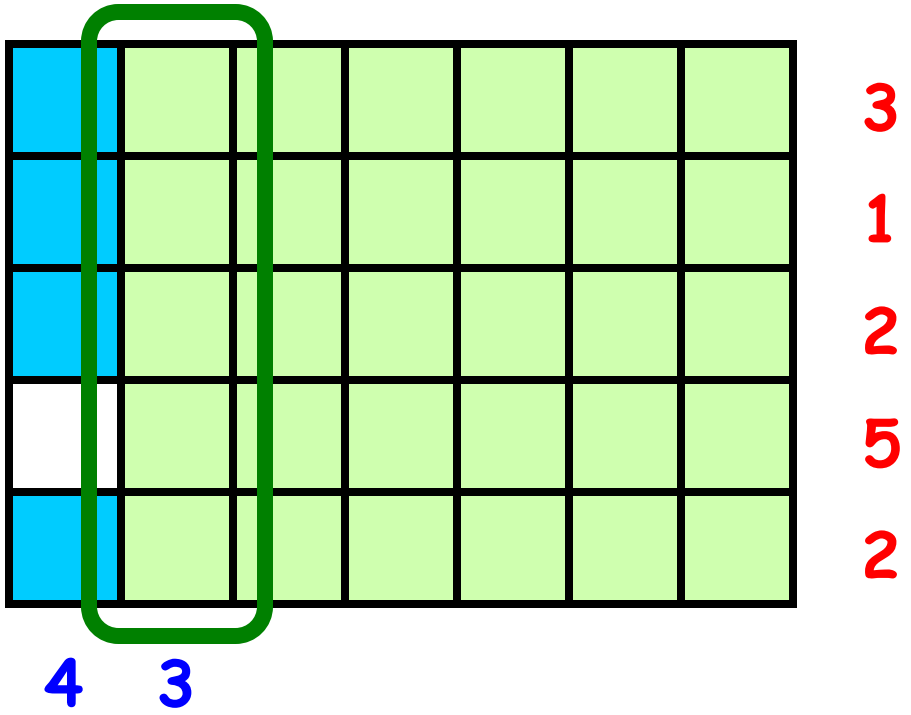

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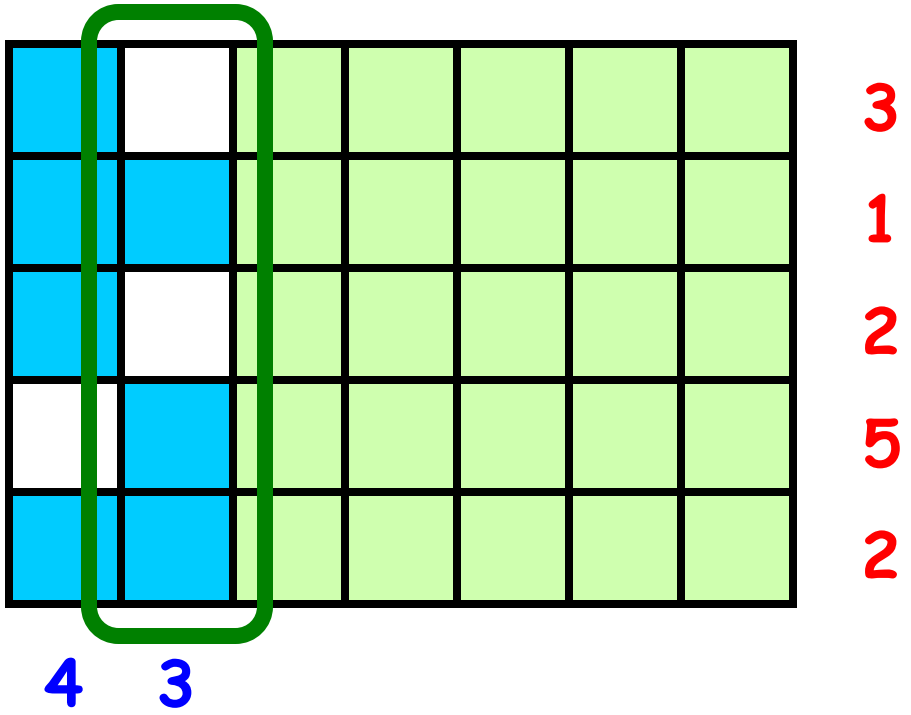

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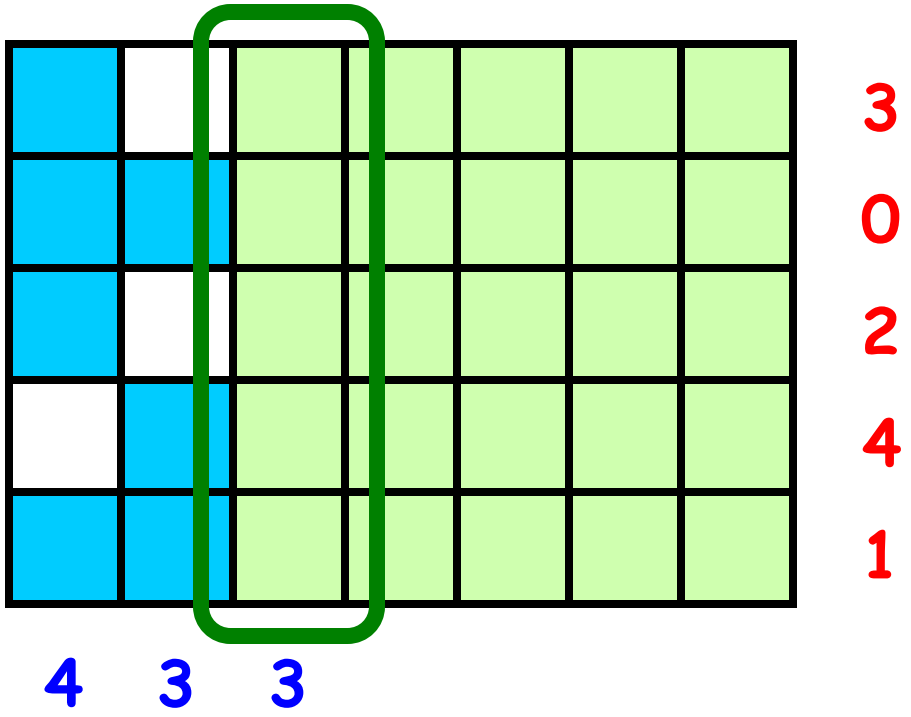

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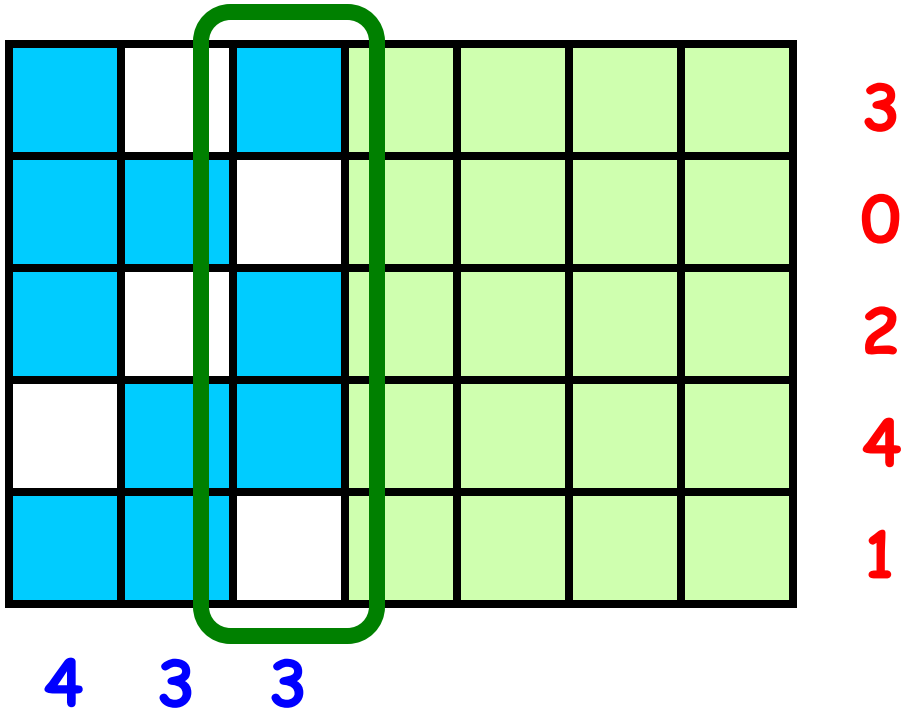

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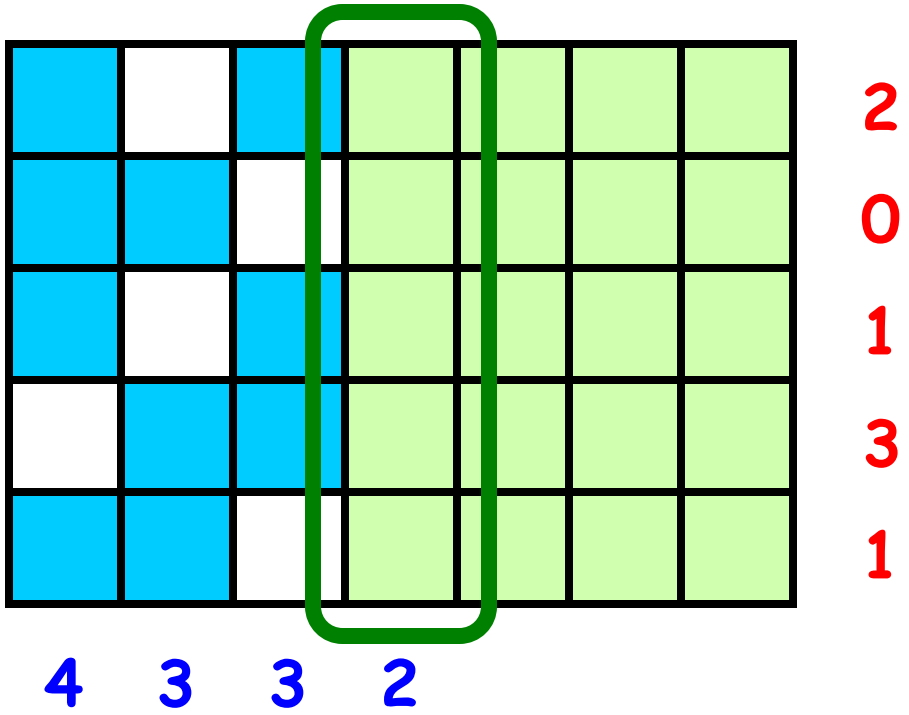

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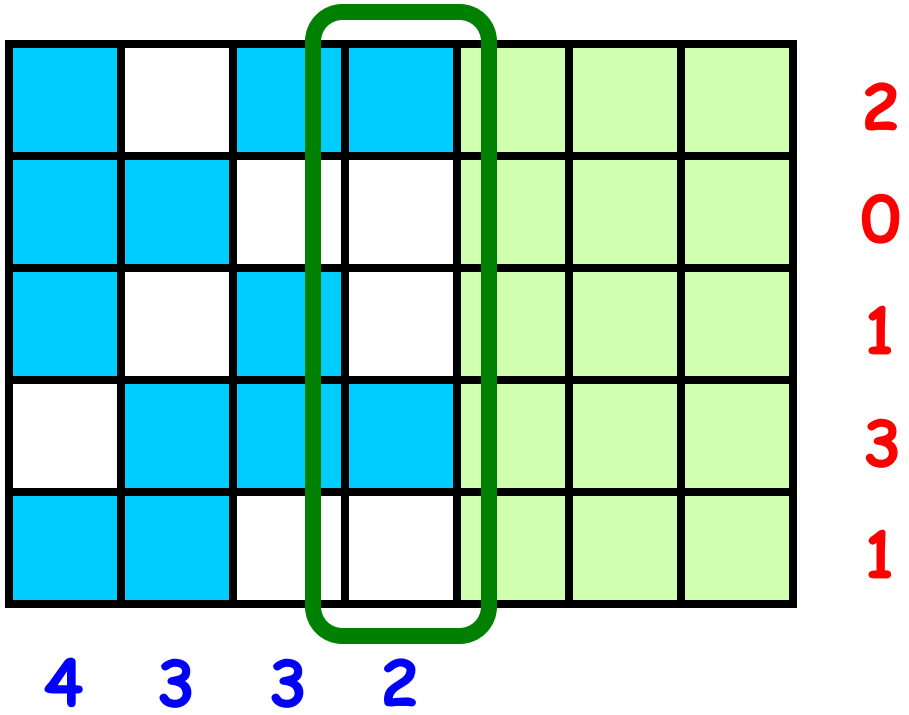

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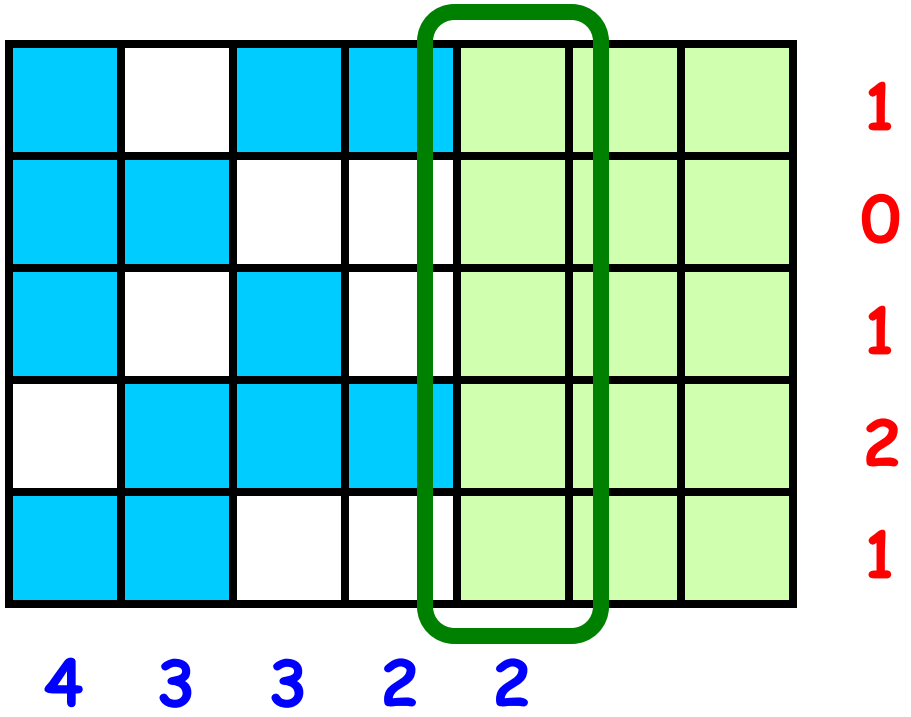

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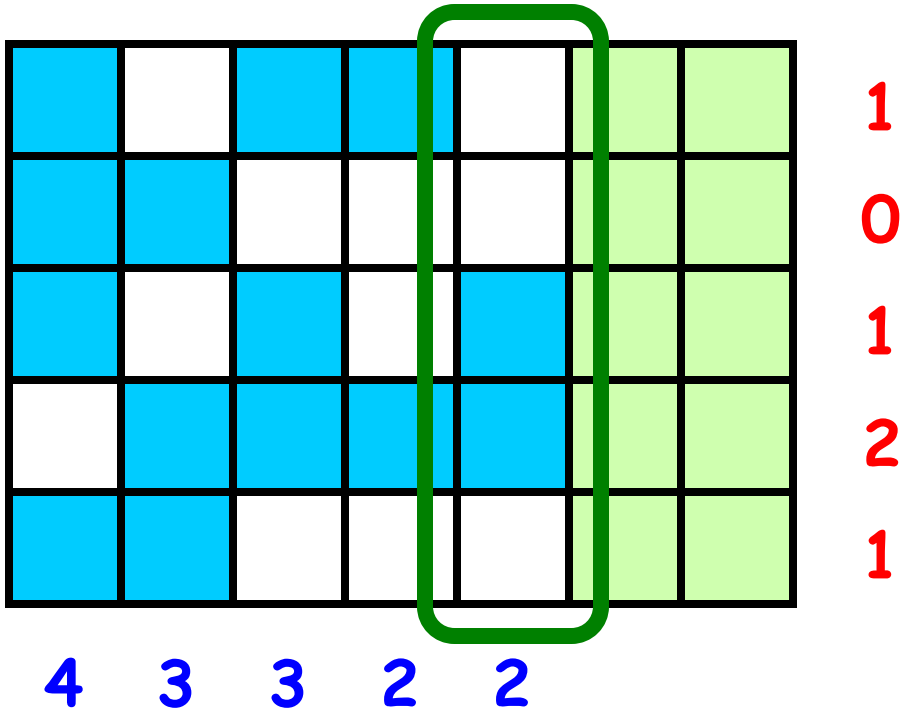

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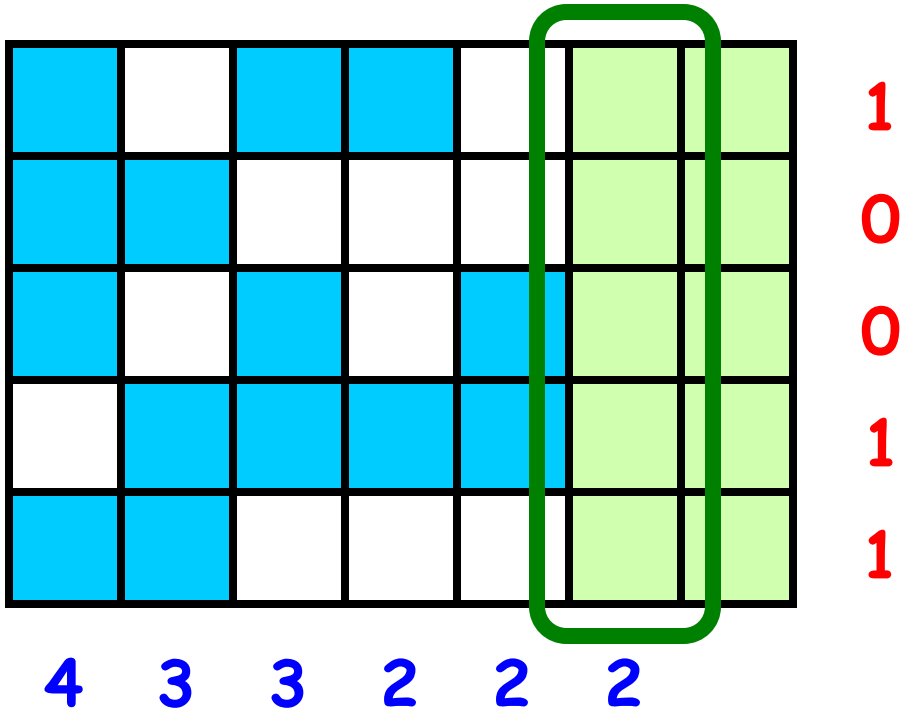

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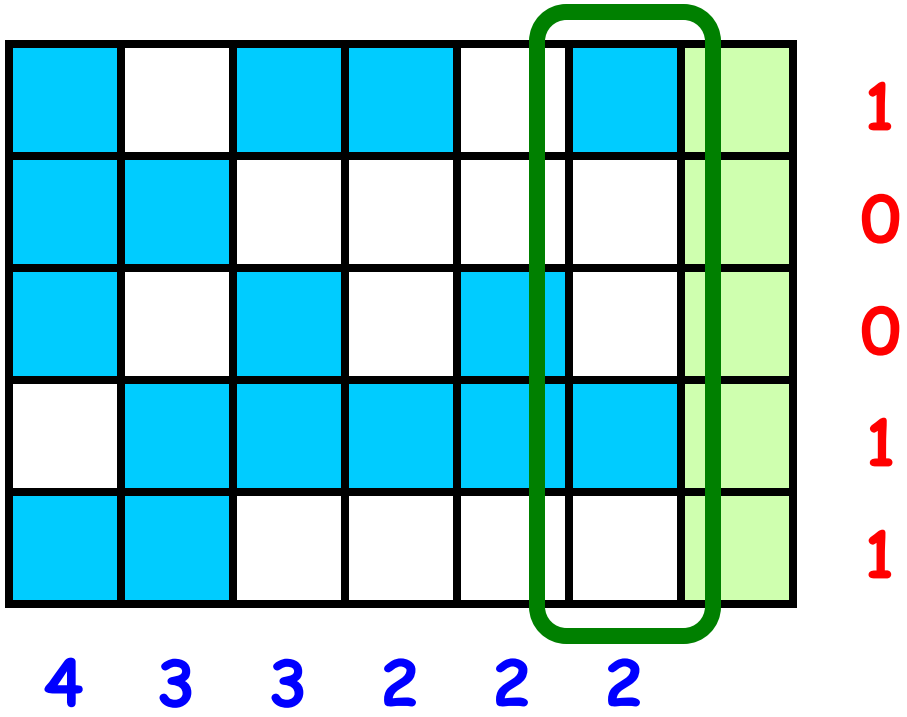

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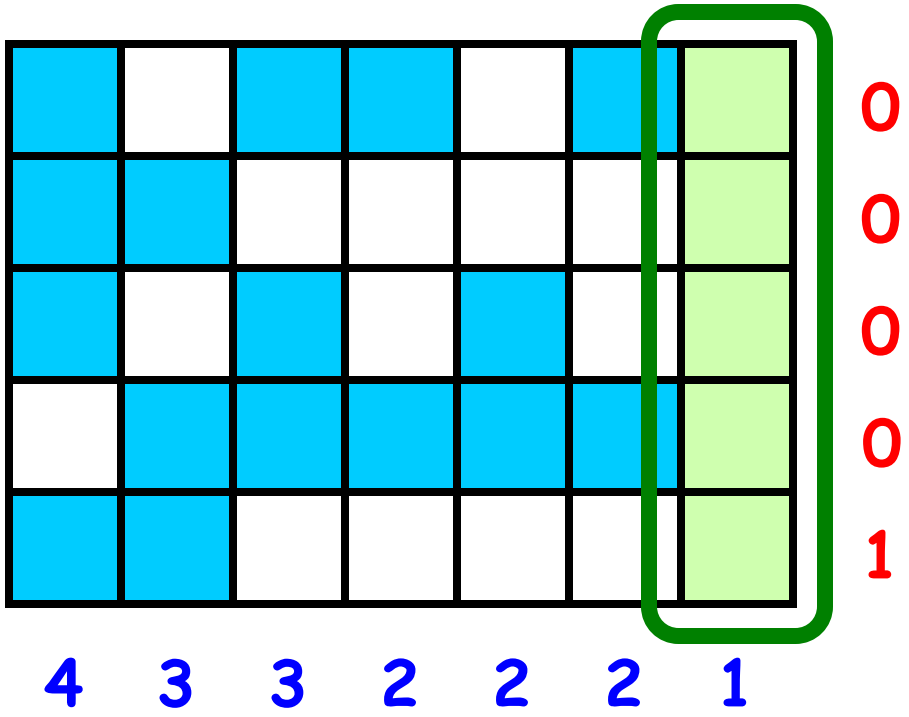

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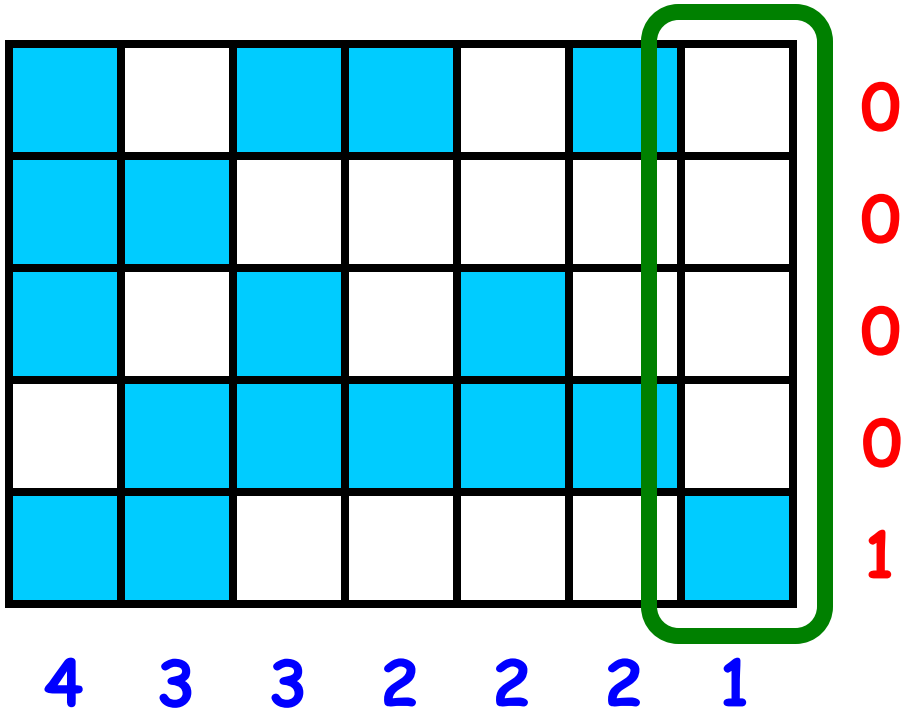

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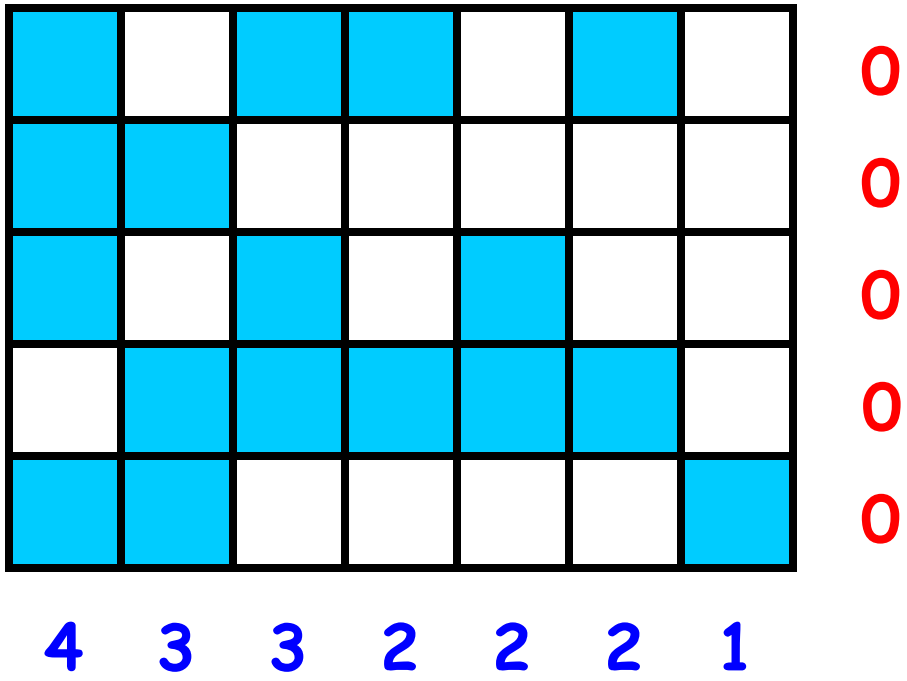

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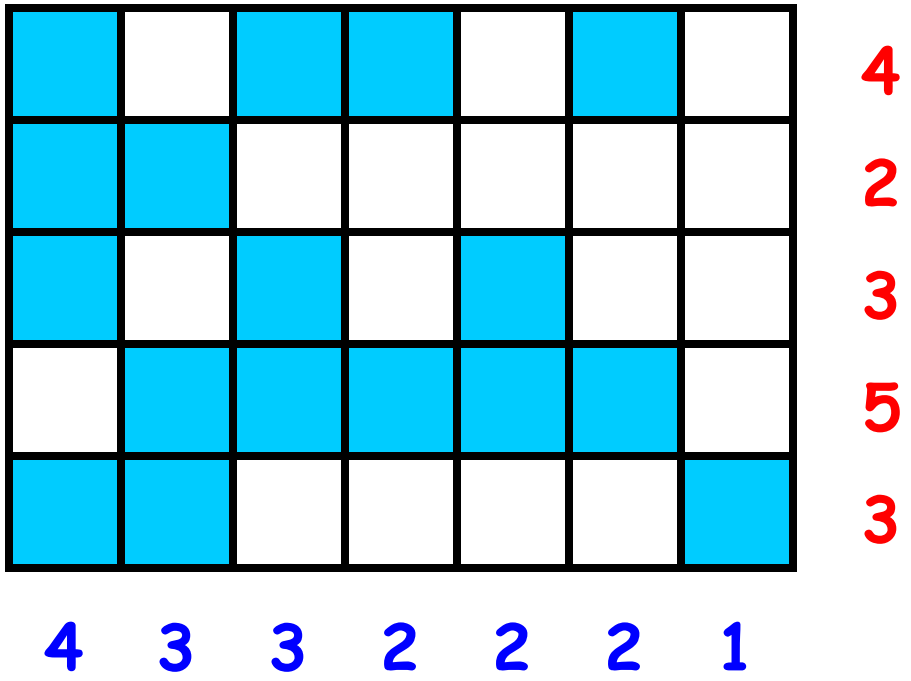
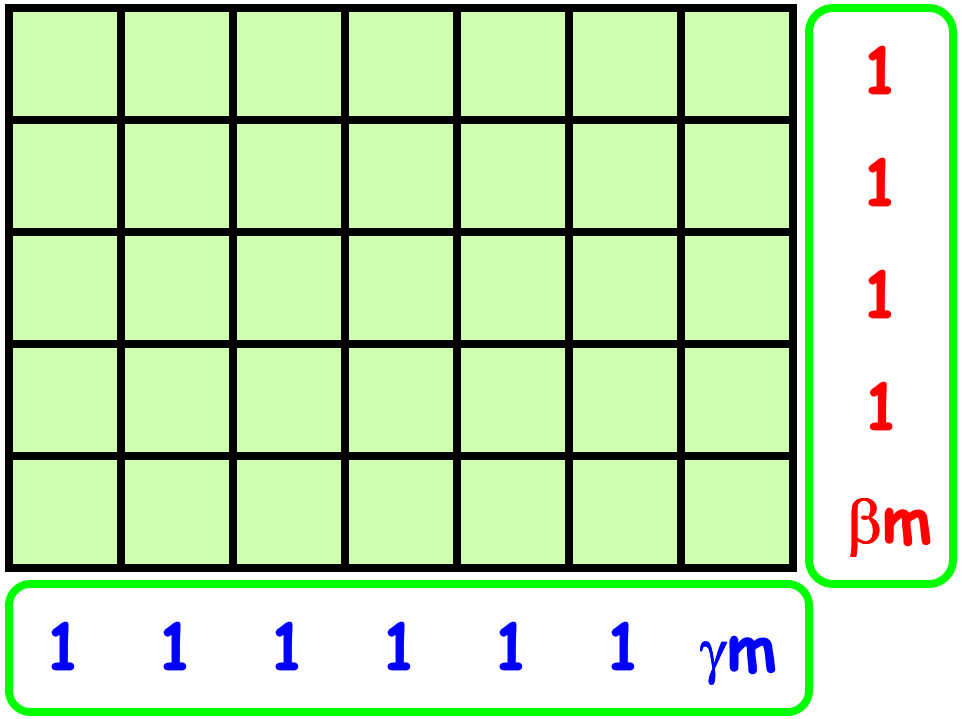


A Counterexample for SIS

Thm [Bezáková-Sinclair-Štefankovič-Vigoda '06]:

For any $\beta \neq \gamma$, SIS output after any subexponential number of trials is **off by an exponential factor** (with high probability).



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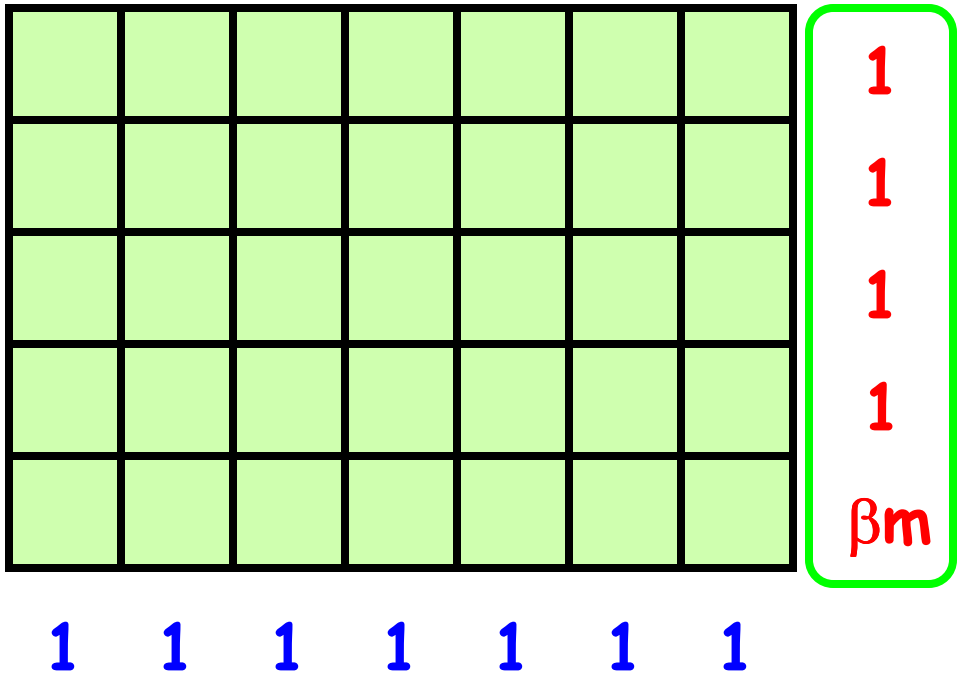

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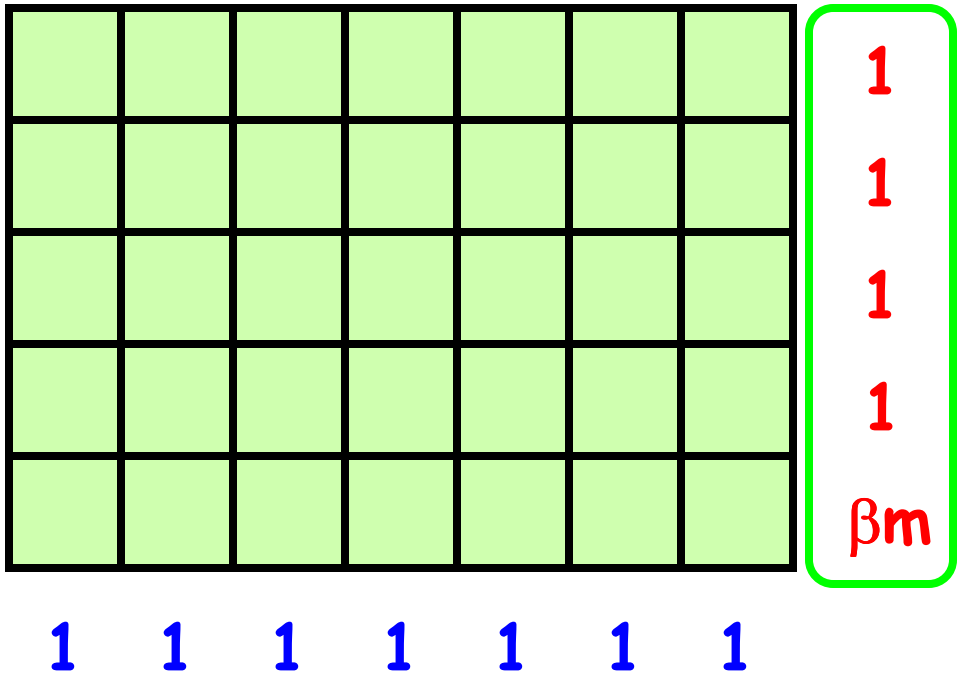

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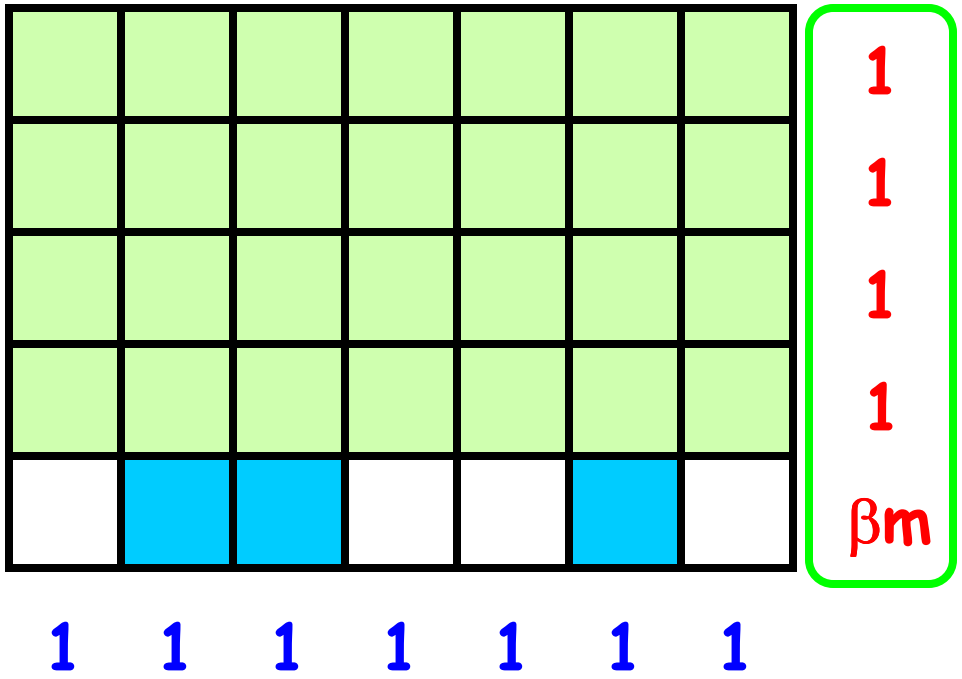

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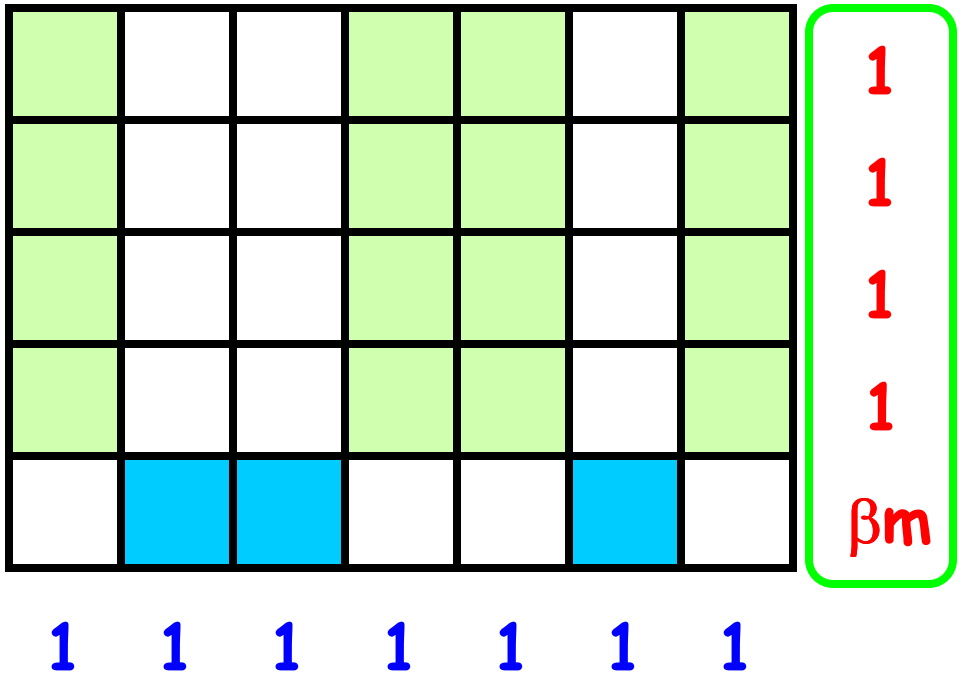

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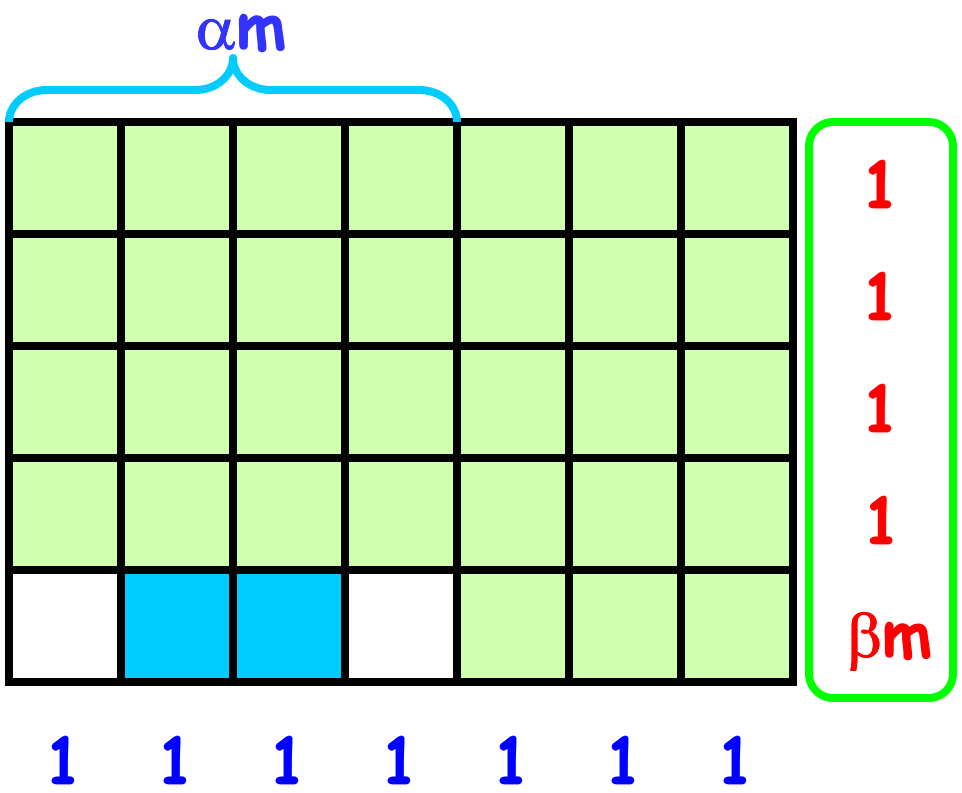

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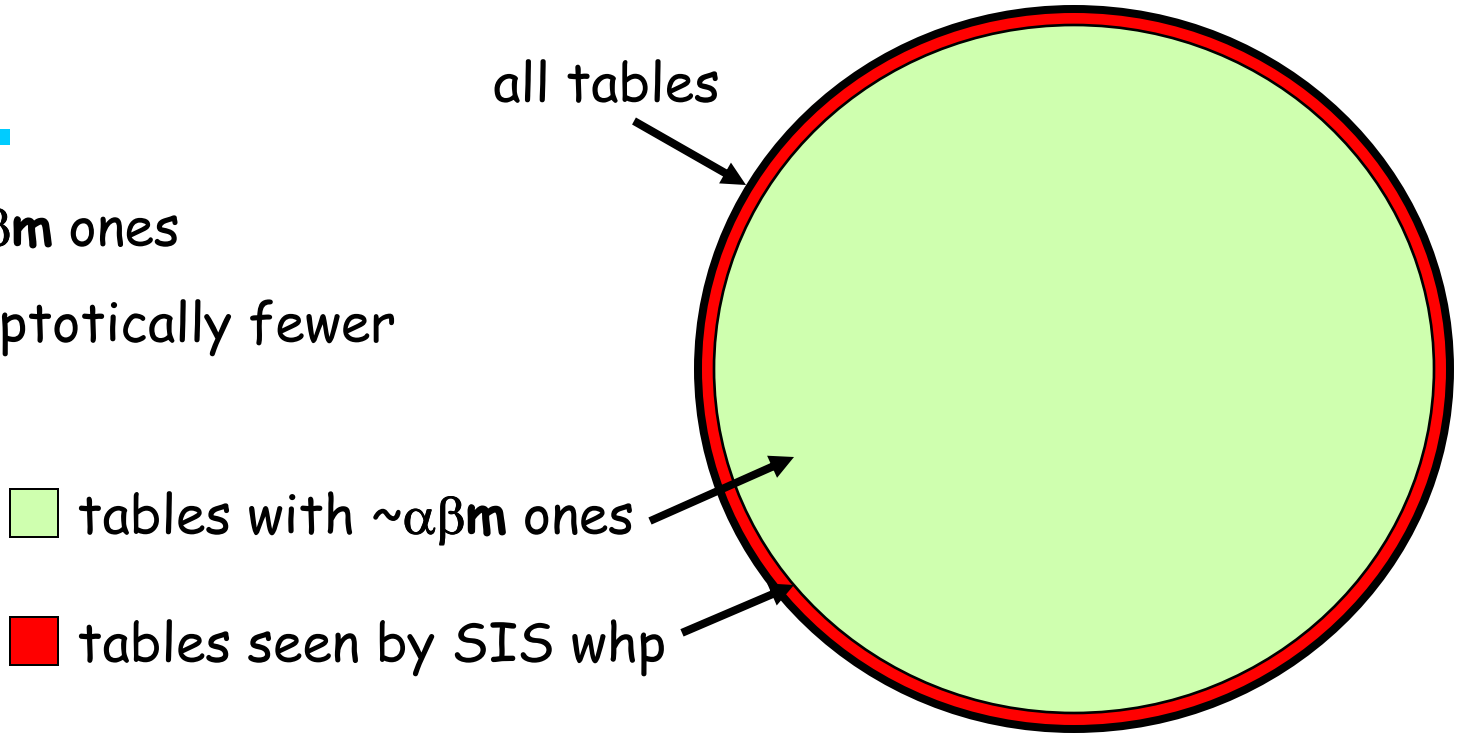
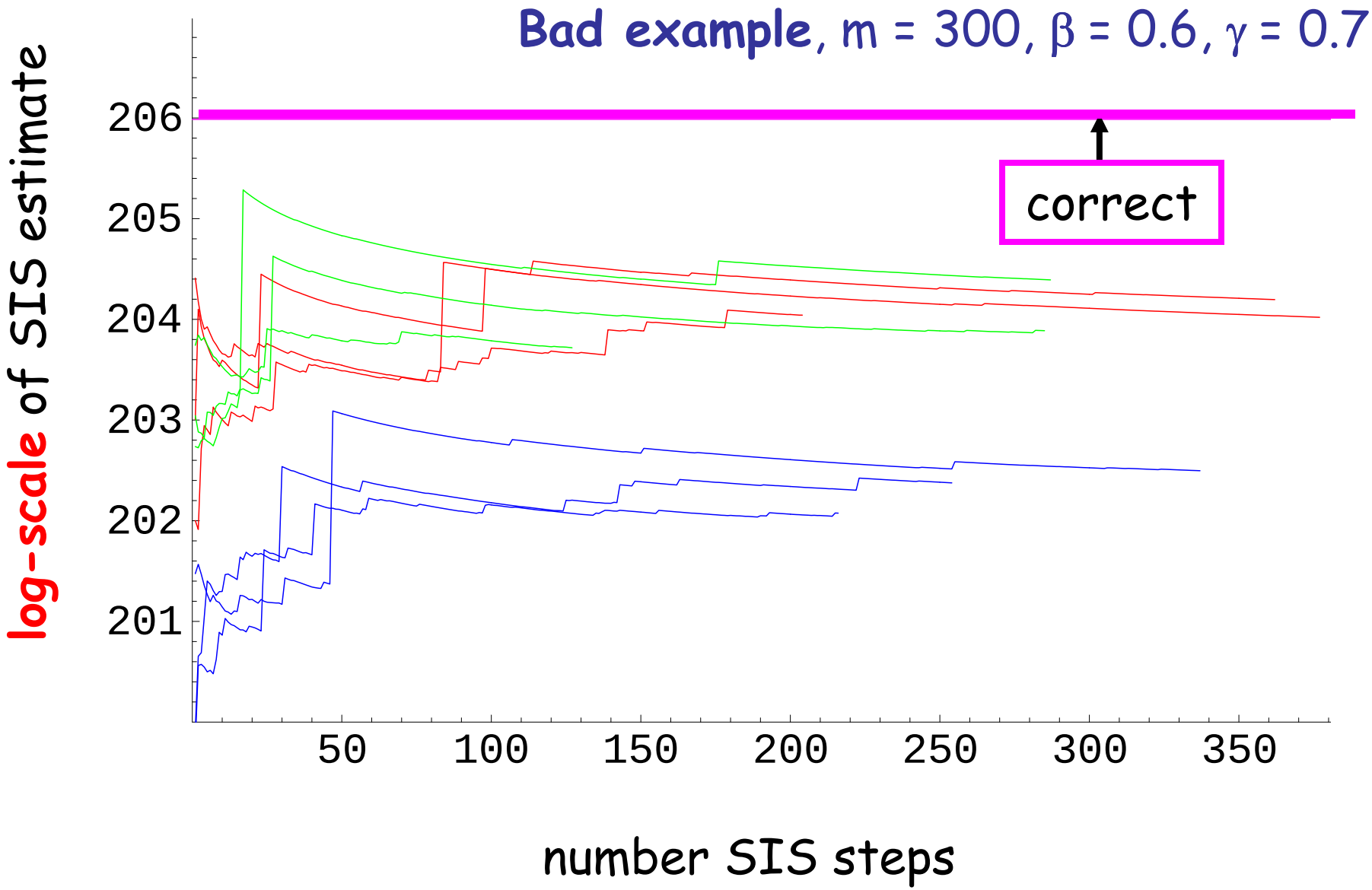


SIS - Experimental Results



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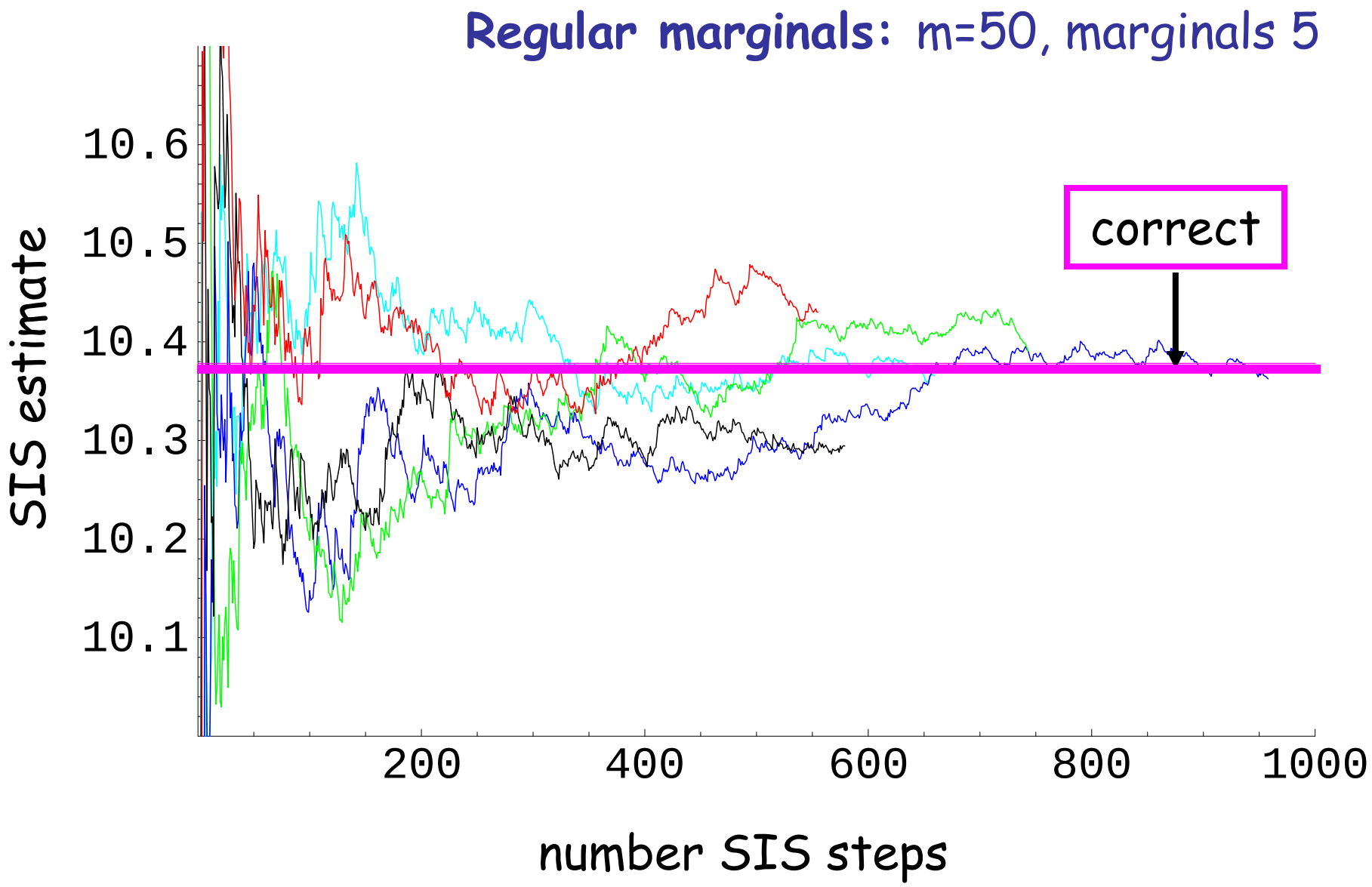

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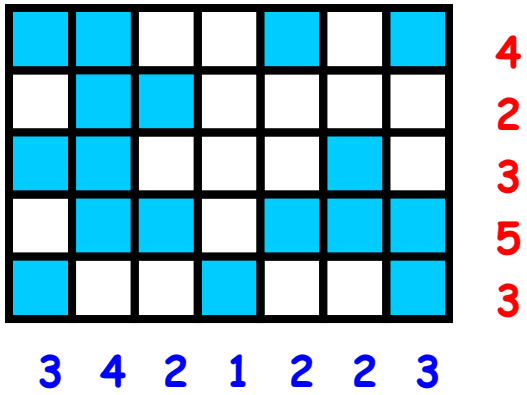

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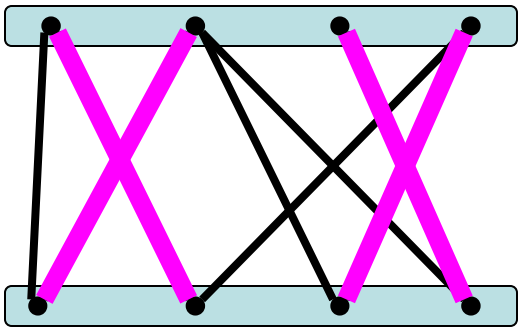

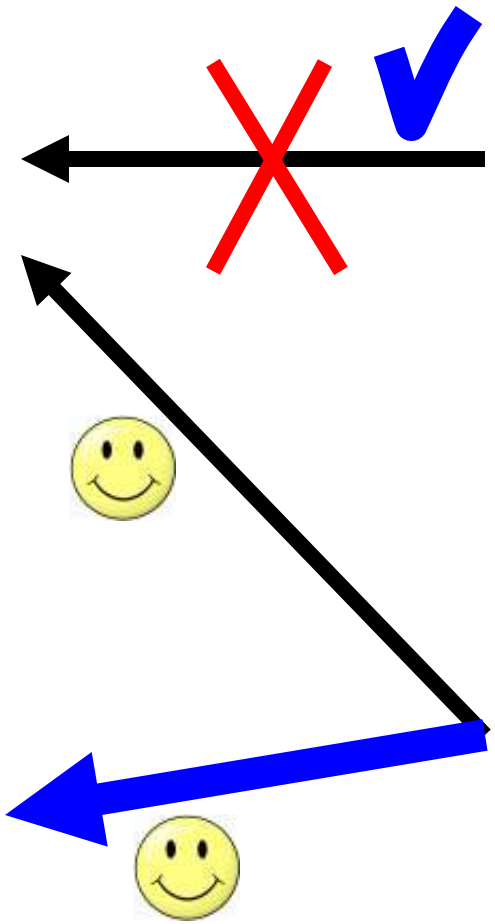

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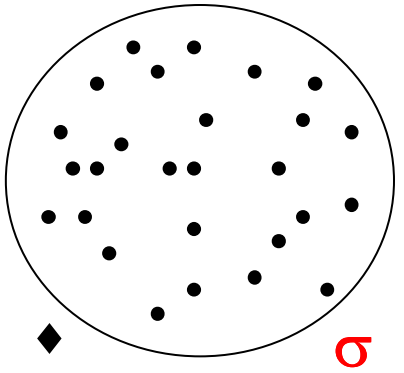


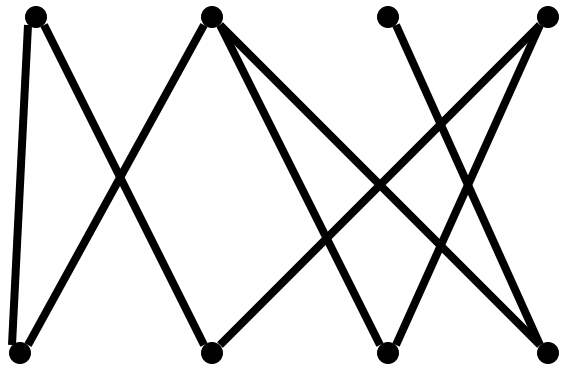
Simulated annealing

Broder Chain

[Broder '88]

What for: uniform sampling of perfect matchings

How: Markov chain on perfect + near-perfect matchings



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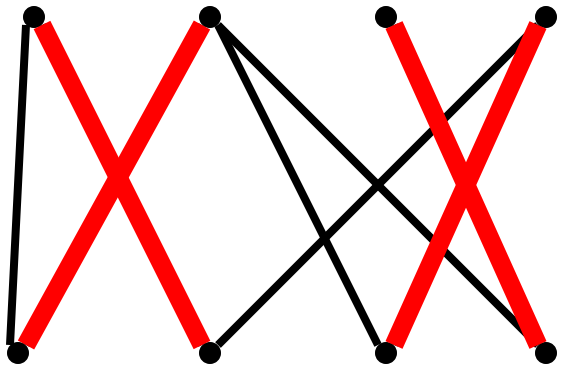

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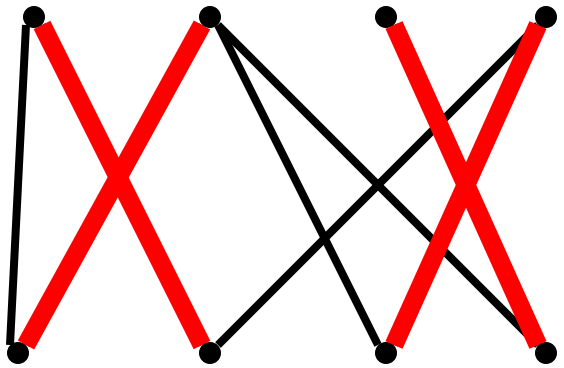

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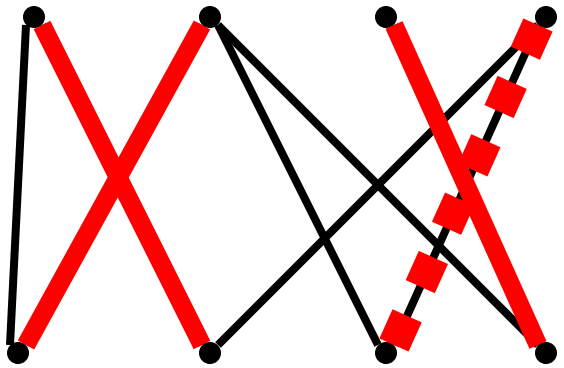

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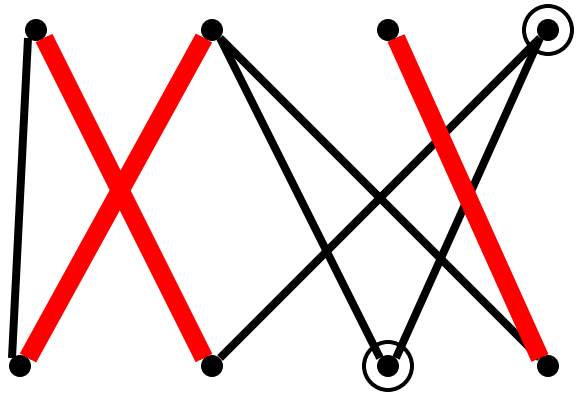

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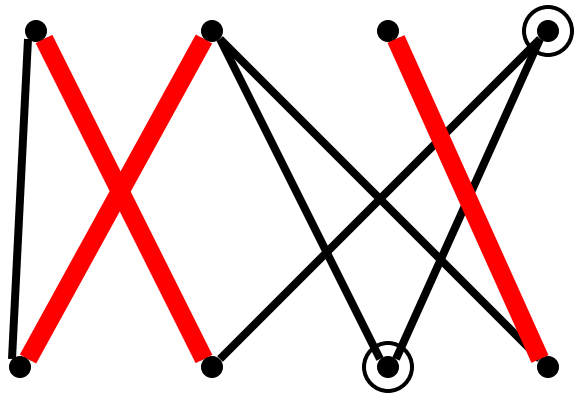

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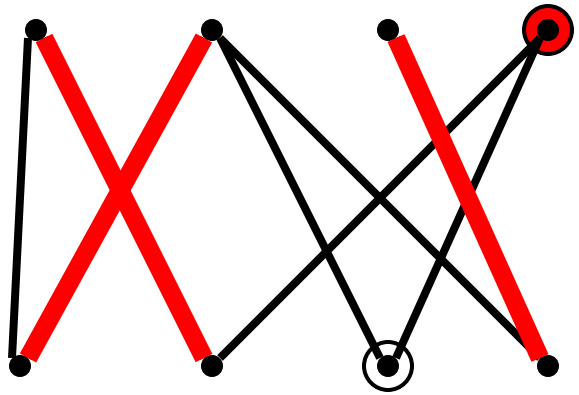

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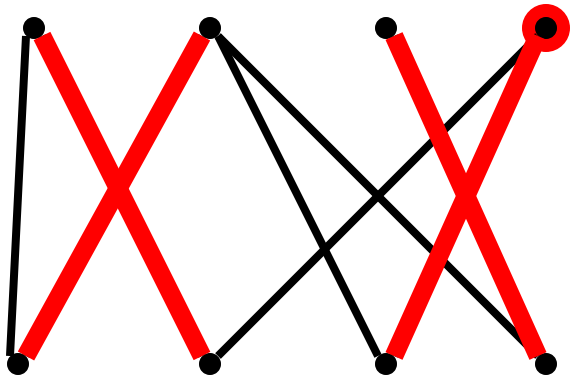

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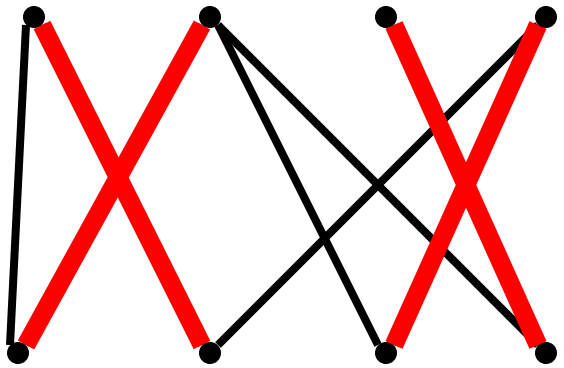

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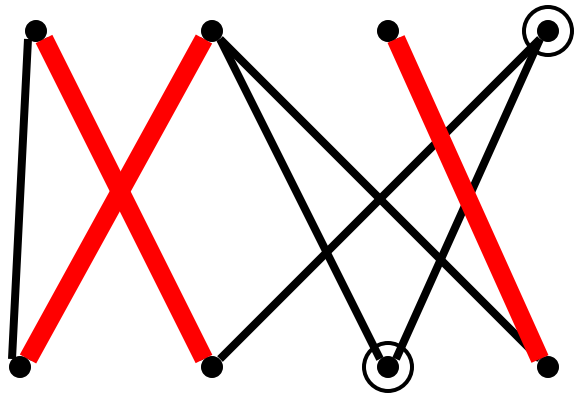

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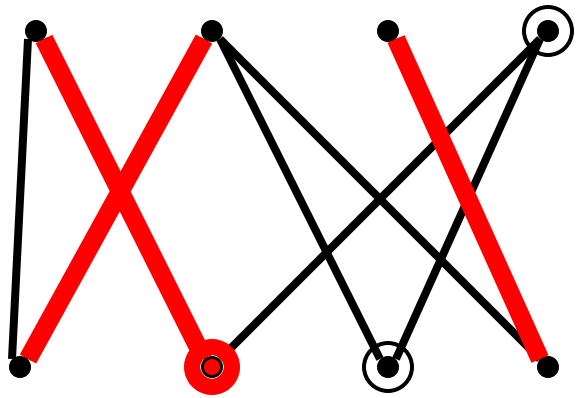

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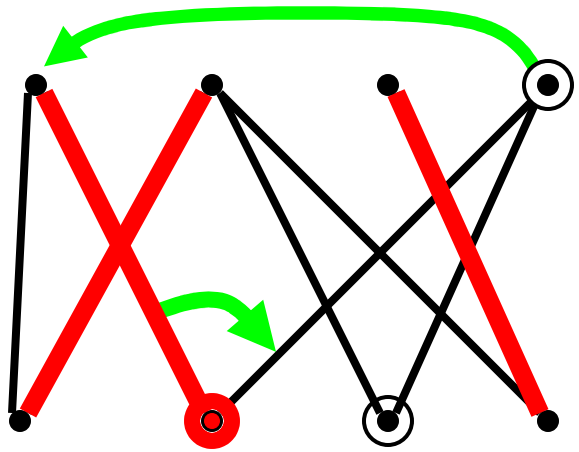

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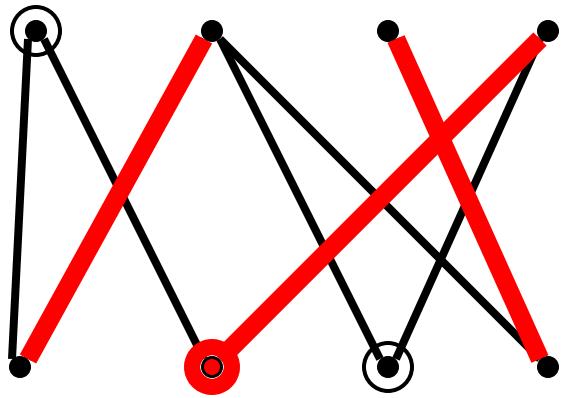

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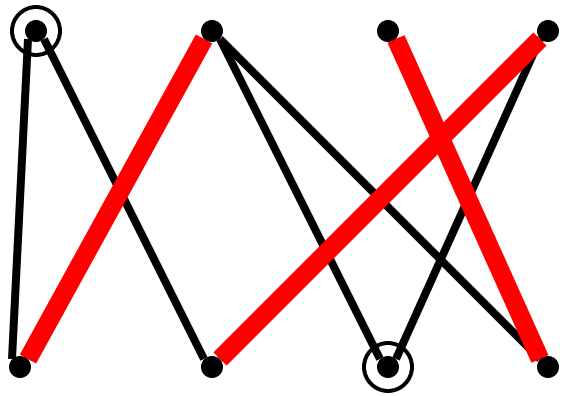

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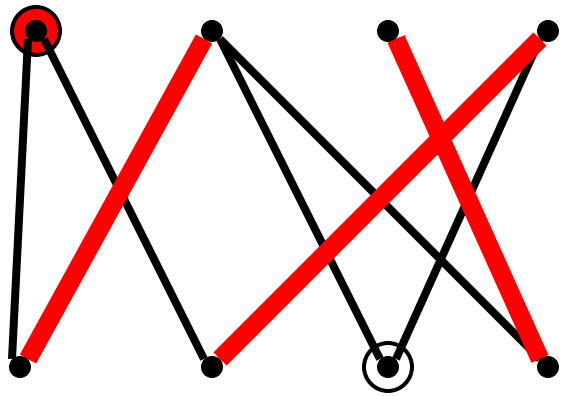

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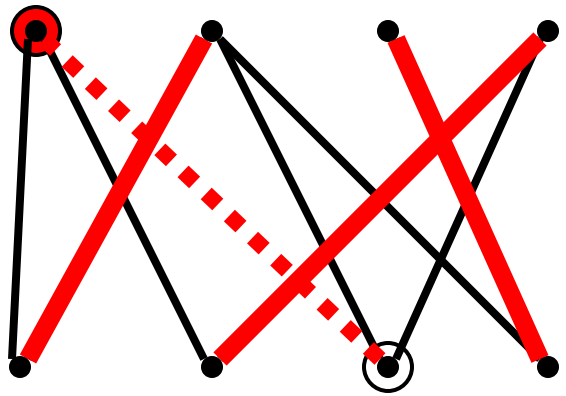

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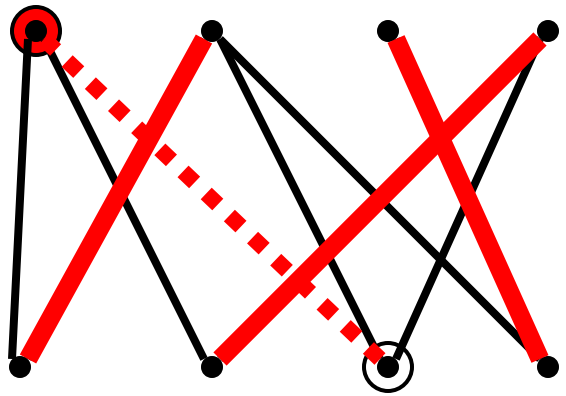

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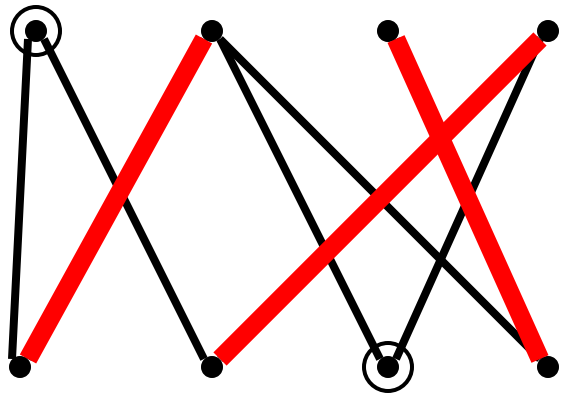

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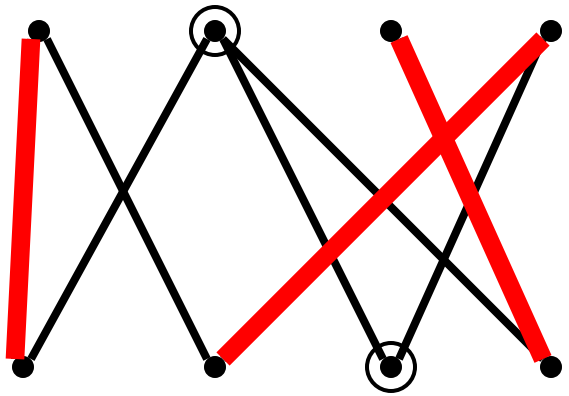

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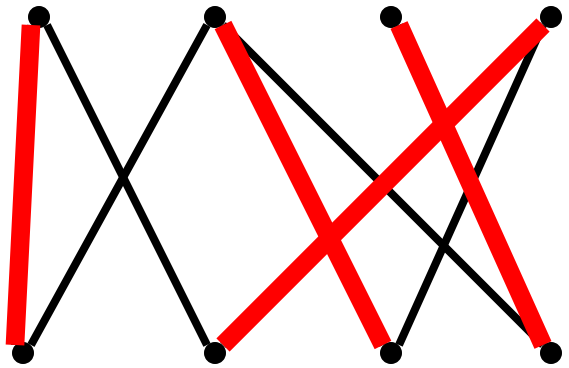

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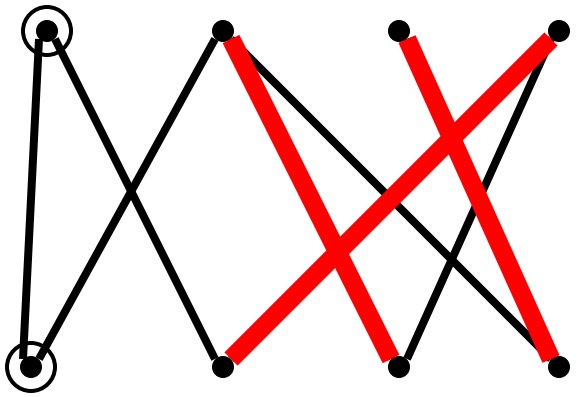

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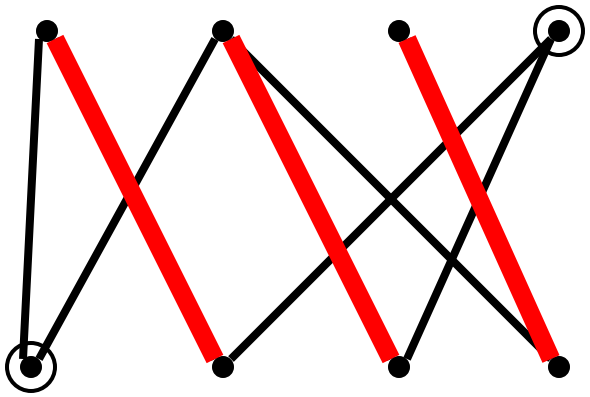

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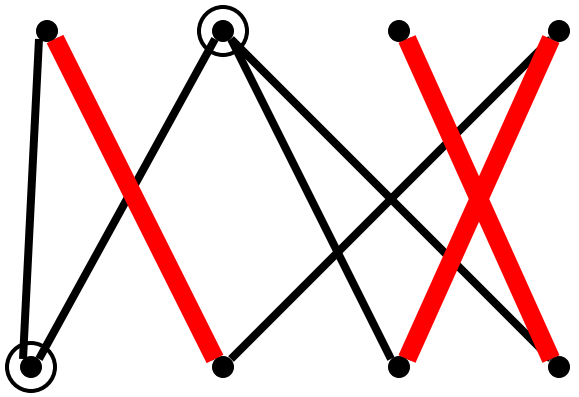

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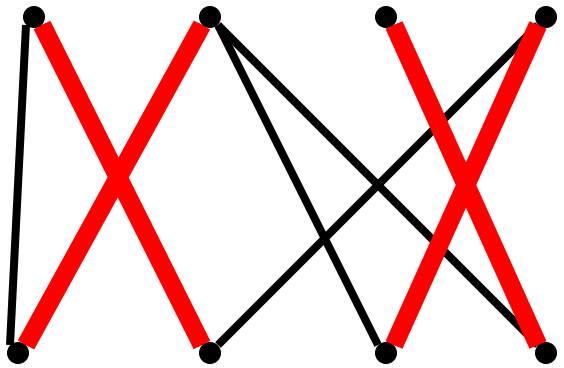

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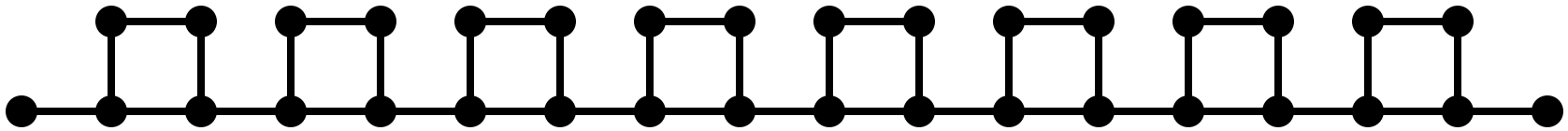
Even if it did...



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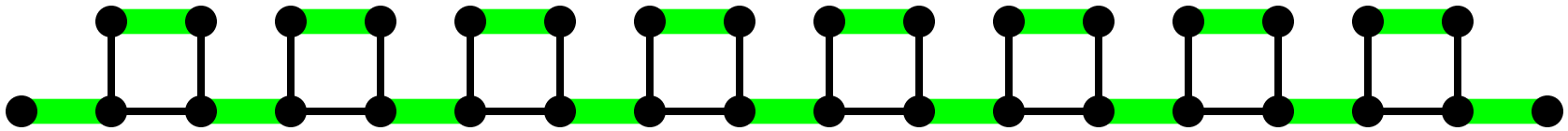

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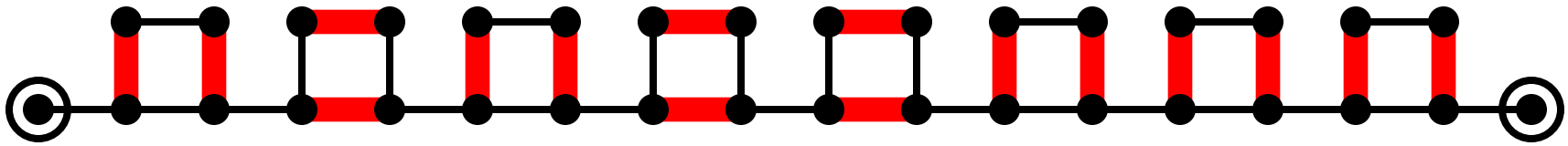
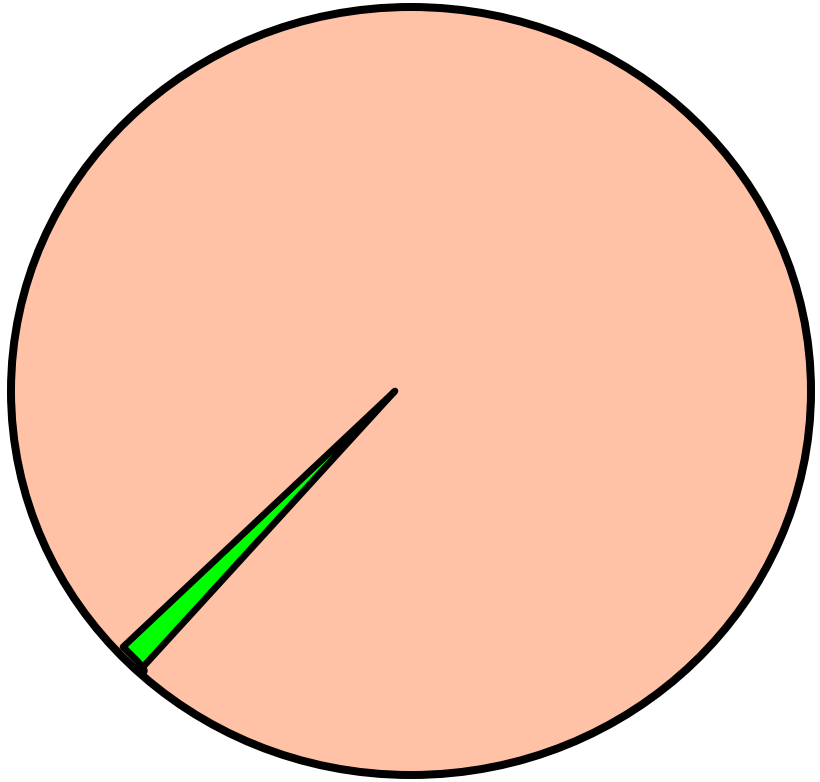


1 perfect matching

$\geq 2^{(n/4)}$ near matchings



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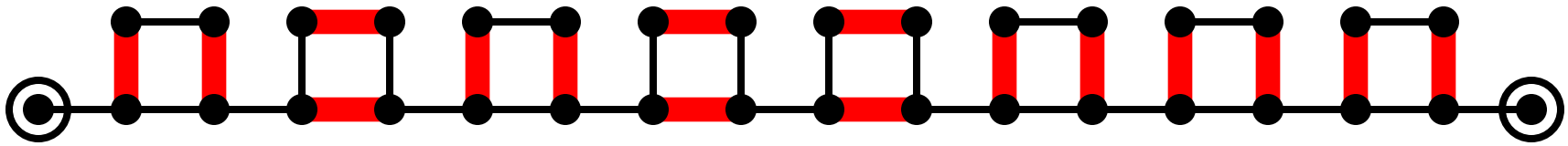

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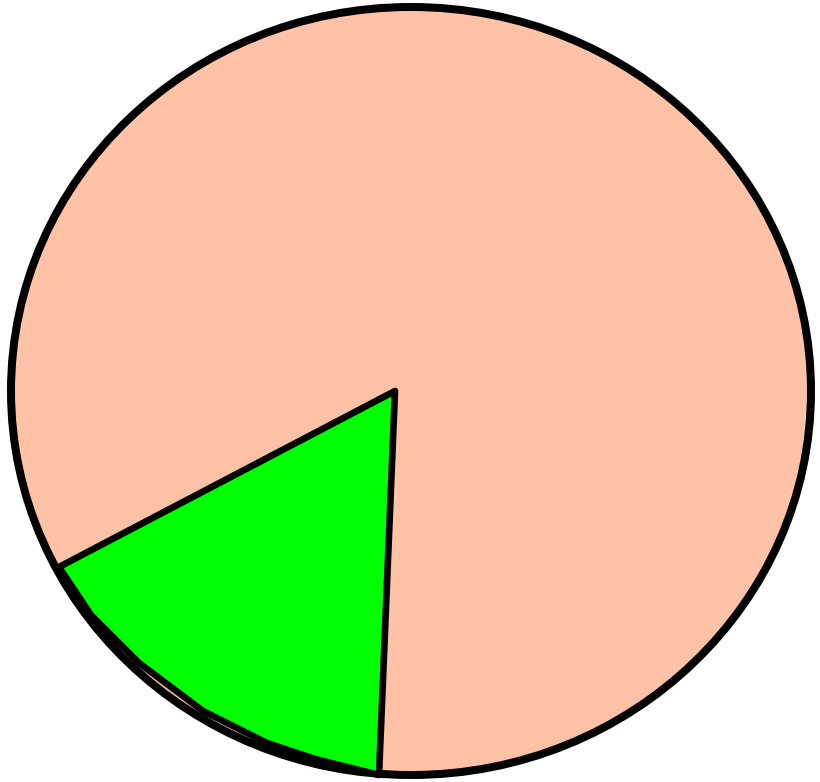


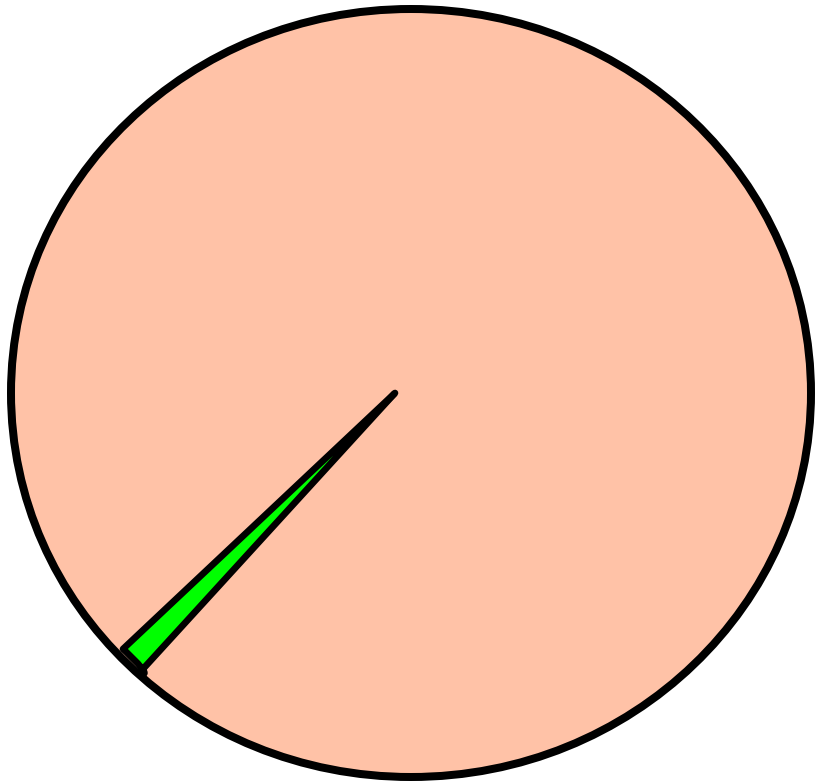
Thm [Jerrum-Sinclair '89]:

Rapid mixing if perfects **polynomially** related to nears.

Broder Chain

Idea [Jerrum-Sinclair-Vigoda '01]:

Change the **weight** so that **perfect matchings** take **polynomial** fraction.



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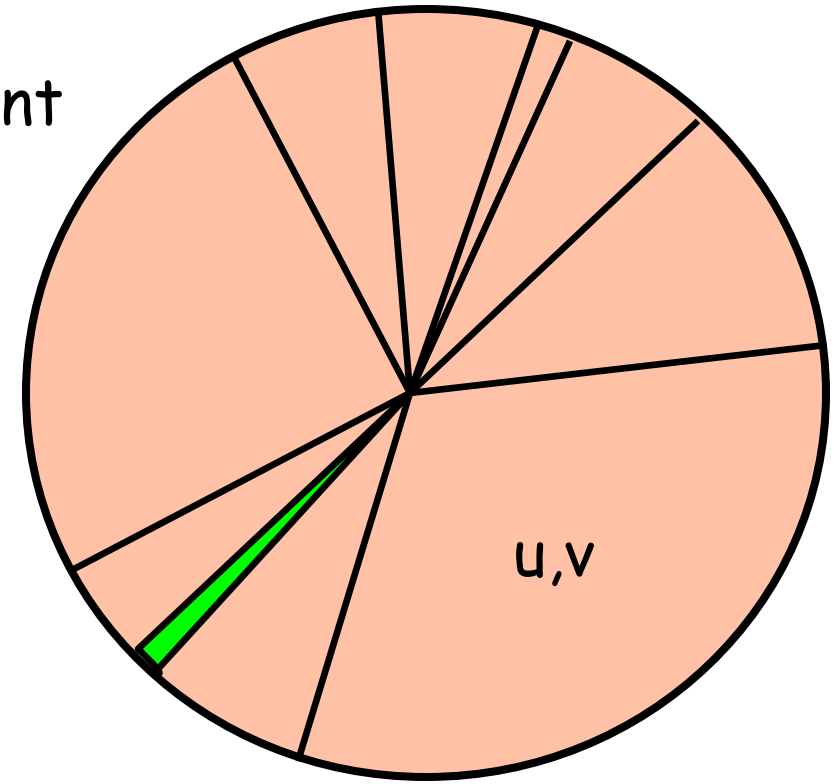
n^2+1 regions, very different size



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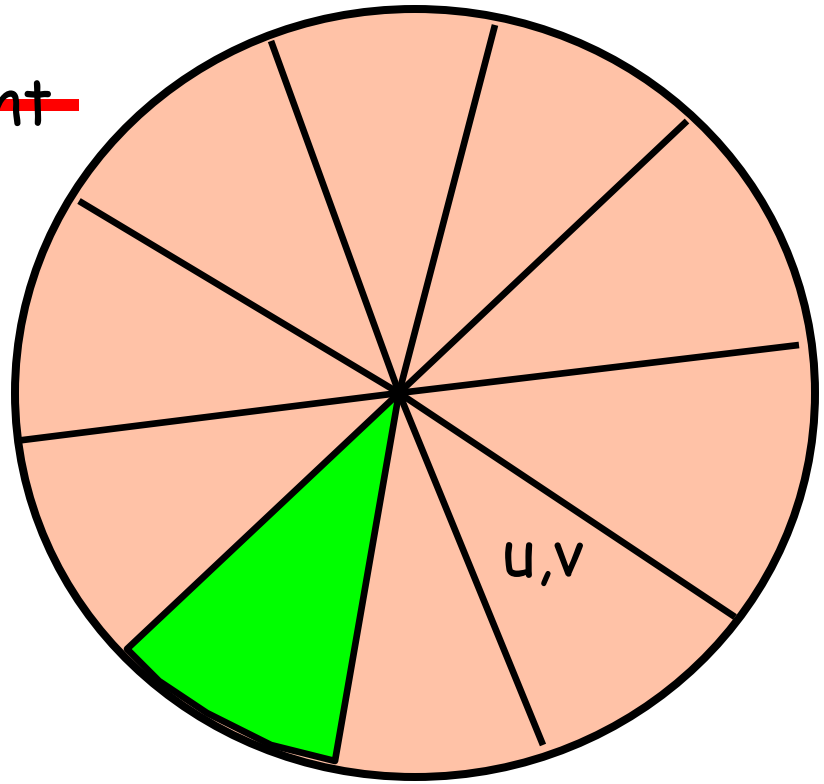

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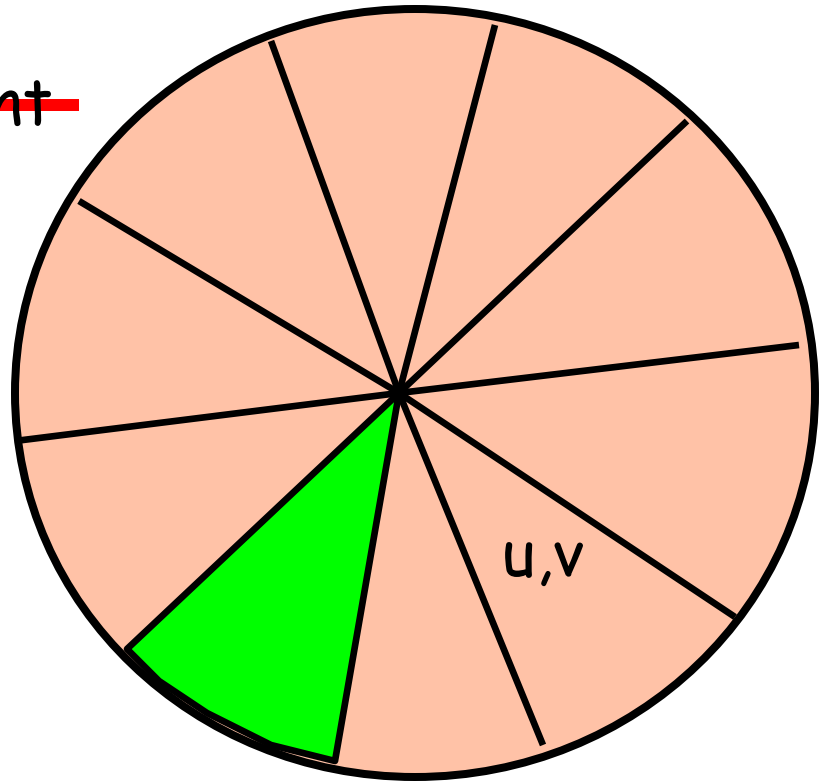

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(for a matching with holes u,v):

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Broder Chain

Good: A perfect matching sampled with prob. $1/(n^2+1)$

Bad: Computing ideal weights as hard as original problem ?

Solution: **Approximate**

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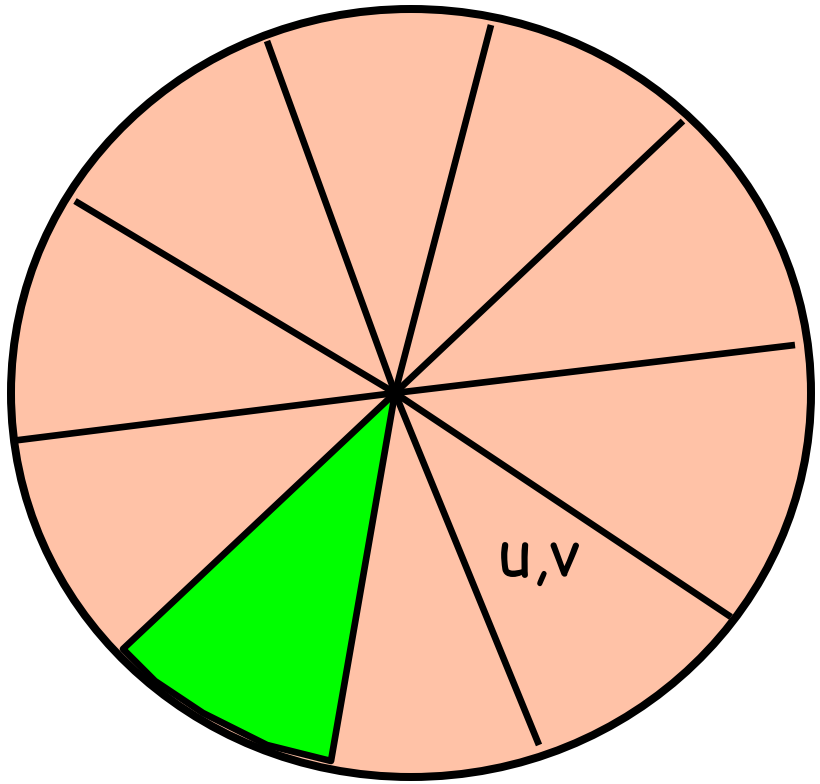

Simulated Annealing for Permanent

Unordered state → Ordered state

(EASY) (DIFFICULT)

G

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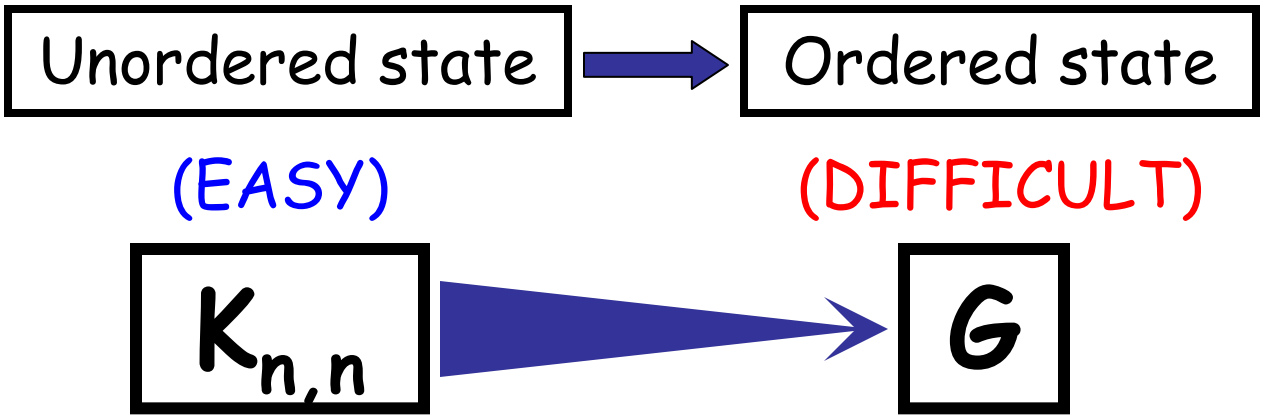

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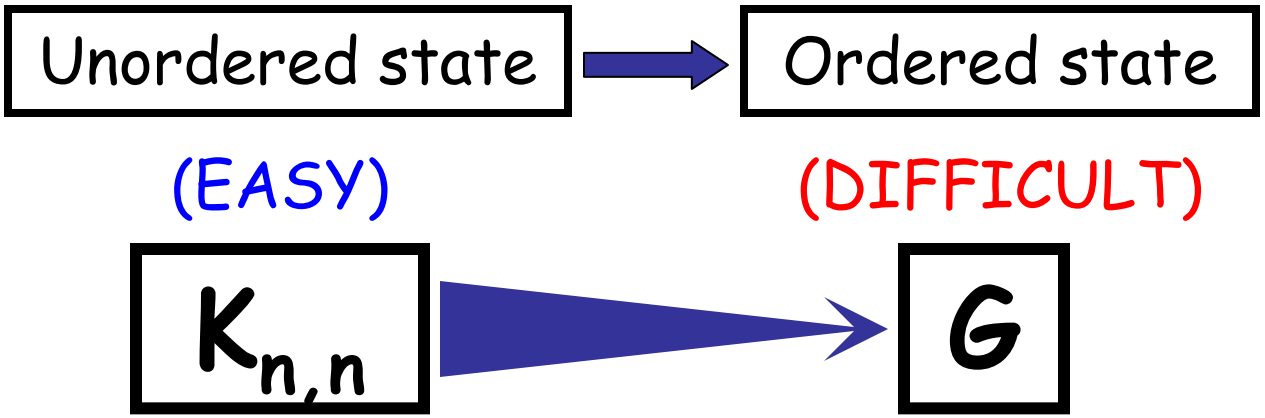

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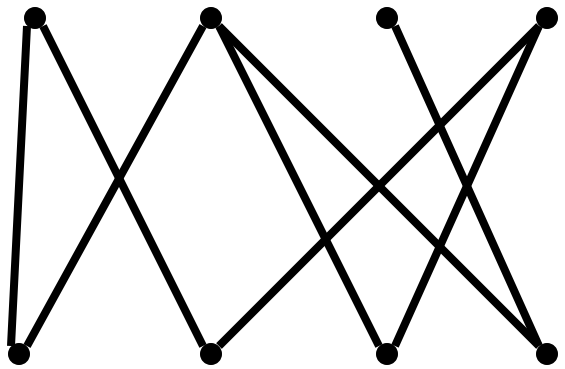

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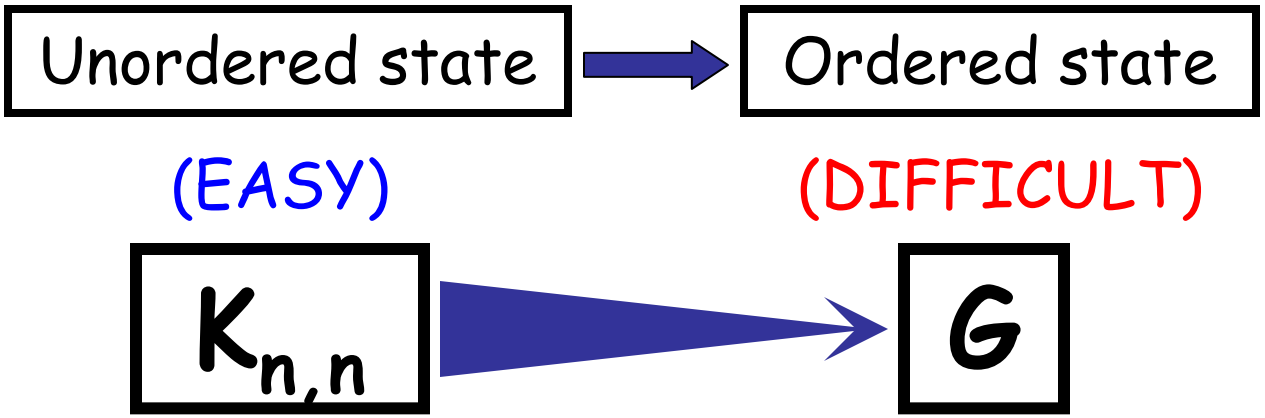

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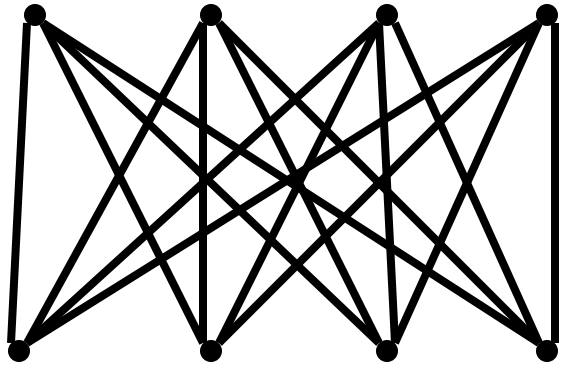

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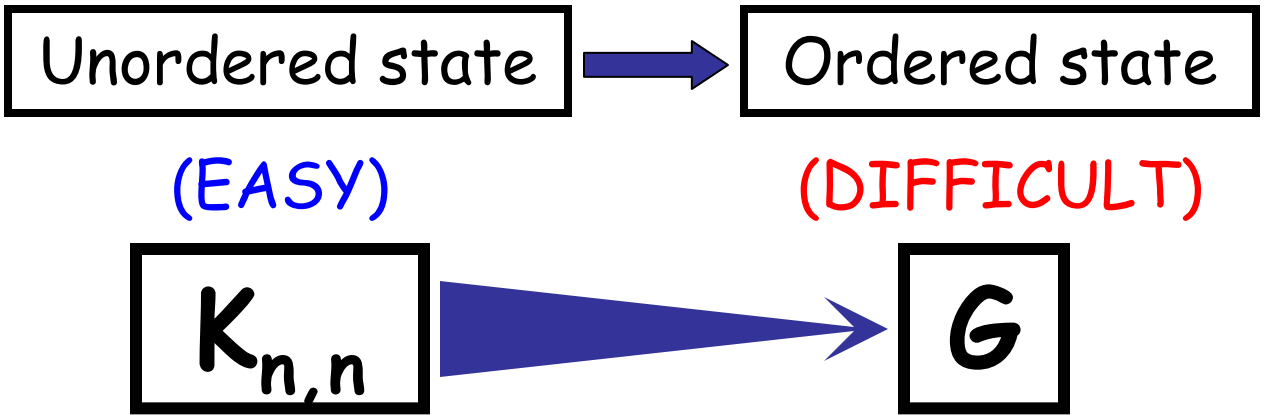

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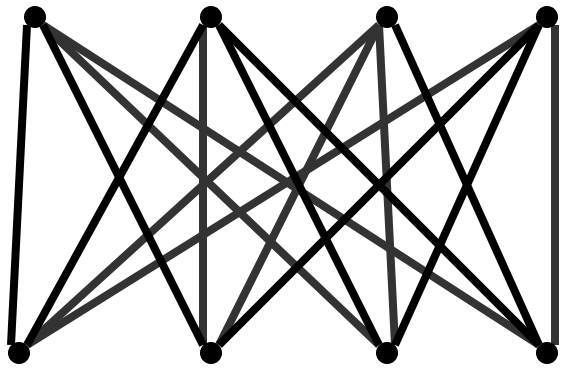

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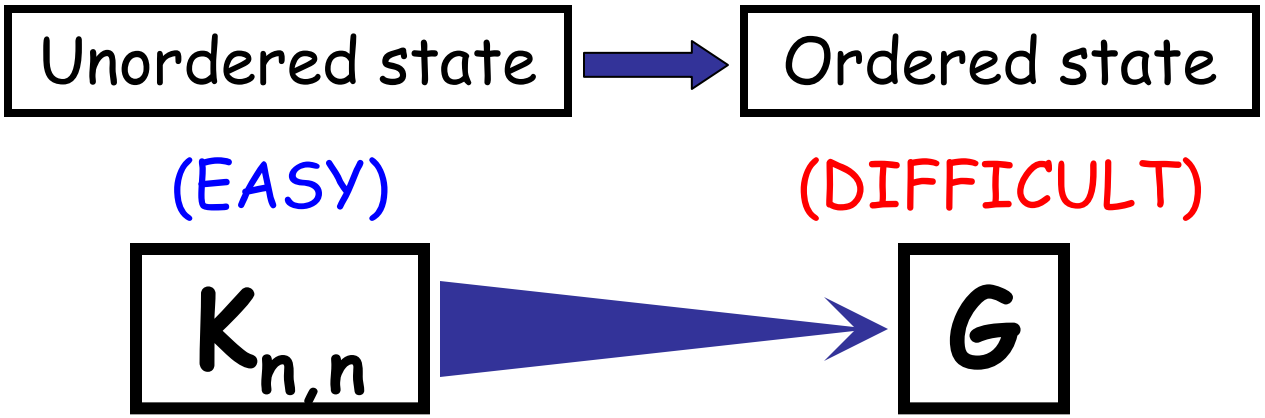

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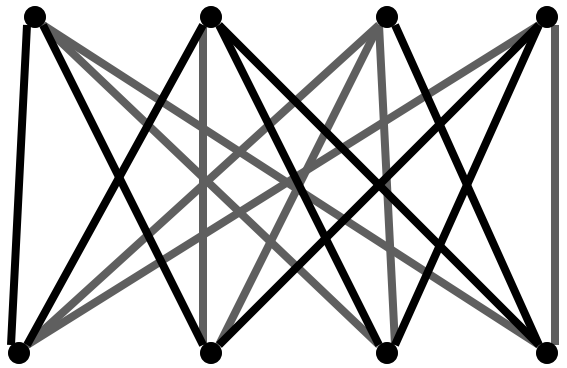

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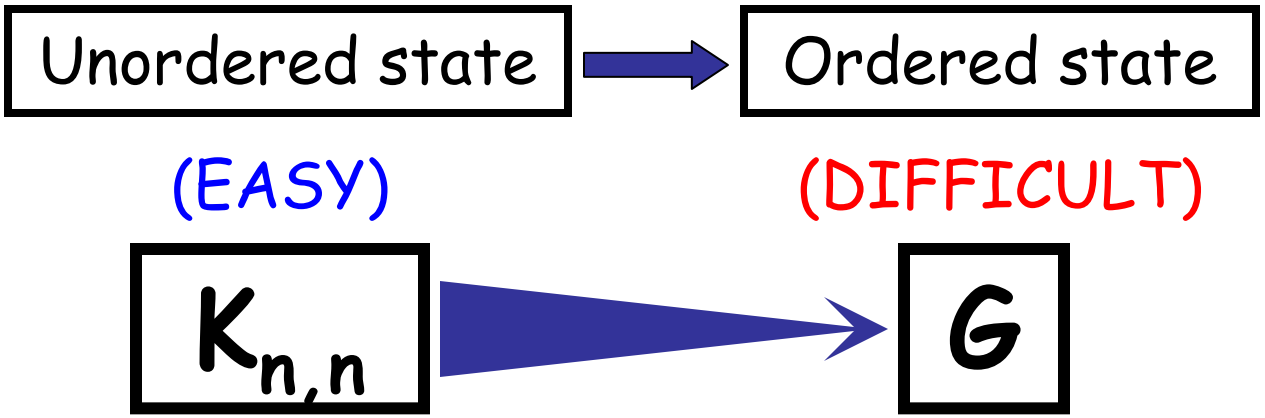

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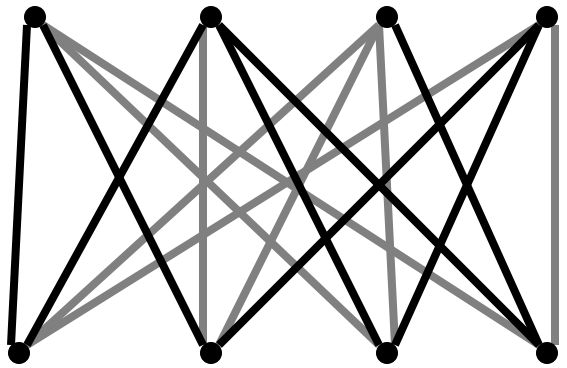

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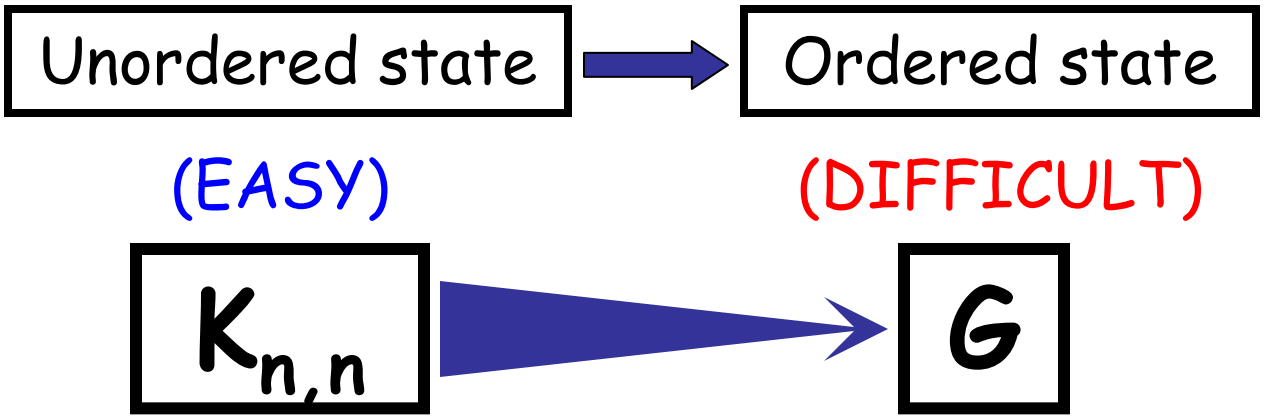

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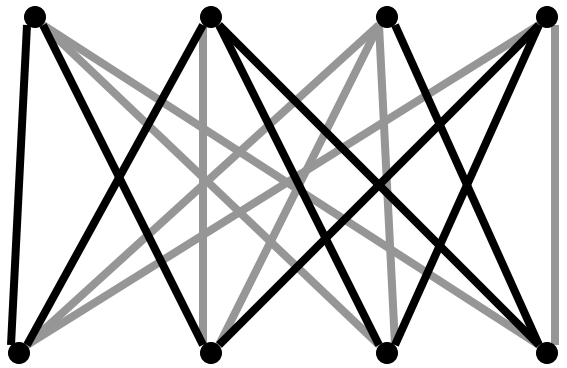

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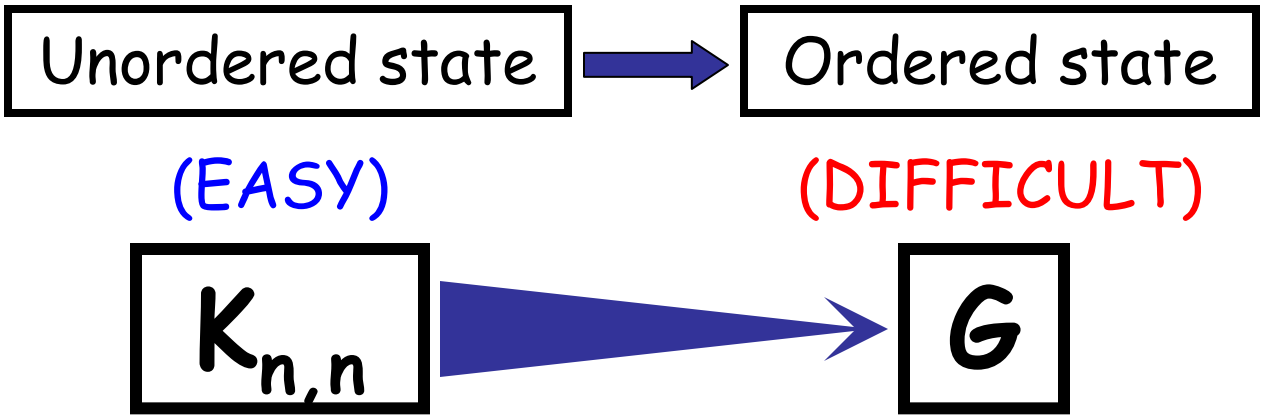

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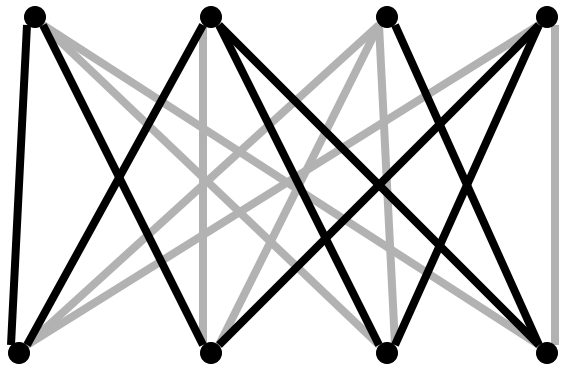
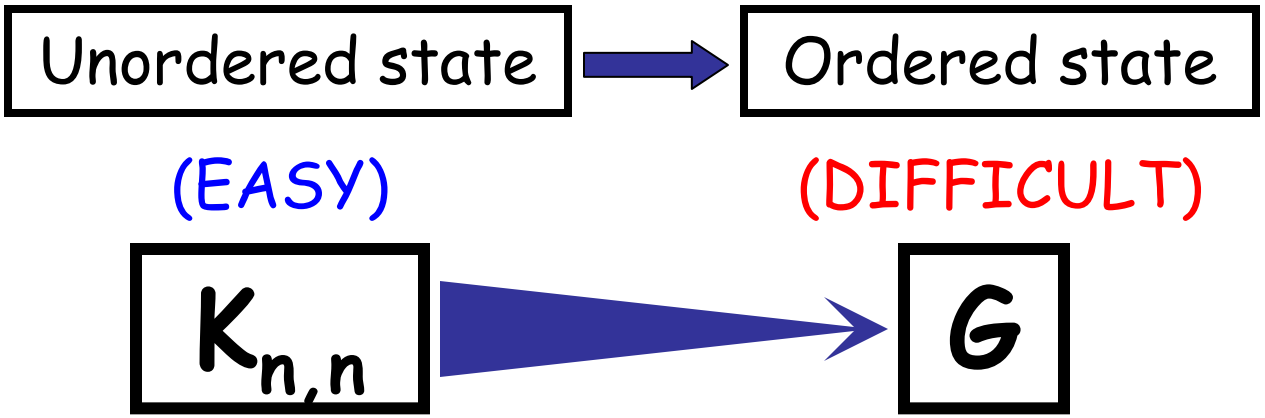
(for a matching with holes u,v):

$$\frac{\text{(\# perfects)}}{\text{(\# nears with holes u,v)}}$$



Simulated Annealing for Permanent



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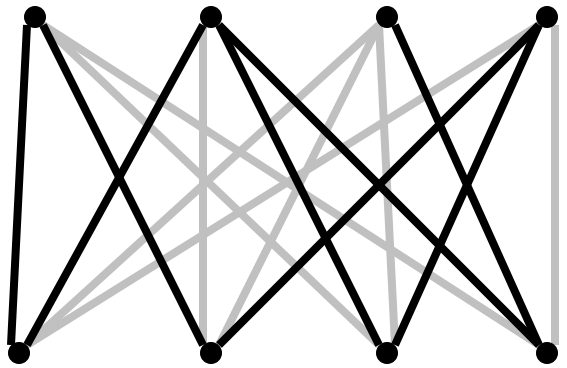

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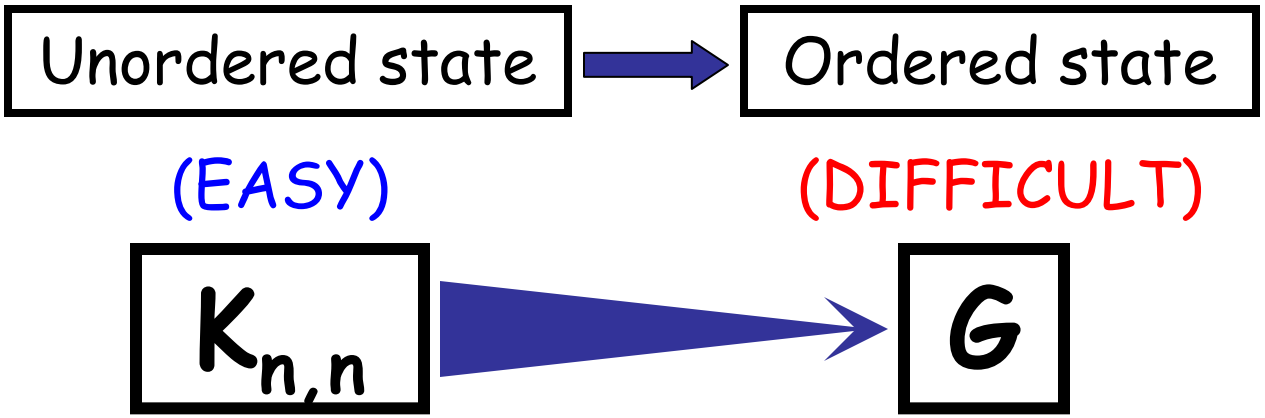

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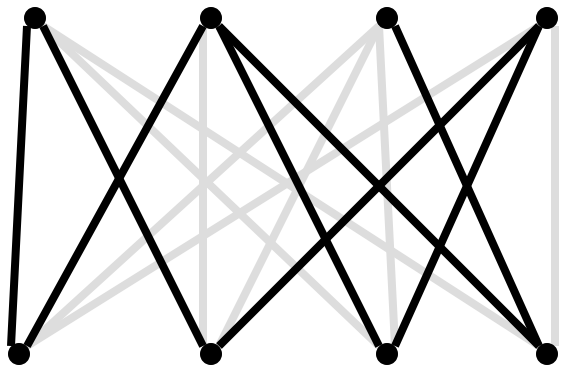

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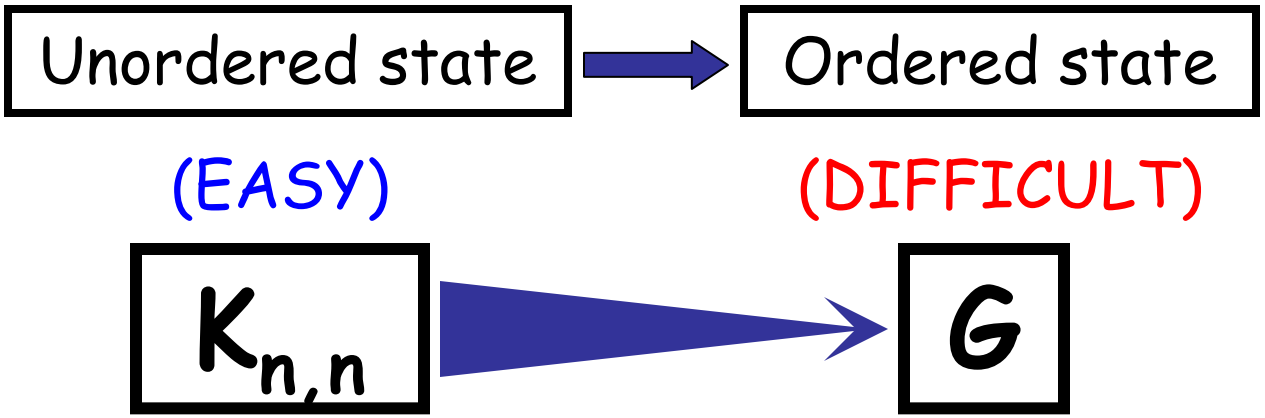

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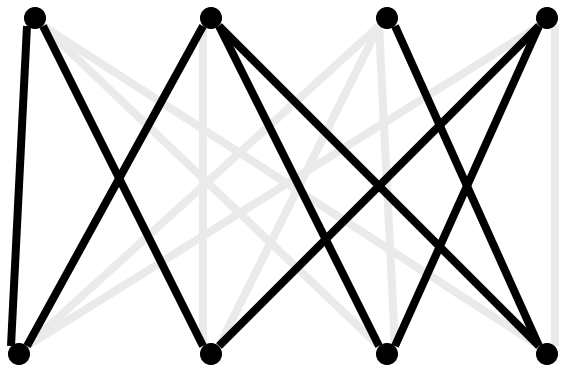

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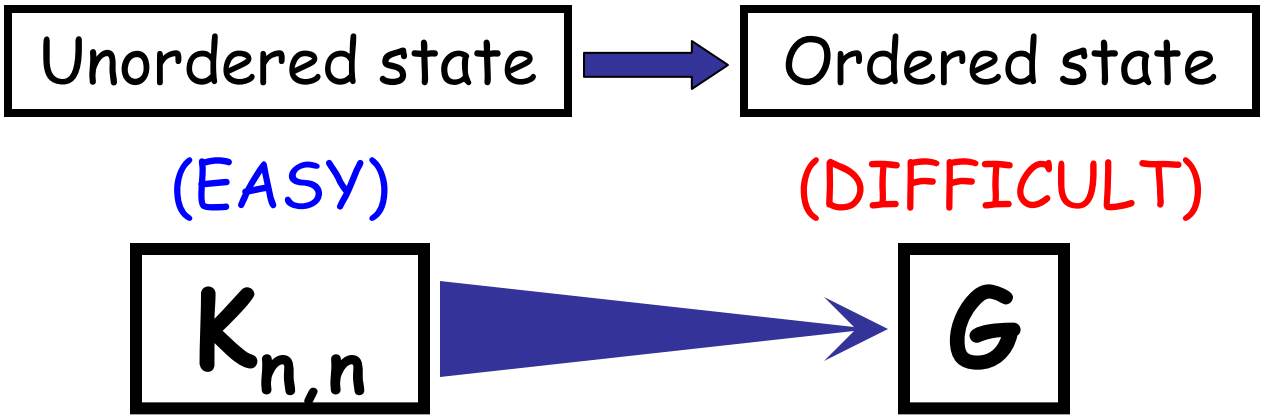

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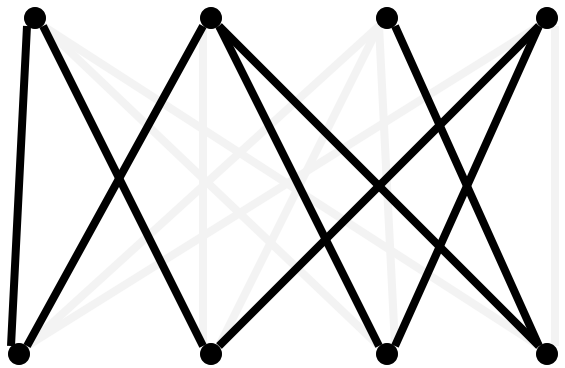

Simulated Annealing for Permanent

Unordered state → Ordered state

(EASY) (DIFFICULT)

$K_{n,n}$ → G

Solution: **Approximate**

Ideal weights
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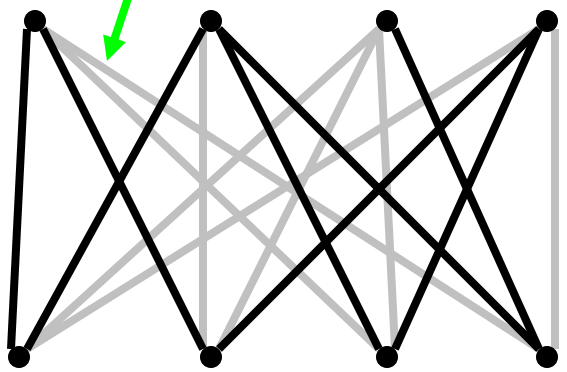
λ = 1 ... ~0



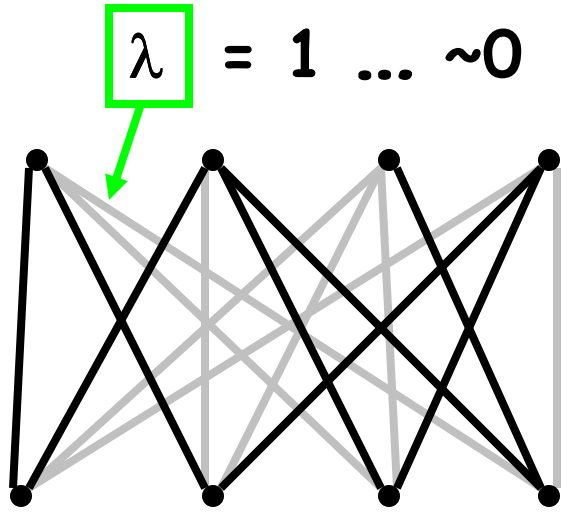
New Cooling Schedule

[Bezáková-Štefankovič-
Vazirani-Vigoda SODA '06]

$$\frac{\text{(\# perfects)}}{\text{(\# nears with holes u,v)}}$$

← ratio of polynomials in λ
(don't know coefficients !)

Want: decrease λ so that **polynomials drop by $\leq$ 2 factor**



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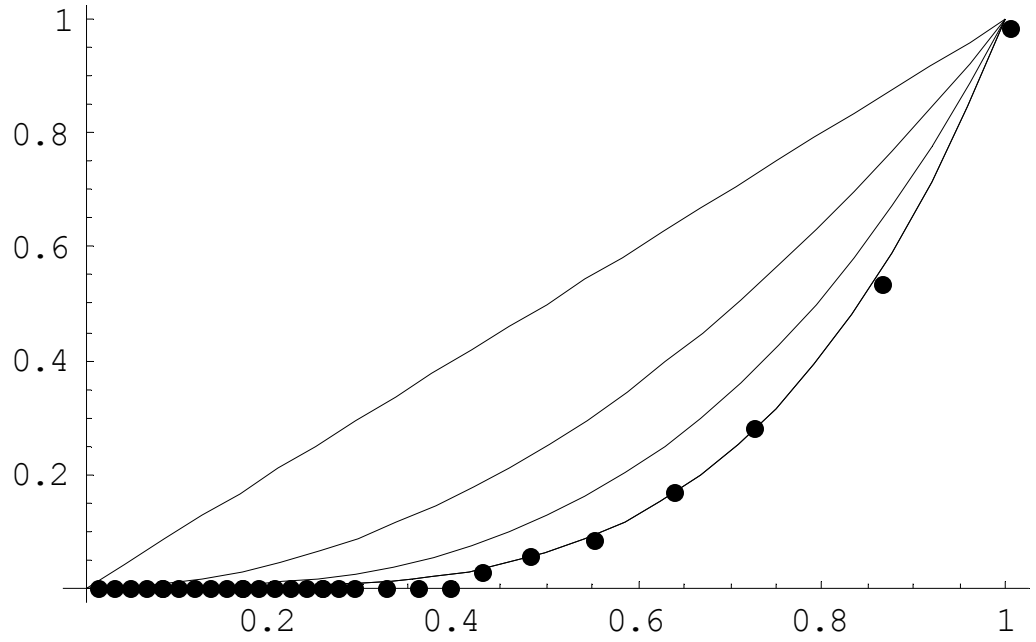
λ^j, **j=1…n**



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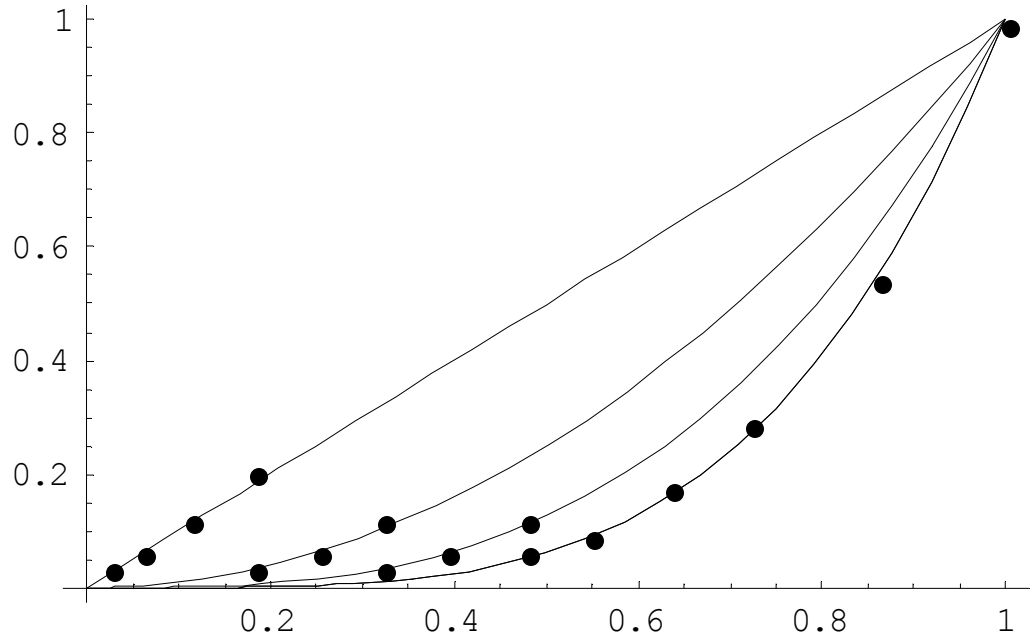
Worst case:

λ^j, **j=1…n**

Idea: make use of low degrees.



New Cooling Schedule

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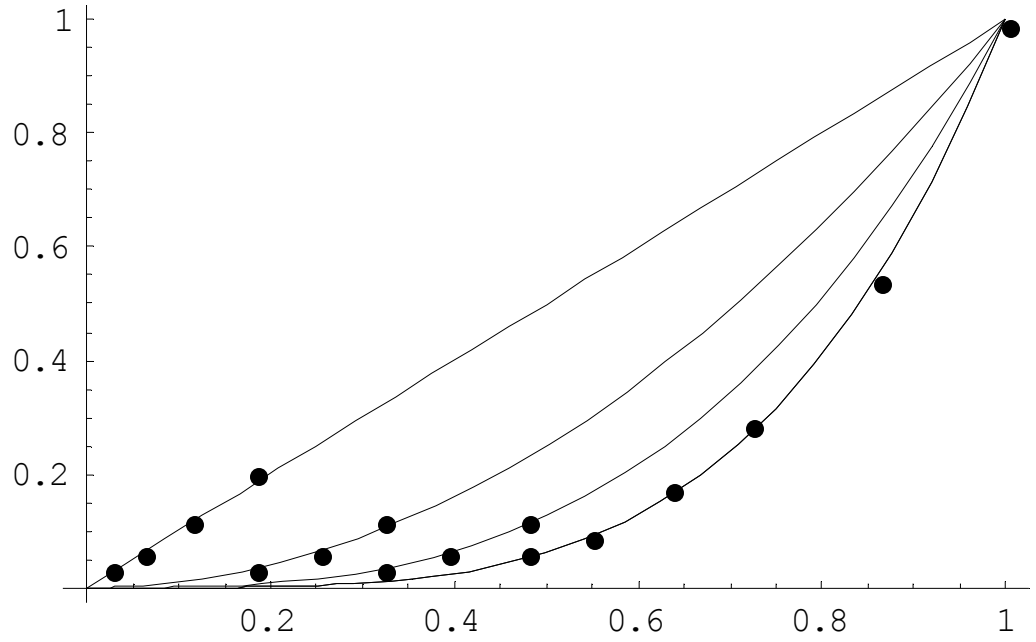
← ratio of polynomials in λ
(don't know coefficients !)

Want: decrease λ so that **polynomials drop by $\leq$ 2 factor**

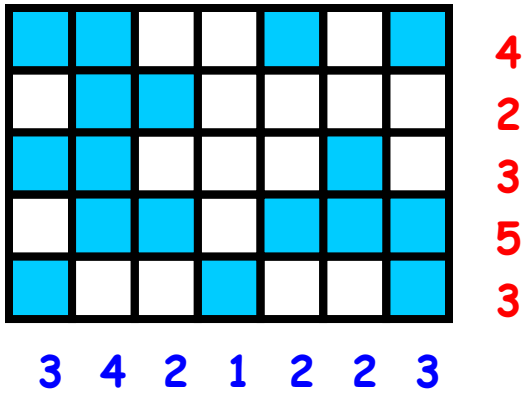
Thm [BŠVV '06]:

Permanent of nonnegative matrix in time $O^*(n^7)$.

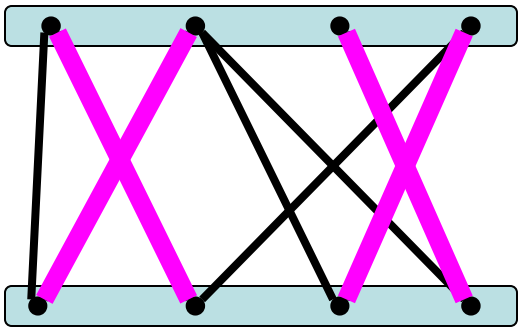


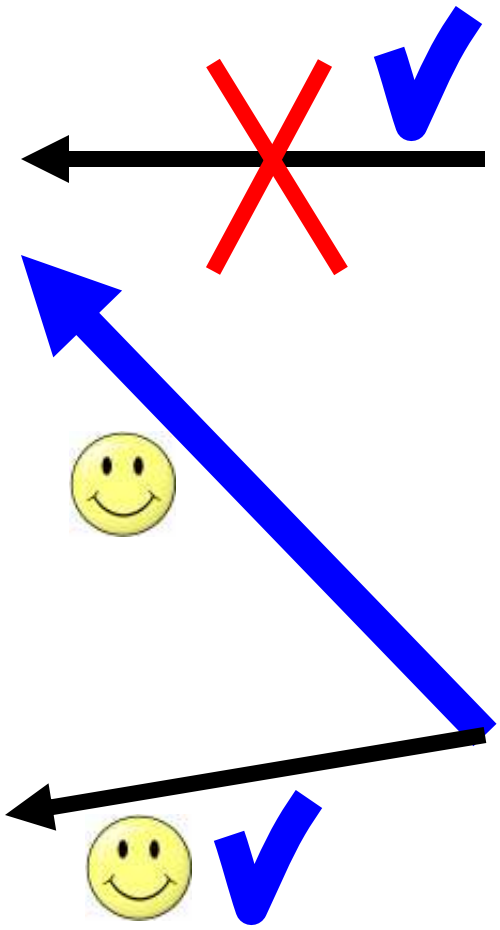
Problems

Binary
contingency tables



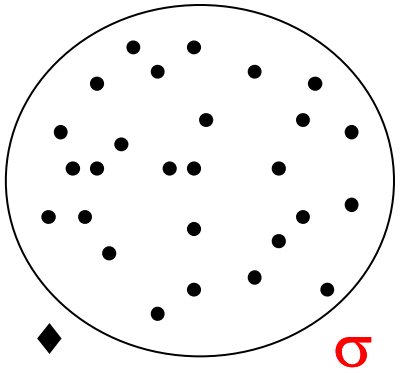
Permanent





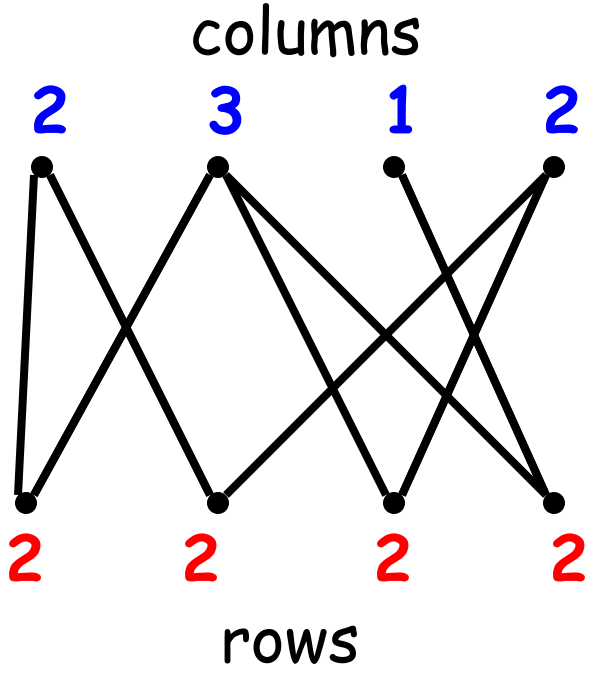
Heuristics

Importance sampling



Simulated annealing

BCT: Bipartite Graphs with Given Degrees



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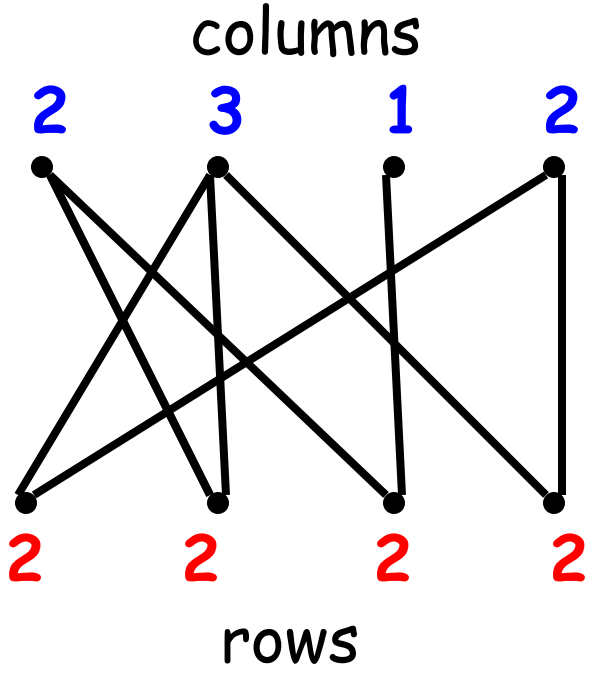
2	3	1	2	

rows

BCT: Bipartite Graphs with Given Degrees



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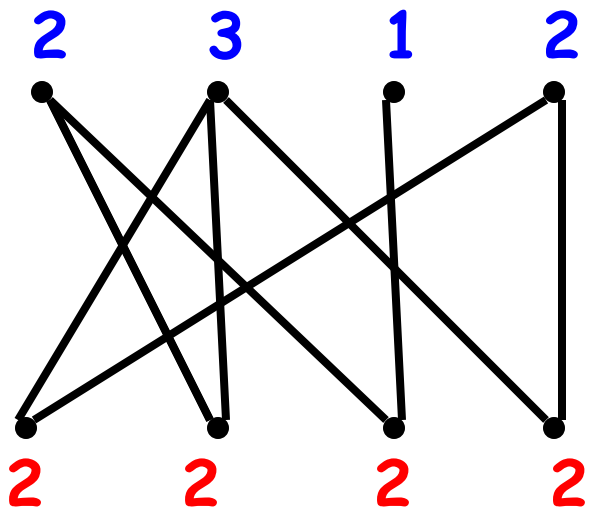

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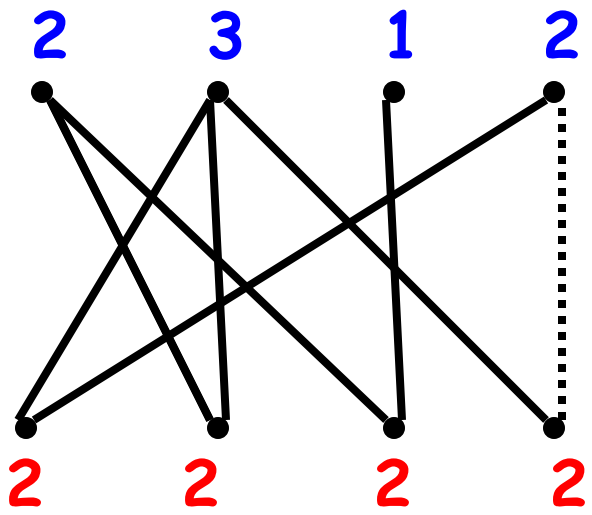
"Sliding" Markov Chain on perfect and near tables

Perfect: remove a random edge

Near: slide edges or match

BCT: Bipartite Graphs with Given Degrees



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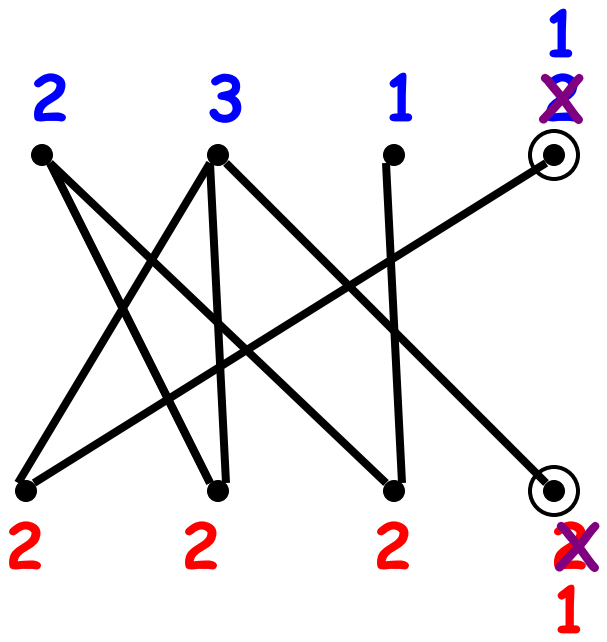

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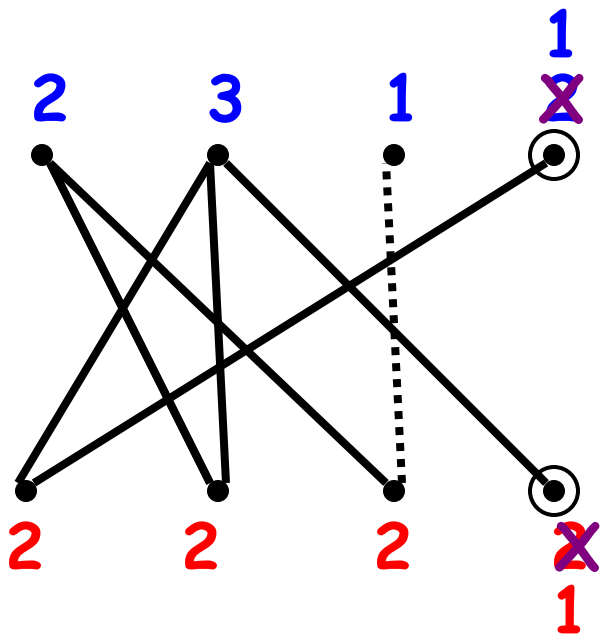

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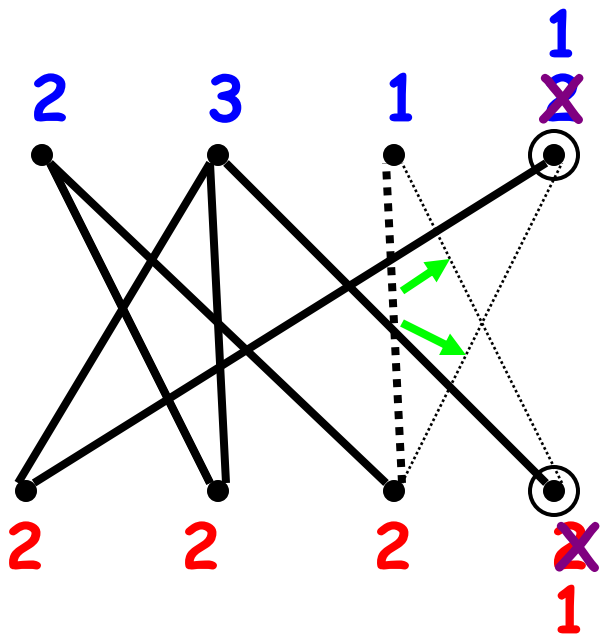

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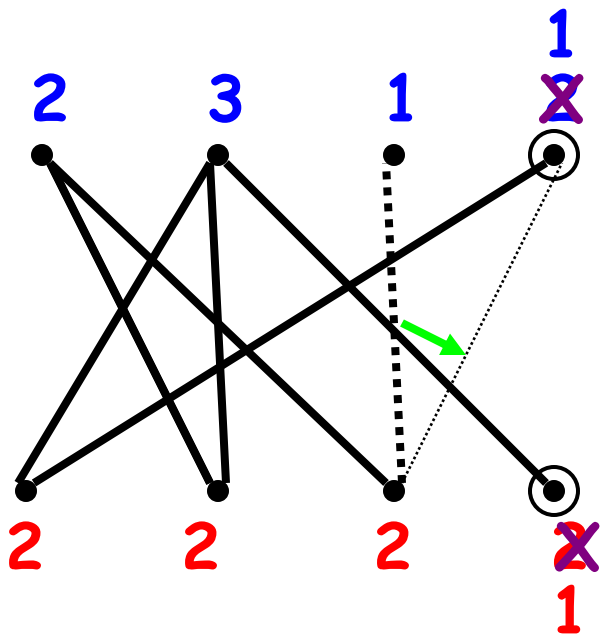

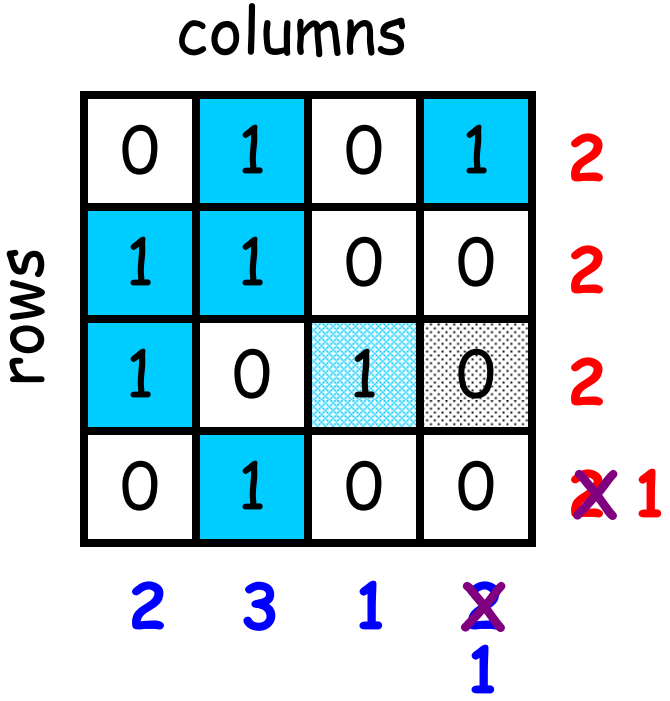

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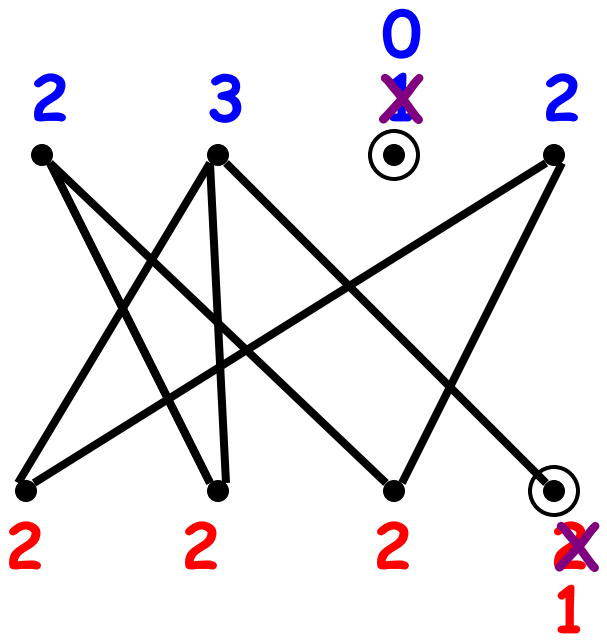

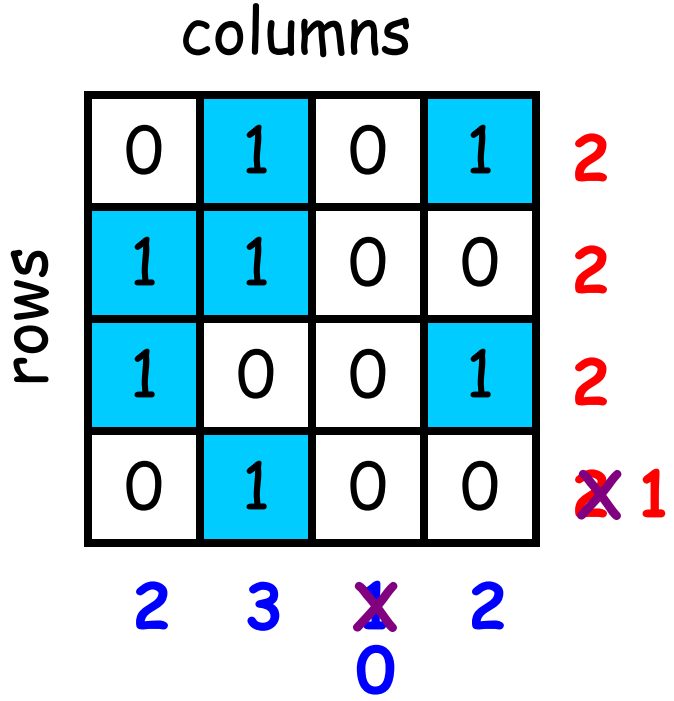

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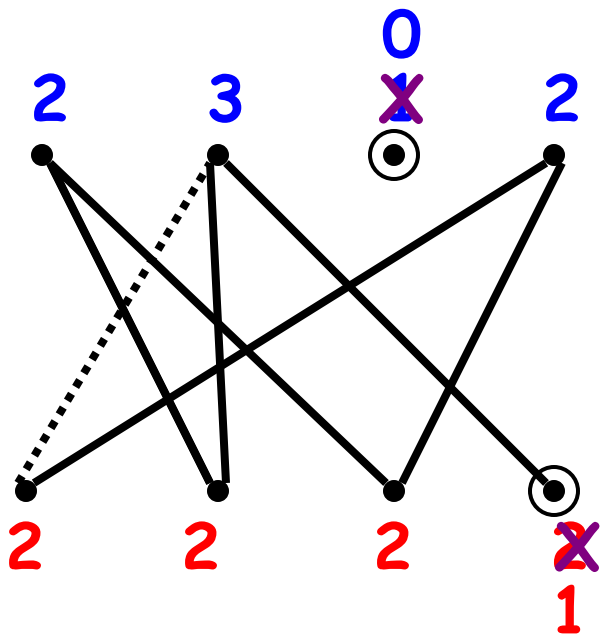

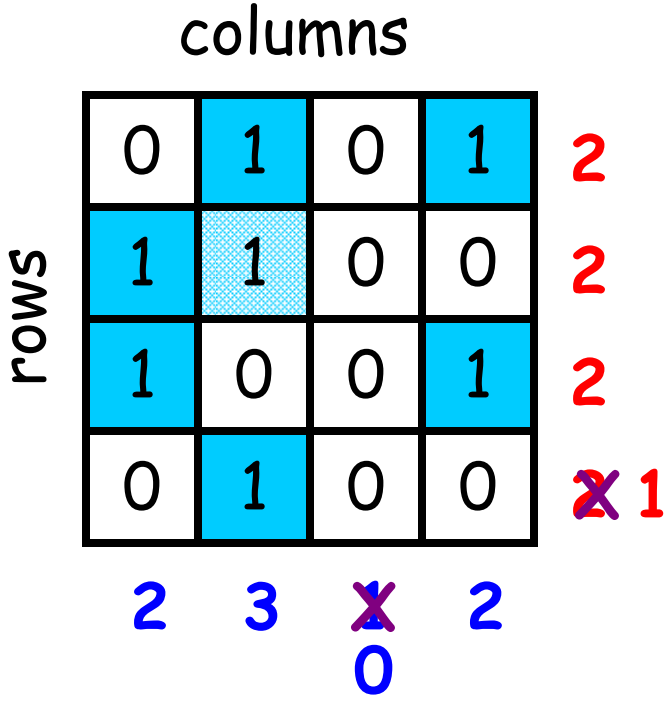

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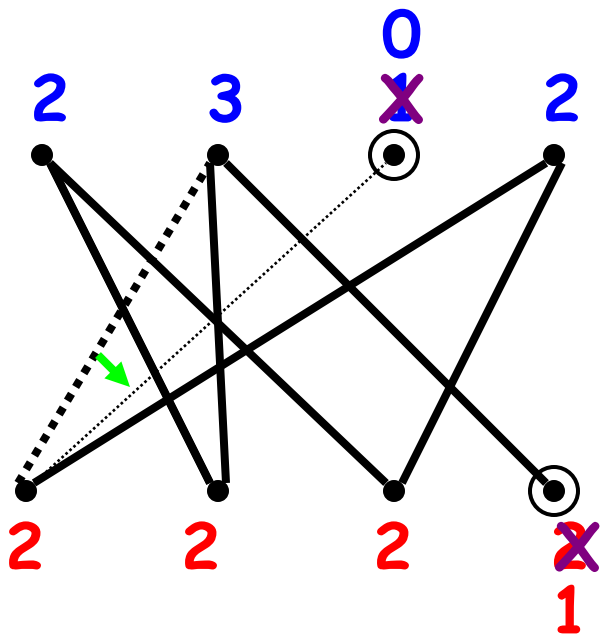

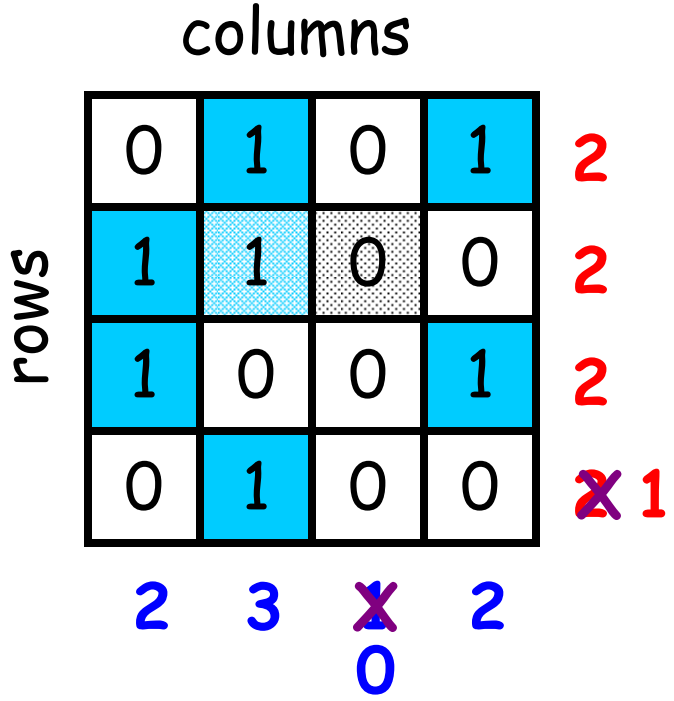

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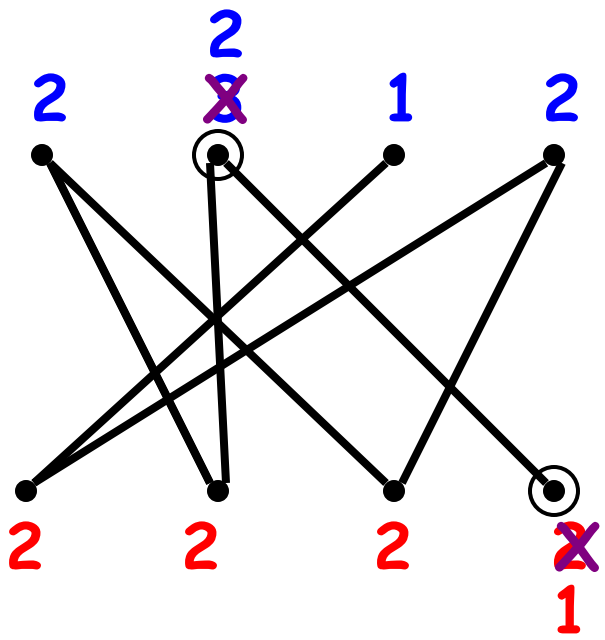

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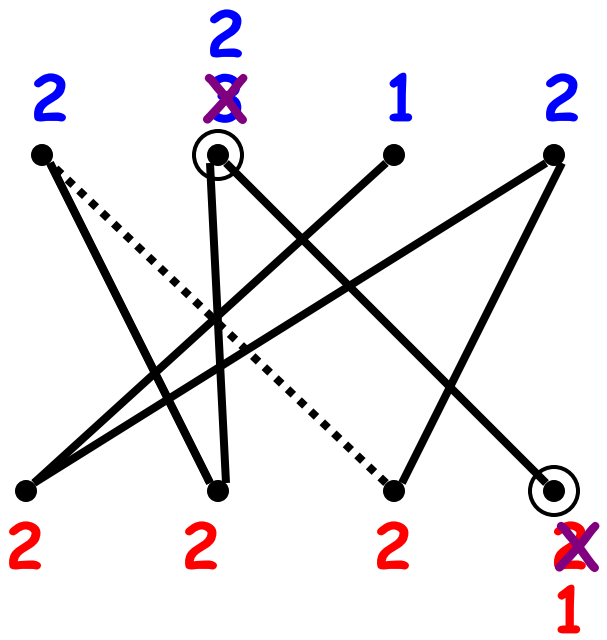

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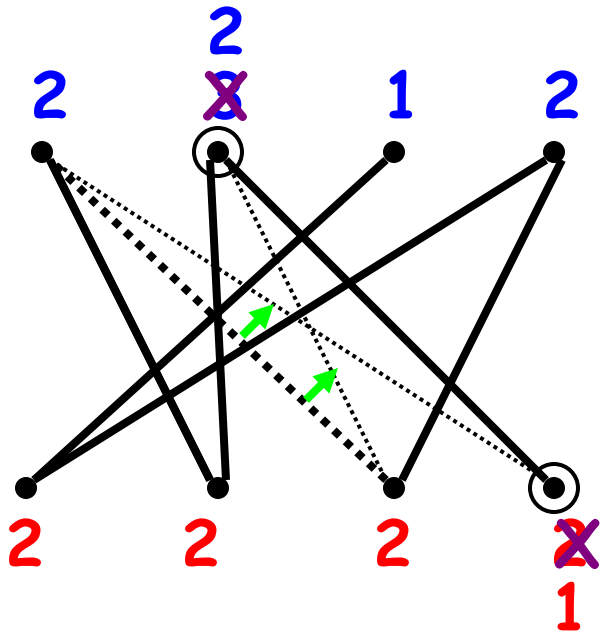

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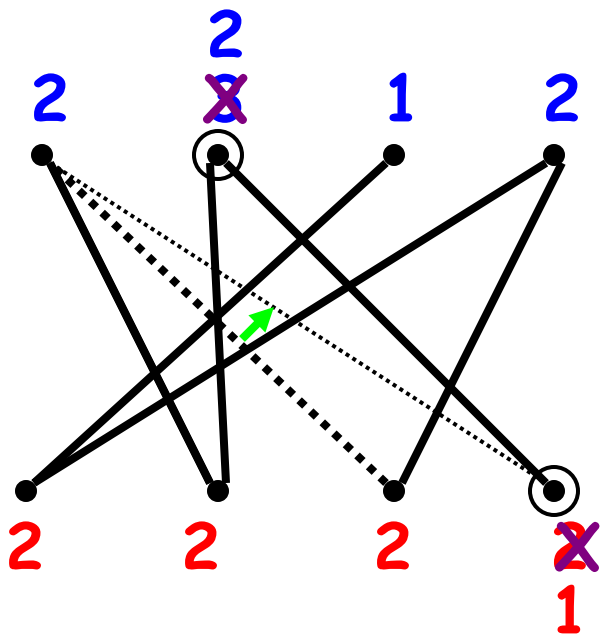

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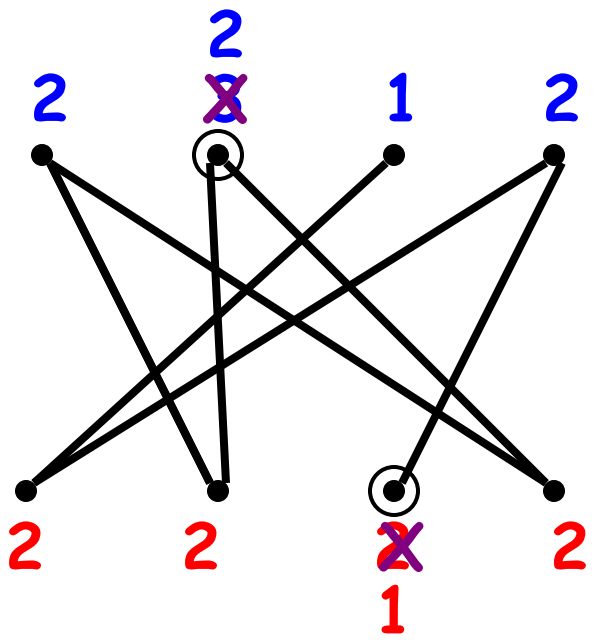

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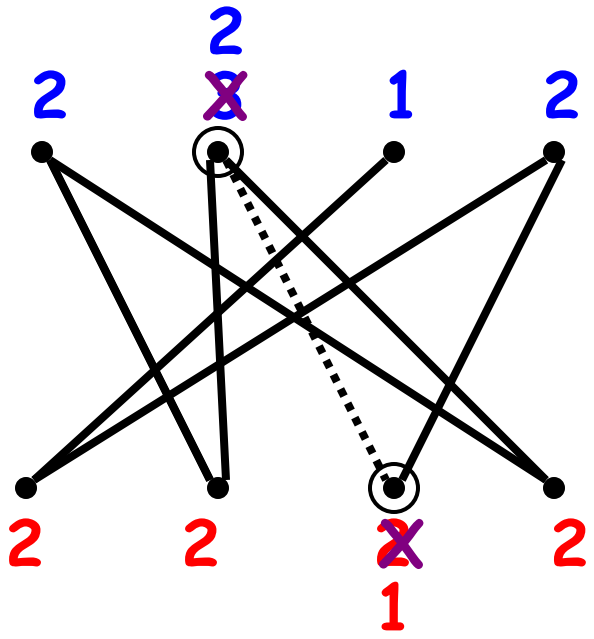

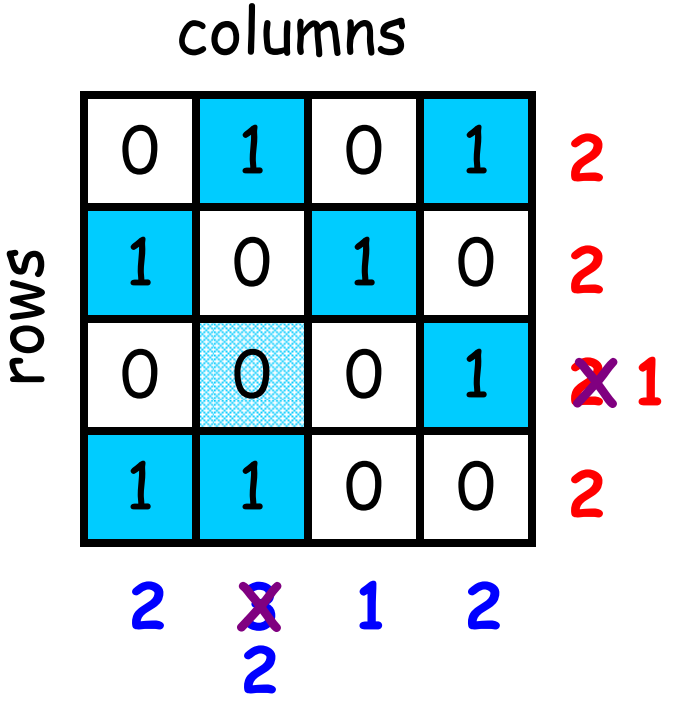

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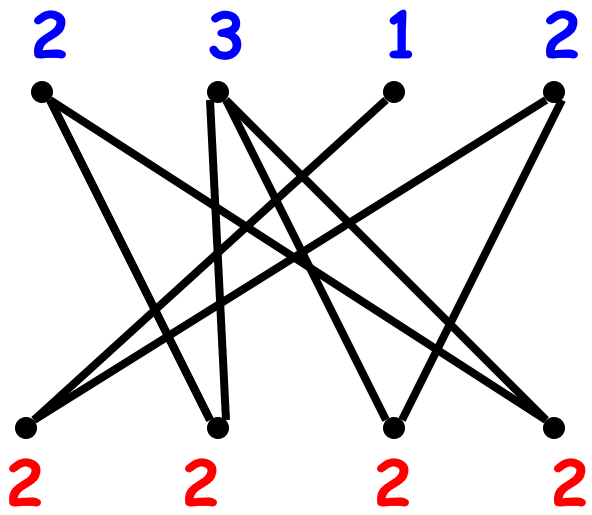

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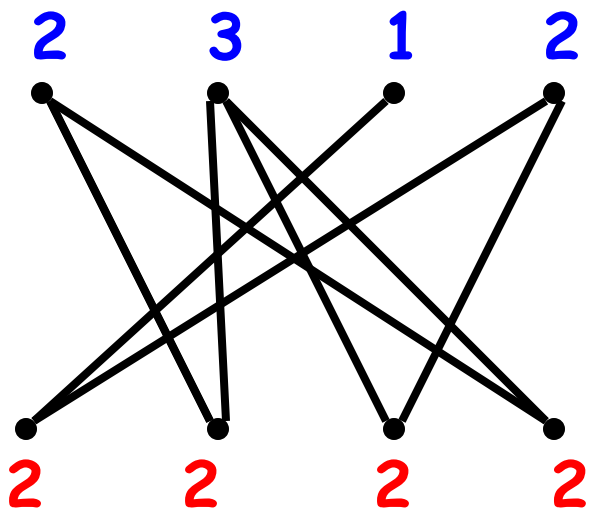
Simulated Annealing for BCT ?

[Bezáková-Bhatnagar-Vigoda SODA '06]

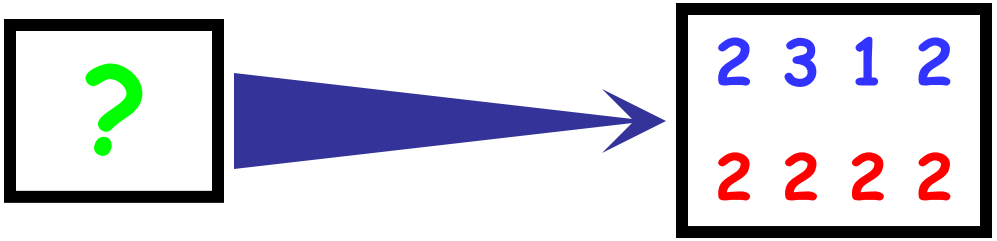


Ideal weights

$$\frac{\text{(\# perfects)}}{\text{(\# nears with holes u,v)}}$$

Unordered state → Ordered state

(EASY) (DIFFICULT)



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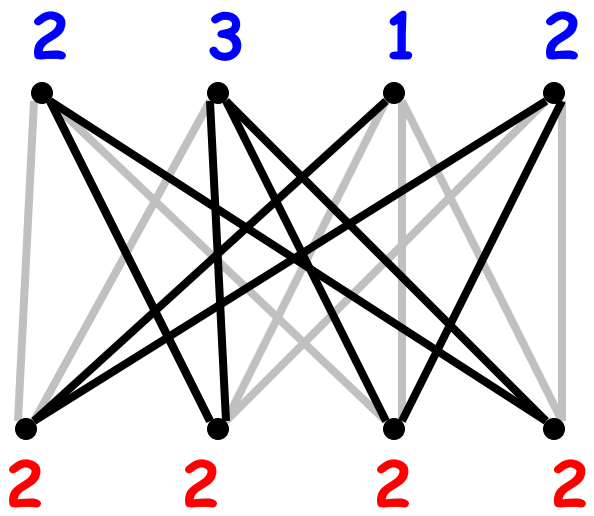
[Bezáková-Bhatnagar-Vigoda SODA '06]



Ideal weights

$$\frac{\text{(\# perfects)}}{\text{(\# nears with holes u,v)}}$$

Unordered state → Ordered state

(EASY) (DIFFICULT)

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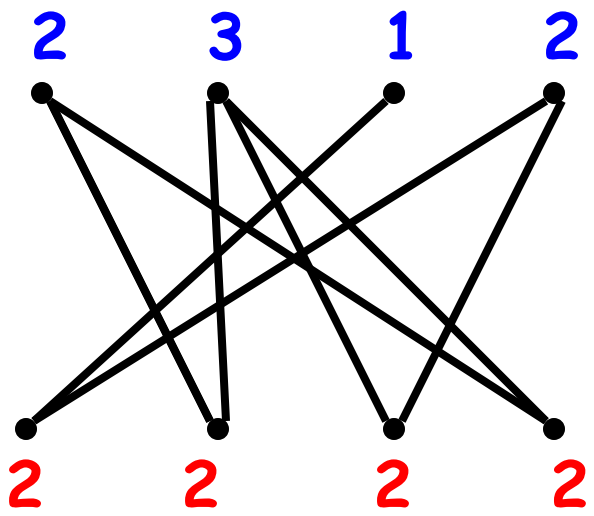

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(EASY) (DIFFICULT)

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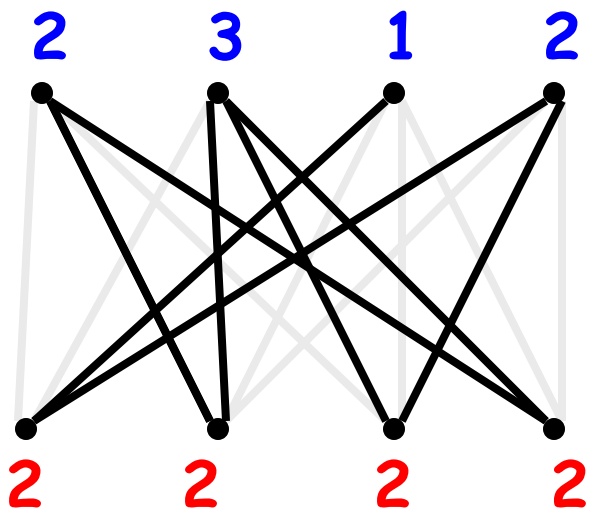

Thm [BBV '06]:

G* s.t. between any two vertices exists an "alternating" path of length $\leq$ **5**.

Unordered state → Ordered state

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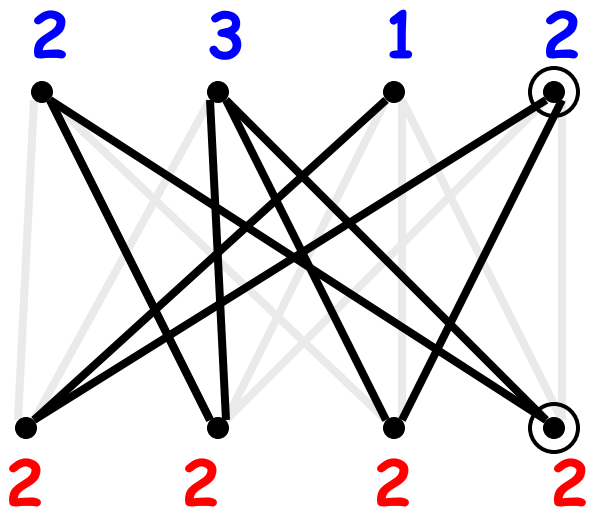

Thm [BBV '06]:

G^* s.t. between any two vertices exists an "alternating" path of length ≤ 5.

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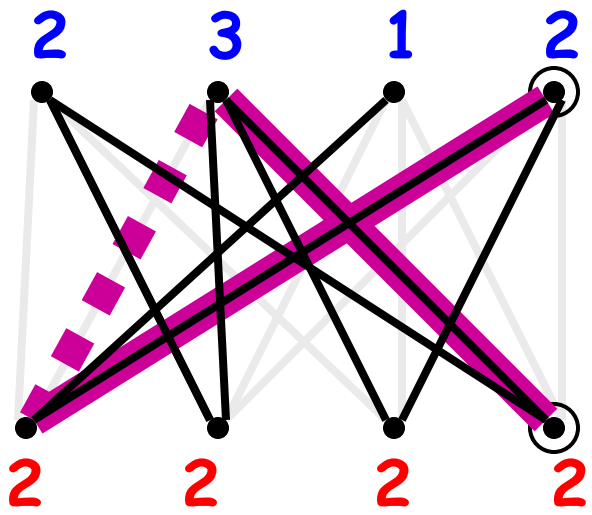

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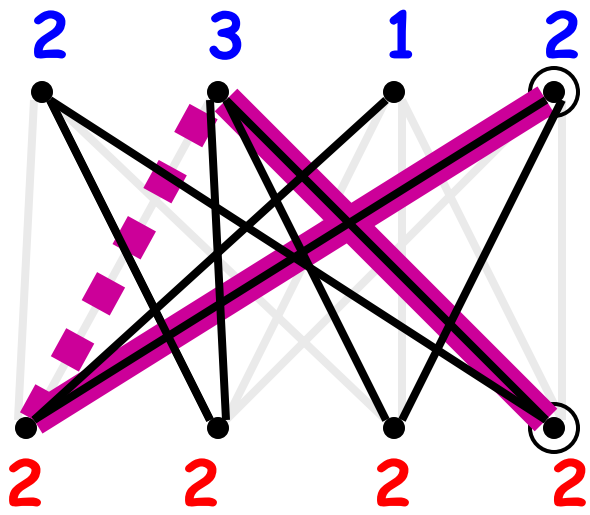

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Counting **subgraphs** (of a bipartite graph) **with given degrees** in poly-time.

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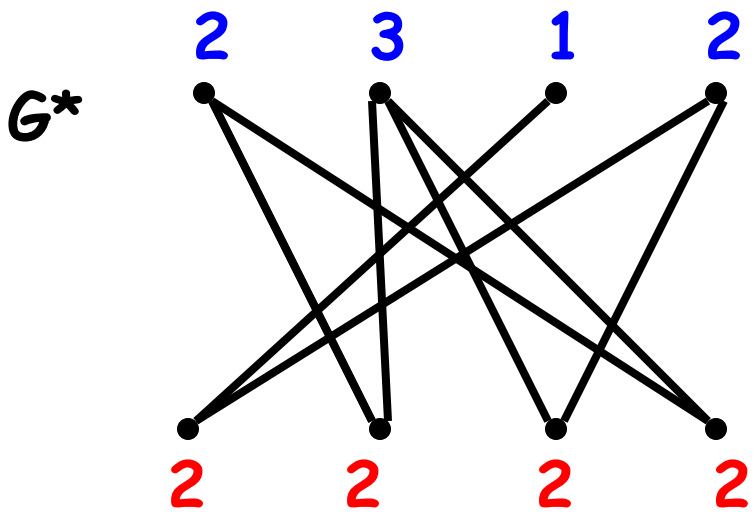
[Bezáková-Bhatnagar-Vigoda SODA '06]



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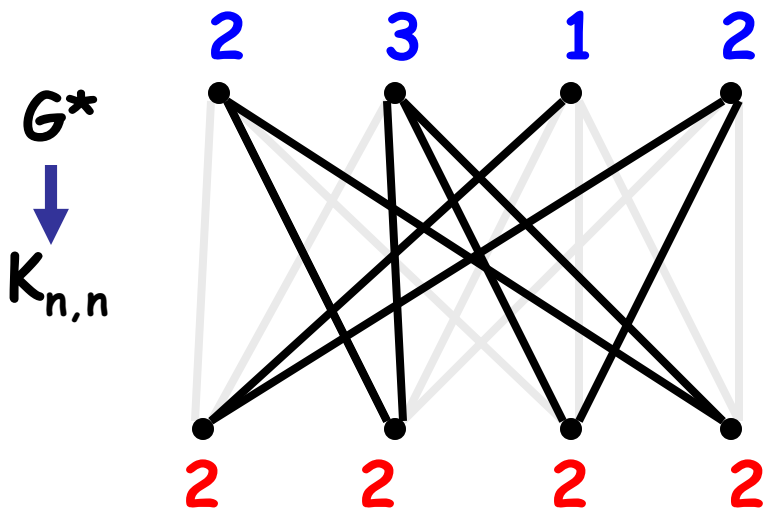

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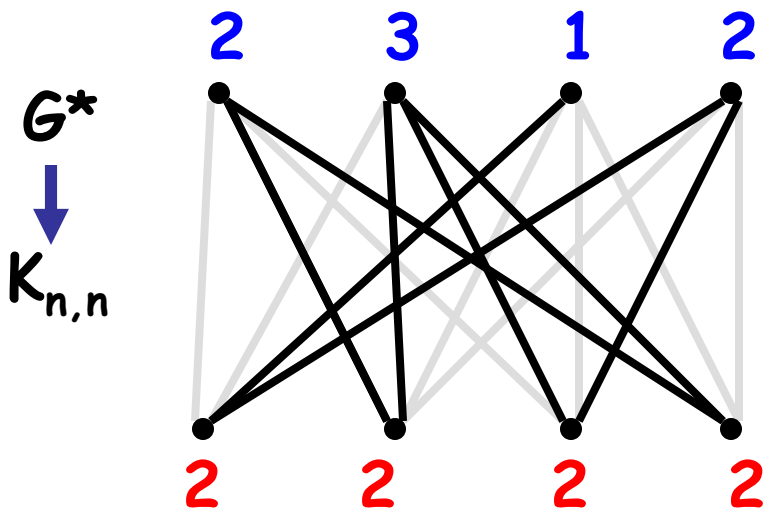

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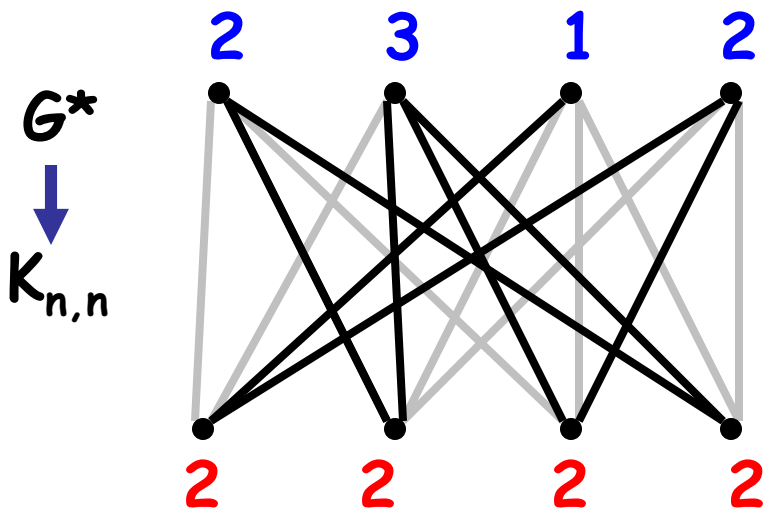

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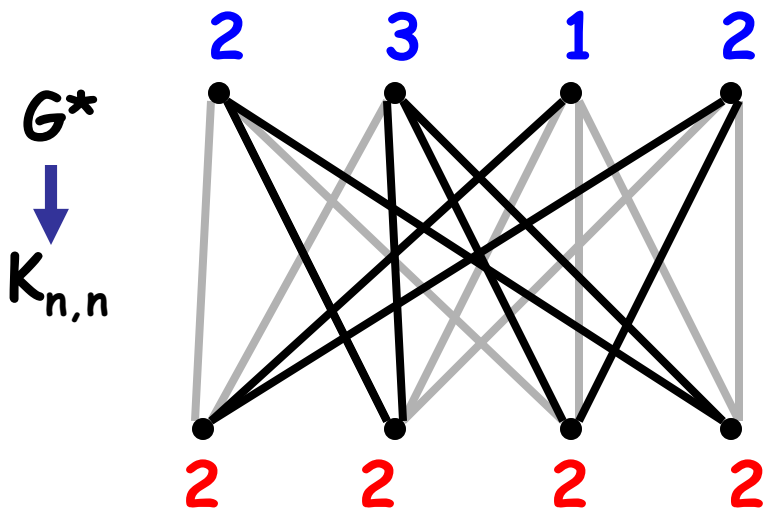

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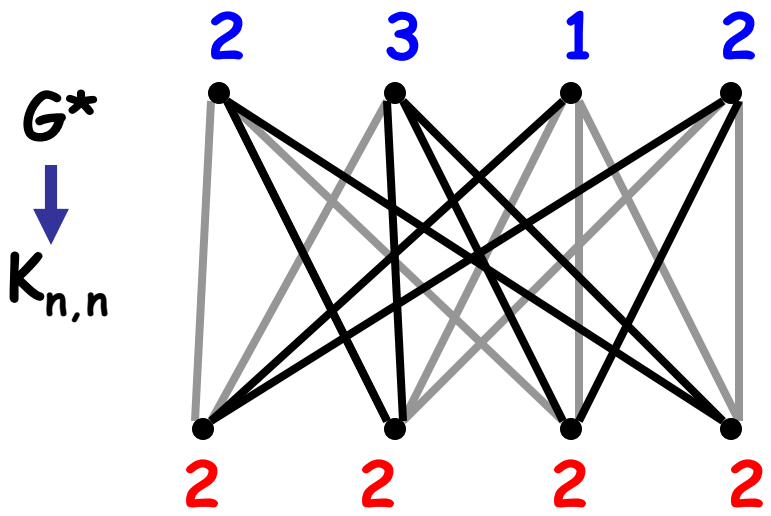

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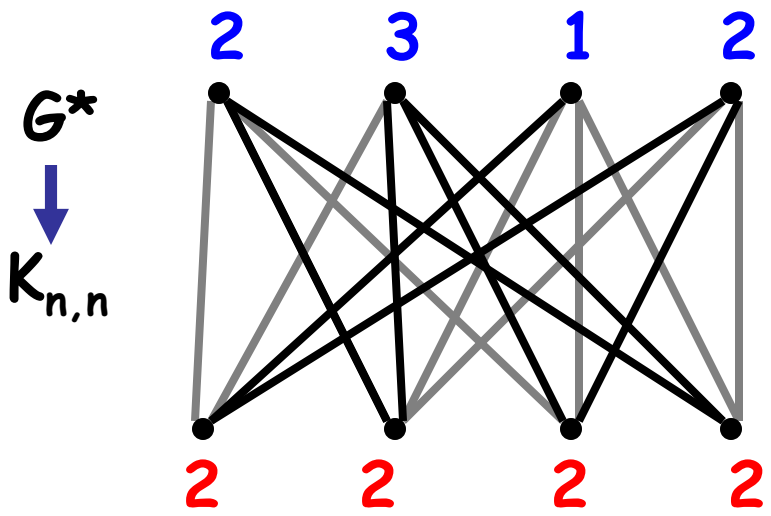

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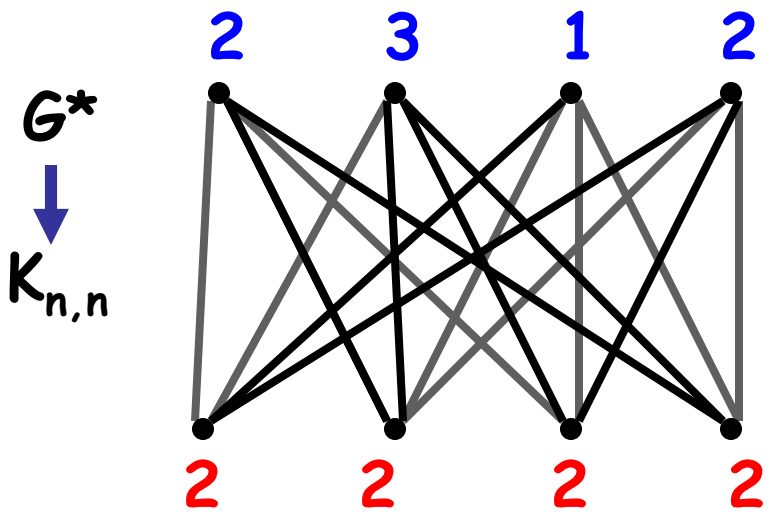

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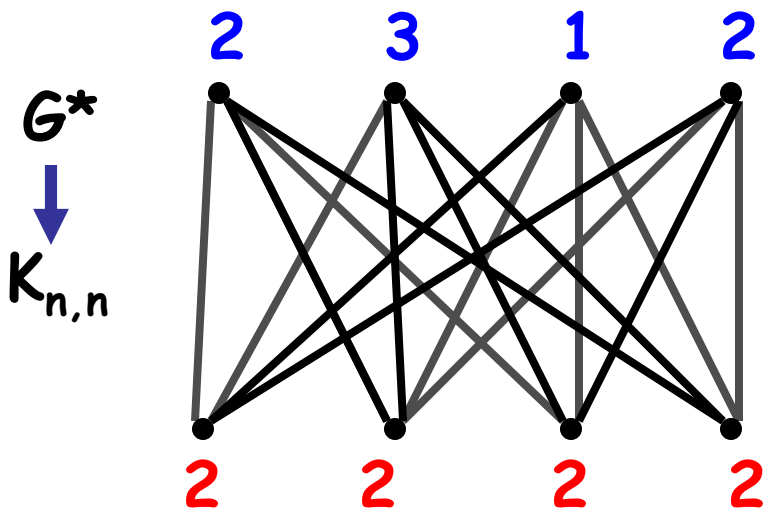

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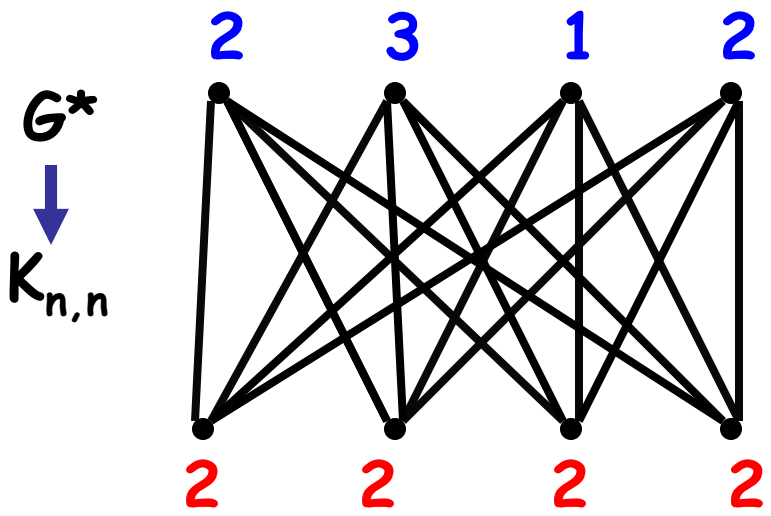

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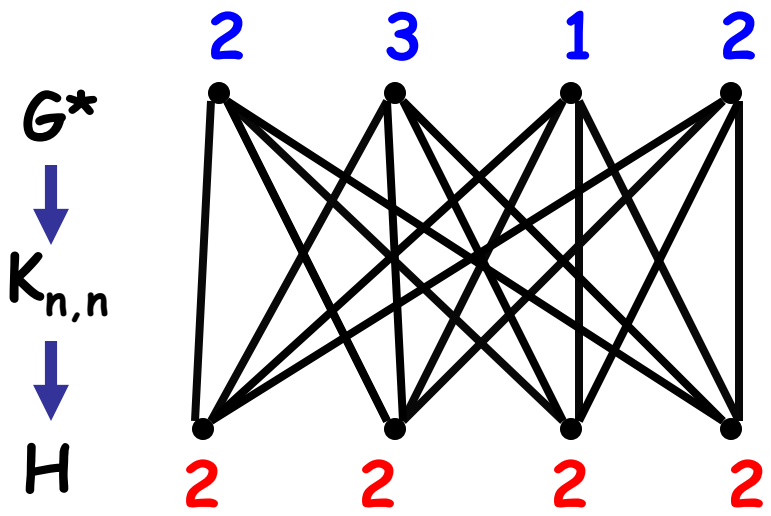

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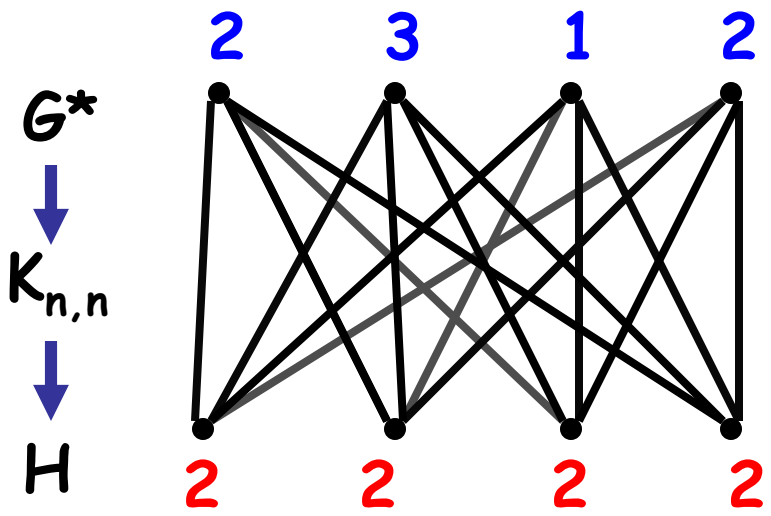

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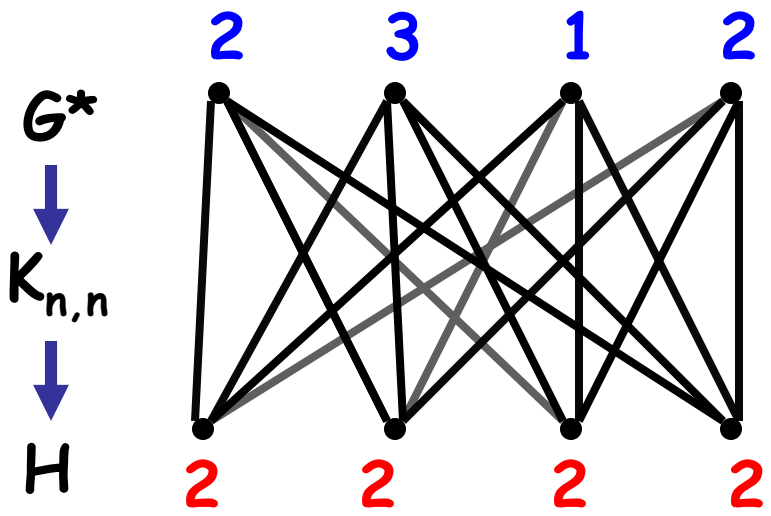

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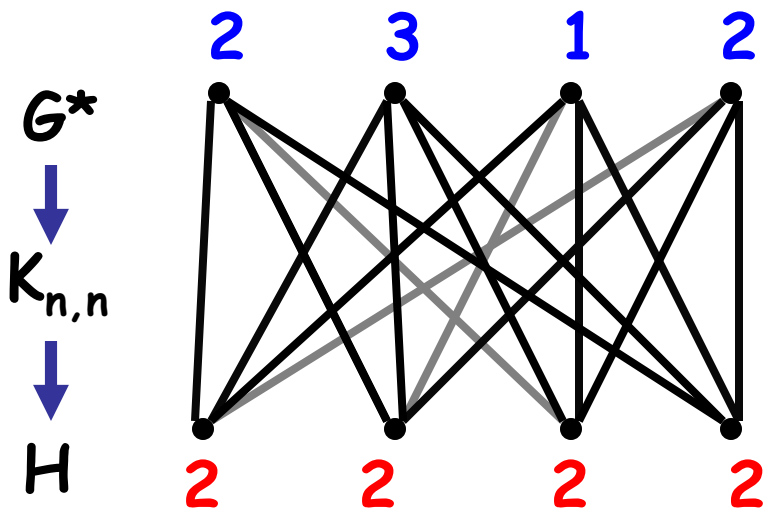

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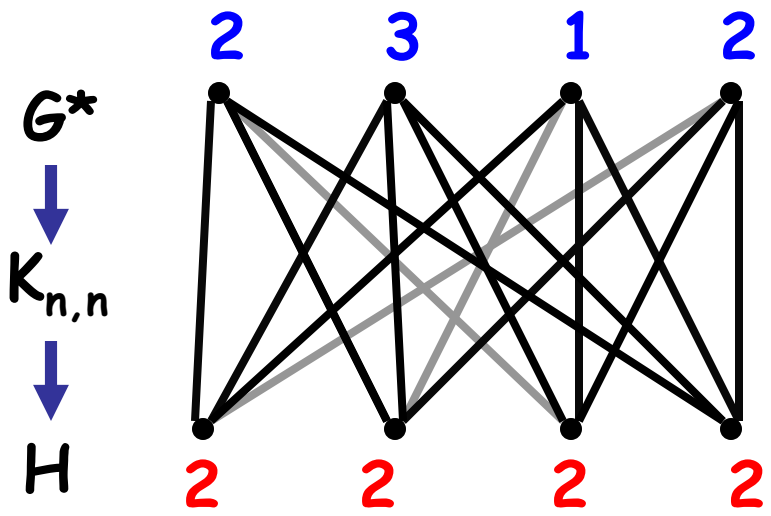

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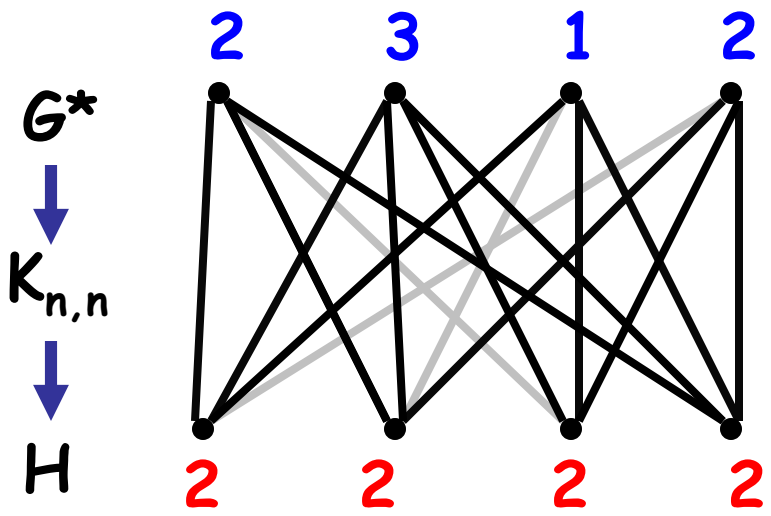

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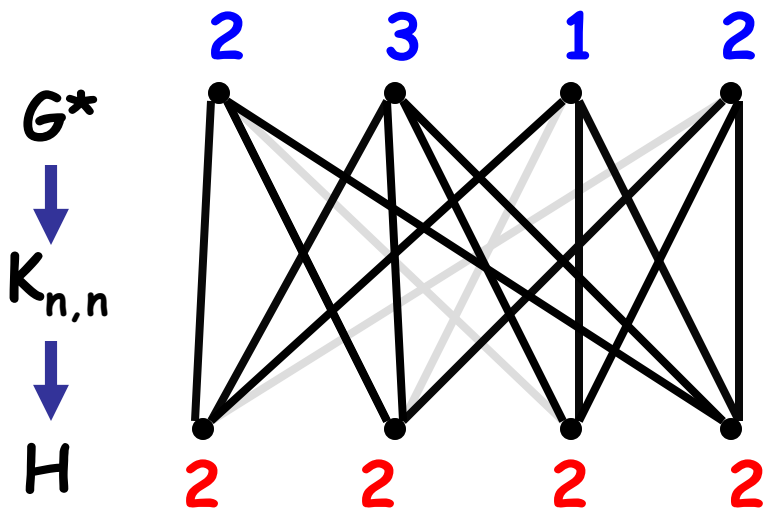

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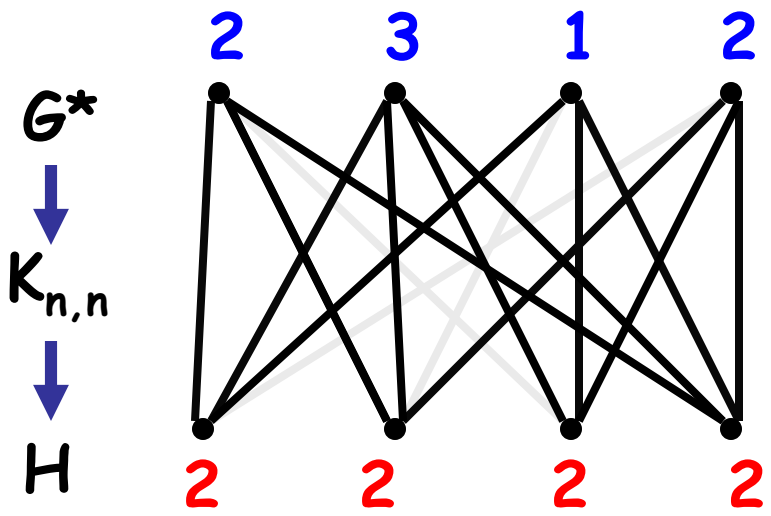

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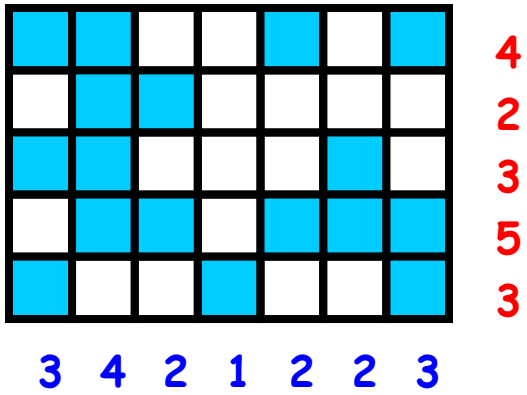
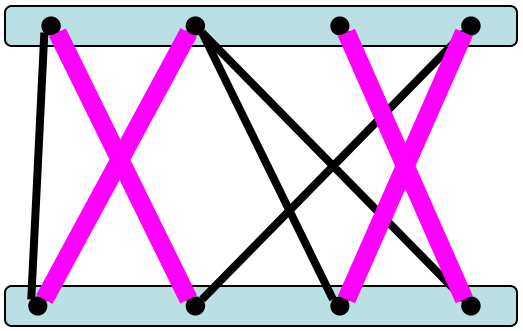
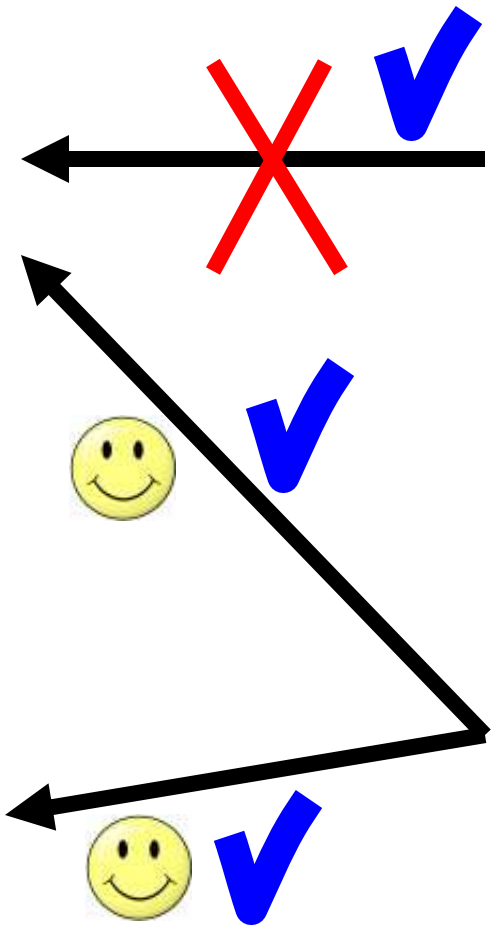
Problems

Binary
contingency tables



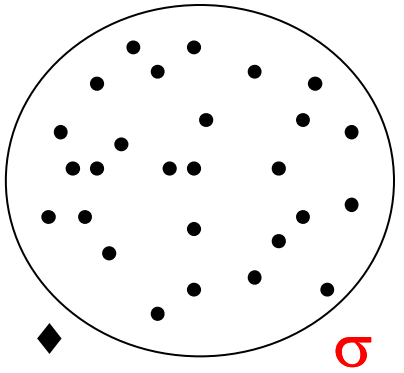
Permanent





Heuristics

Importance sampling



Simulated annealing