Faster Simulated Annealing Algorithms for Combinatorial Counting

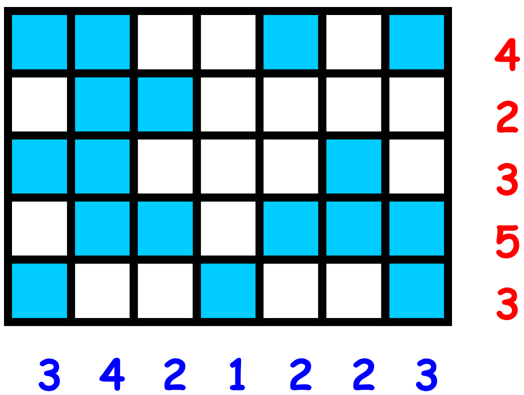
Ivona Bezáková

Rochester Institute of Technology

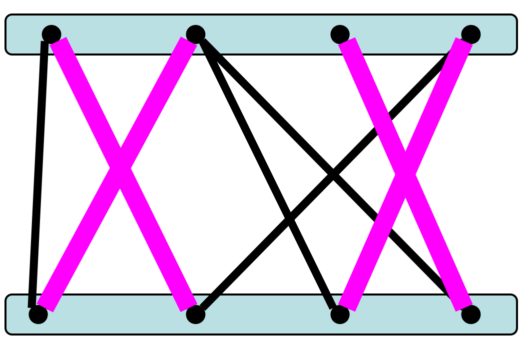
September 22, 2006

Problems

Binary contingency tables

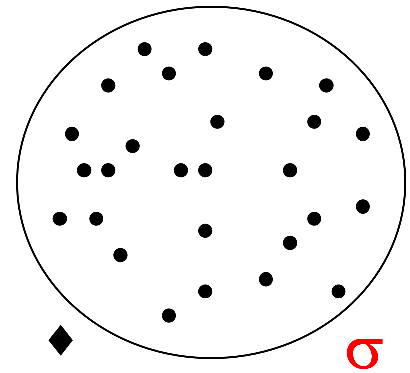


Permanent



Heuristics

Importance sampling



Simulated annealing

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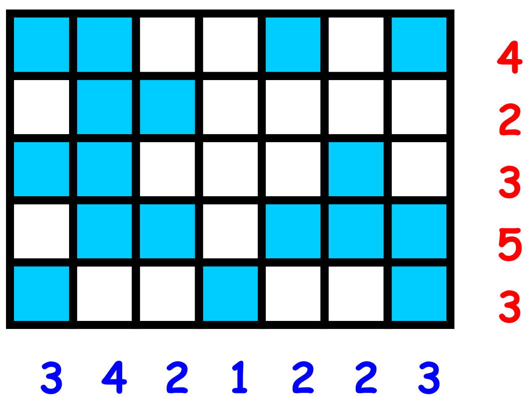

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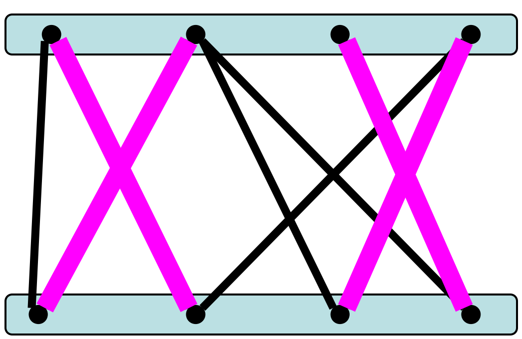

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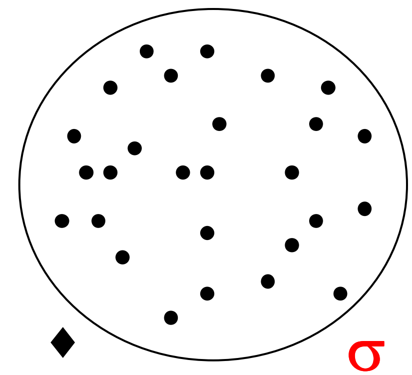
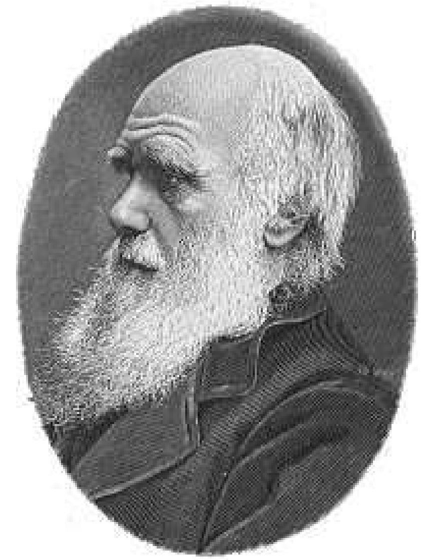
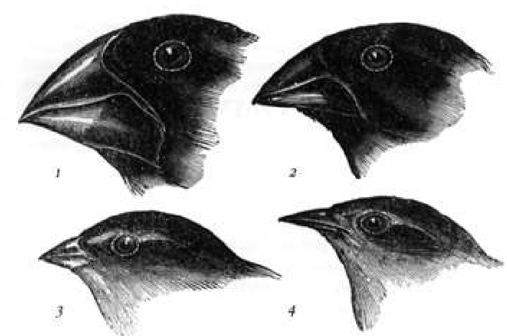


Simulated annealing

Darwin's Finches





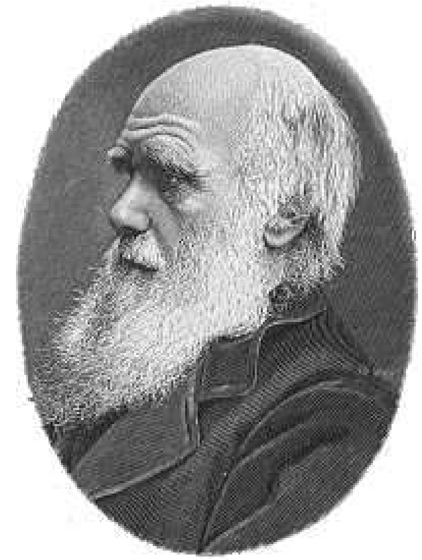
The Voyage of the Beagle

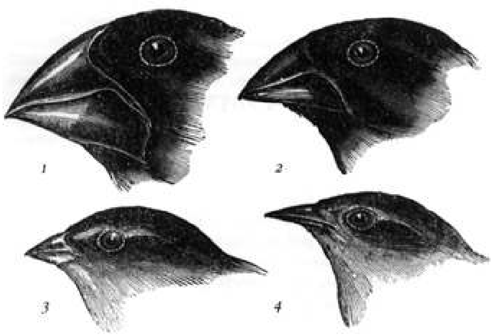
Galápagos archipelago (1835)

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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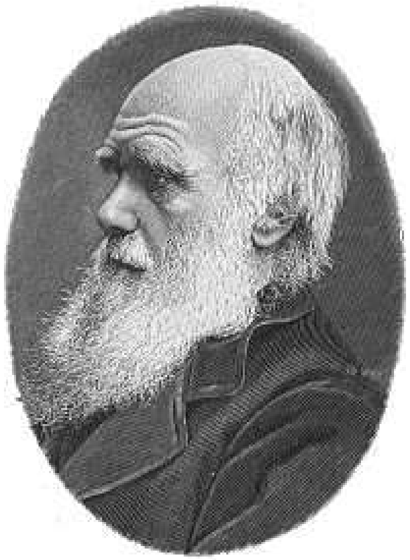
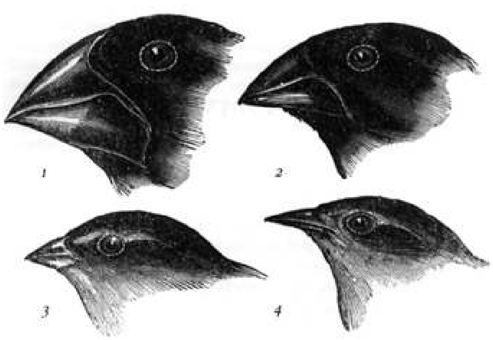
Large Ground Finch	●						●	●	●	●
Cactus Ground Finch	●	●	●	●		●	●		●	●
Large Cactus Ground Finch					●					
Sharp-beaked Ground Finch								●	●	
Vegetarian Finch	●			●		●	●	●	●	●
Small Tree Finch	●		●	●		●	●	●	●	●
Medium Tree Finch						●				
Large Tree Finch	●					●	●	●	●	●
Woodpecker Finch	●			●			●		●	
Mangrove Finch							●	●		
Warbler Finch	●		●	●	●	●	●	●	●	●

8

10

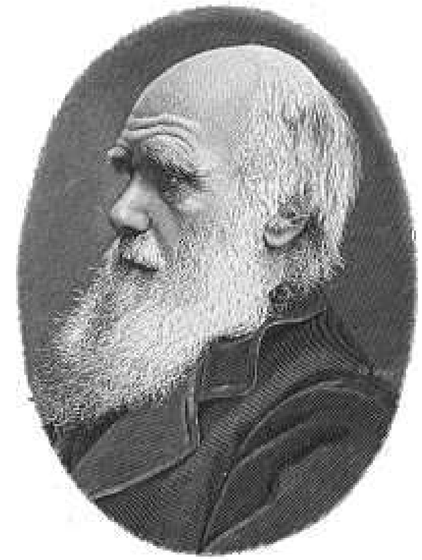




Darwin's Finches

Distribution of Darwin's Finches on Visitor Islands

	Santa Cruz	Plaza	Santa Fe	San Cristobal	Espanola	Floreana	Isabela	Fernandina	Santiago	Rabida	
Small Ground Finch	●	●	●	●	●	●	●	●	●	●	10
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

							4
							2
							3
							5
							3
3	4	2	1	2	2	3	

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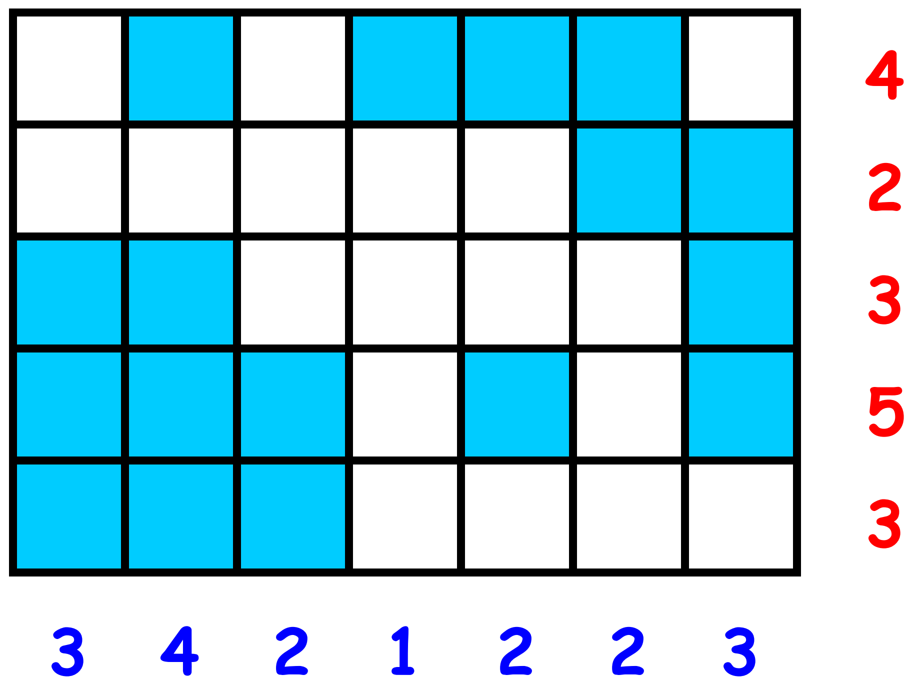

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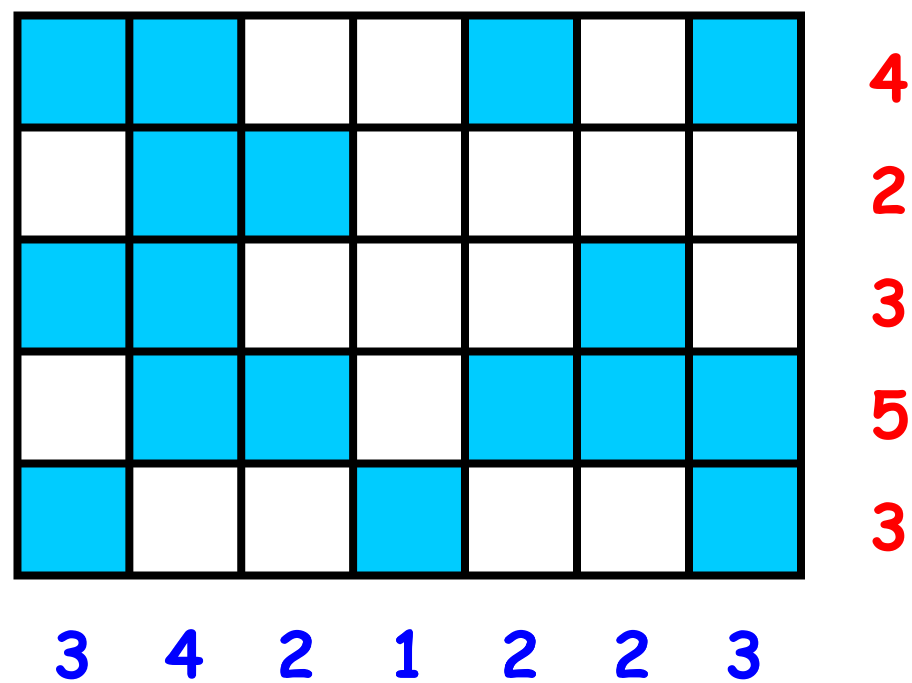

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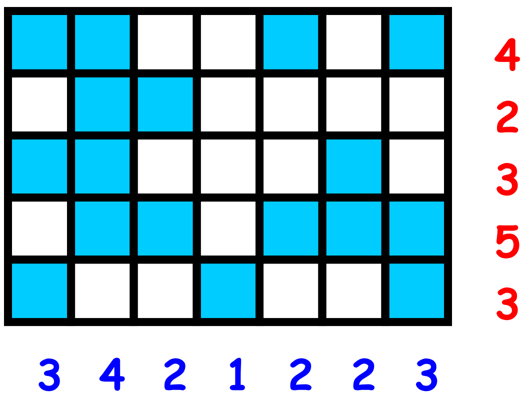
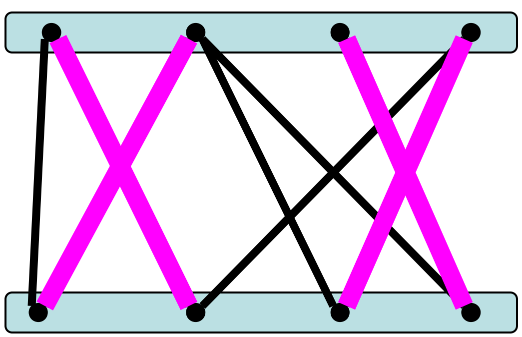


Permanent



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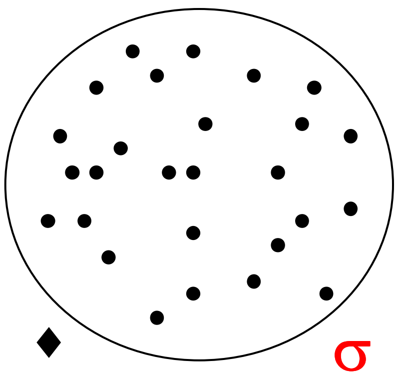


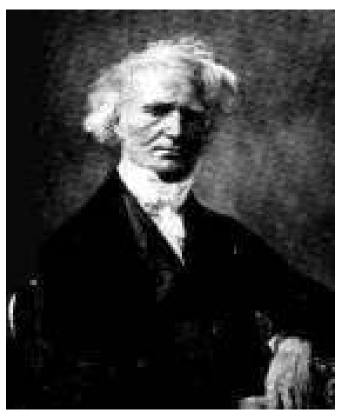
Simulated annealing

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

Permanent of an n x n matrix A

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

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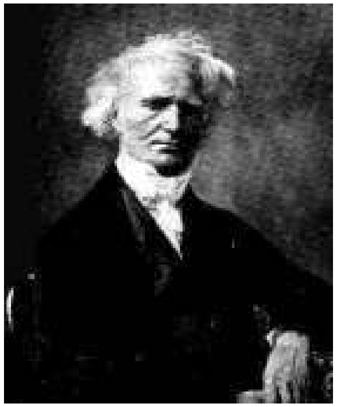

Jacques
Binet

$$A = \begin{bmatrix} 5 & 1 & 0 & 3 & 4 \\ 2 & 0 & 1 & 4 & 4 \\ 5 & 7 & 9 & 2 & 2 \\ 1 & 1 & 6 & 1 & 0 \\ 3 & 3 & 0 & 8 & 7 \end{bmatrix}$$

π

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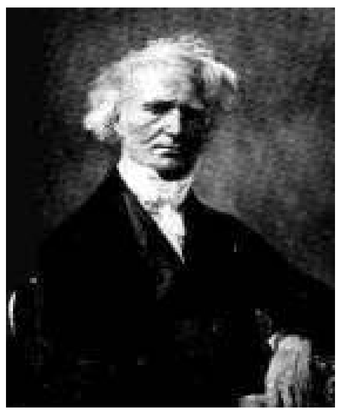

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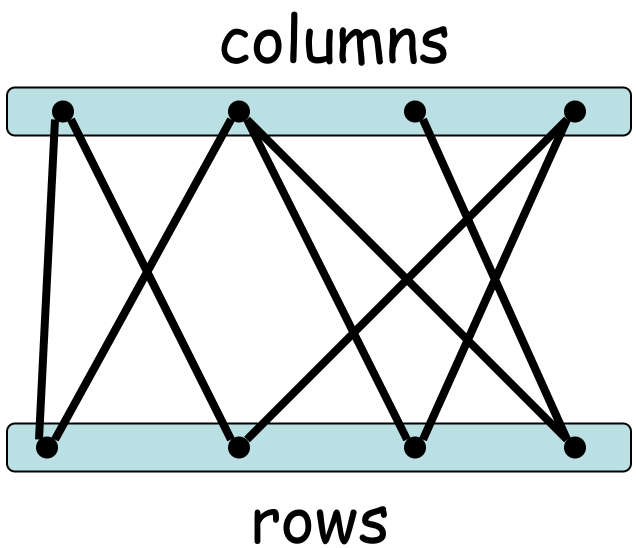


columns

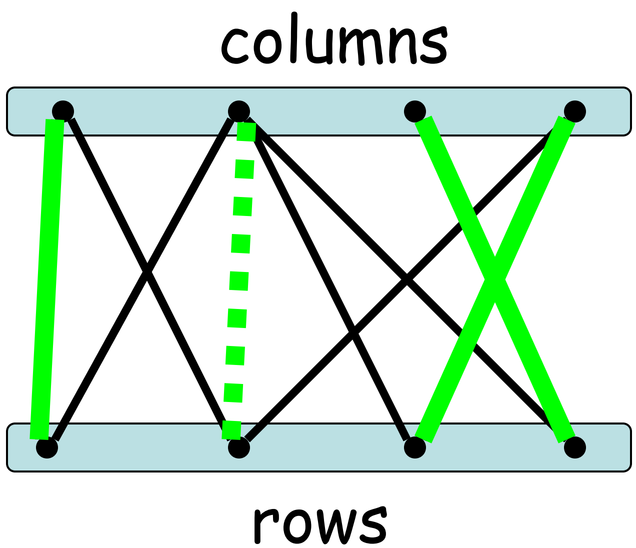
1	1	0	0
1	0	0	1
0	1	0	1
0	1	1	0

rows

Permanent of an $n \times n$ matrix A

0

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



π

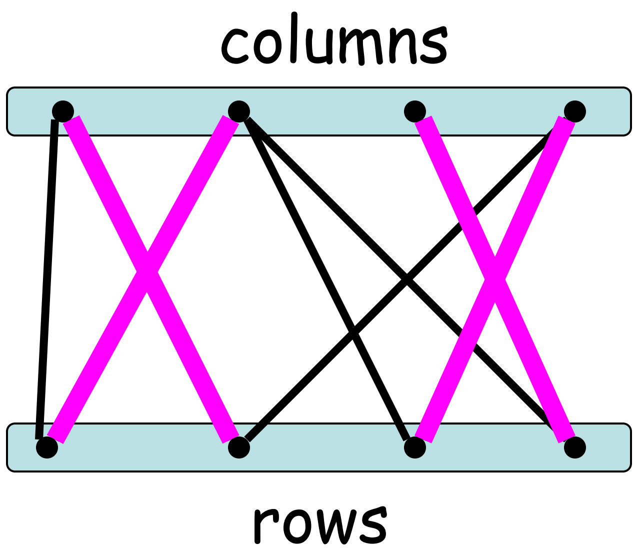
columns

1	1	0	0	rows
1	0	0	1	
0	1	0	1	
0	1	1	0	

Permanent of an n x n matrix A

1

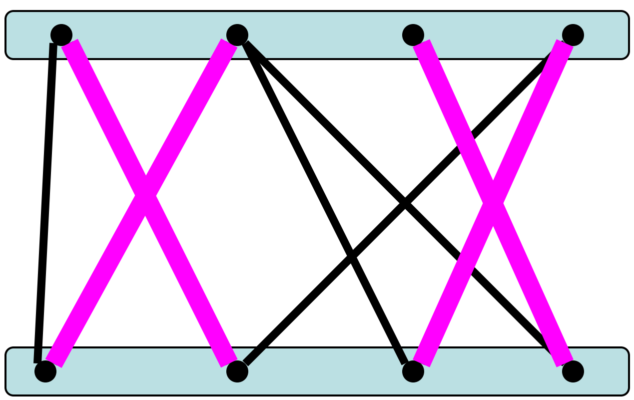
$$\mathrm{Per}(A) = \sum_{\pi \in S_n} \prod_{i=1}^{n} a_{i,\pi(i)}$$



$$\begin{array}{c}
\text{columns} \quad \pi \\
\begin{array}{|c|c|c|c|}
\hline
1 & 1 & 0 & 0 \\ \hline
1 & 0 & 0 & 1 \\ \hline
0 & 1 & 0 & 1 \\ \hline
0 & 1 & 1 & 0 \\ \hline
\end{array} \ \text{rows}
\end{array}$$

Permanent of an n x n matrix A

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

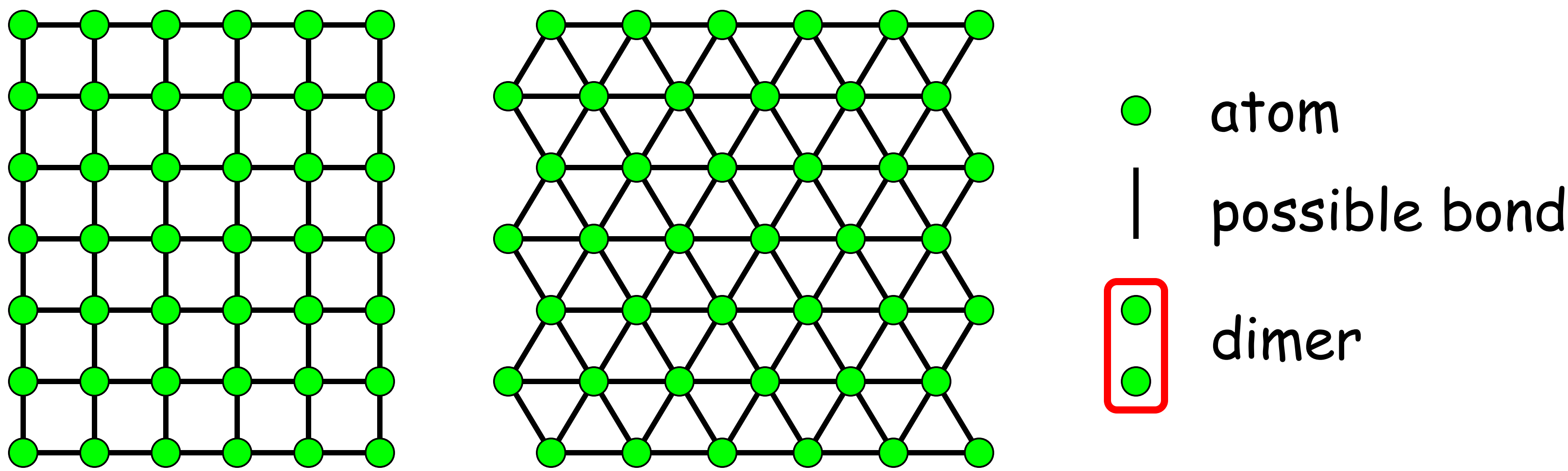


Count perfect matchings of a bipartite graph

Permanent: Counting Perfect Matchings

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

Dimer model



Partition function = permanent (in bipartite case)

- for computation of thermodynamic properties

Permanent: Counting Perfect Matchings

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

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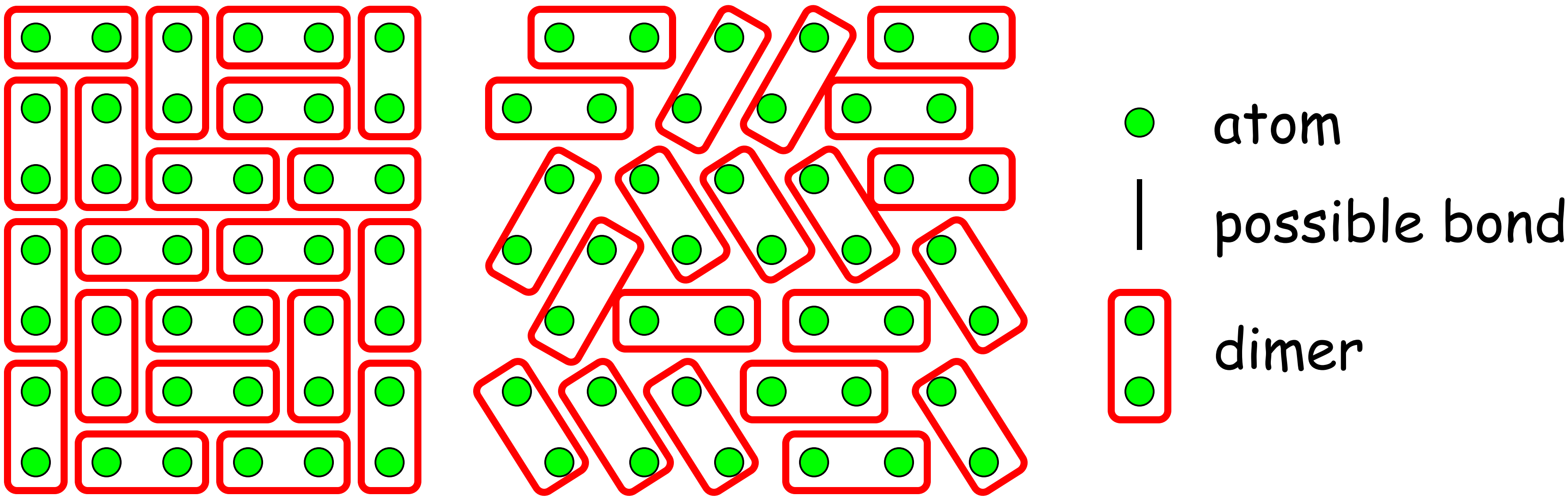

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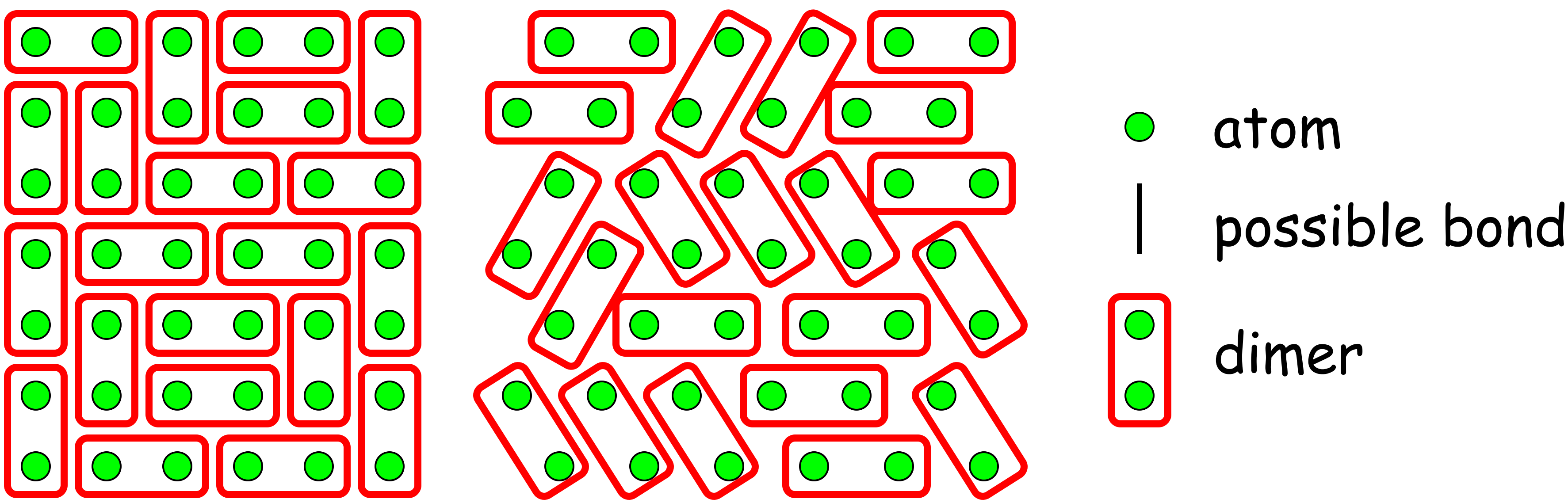
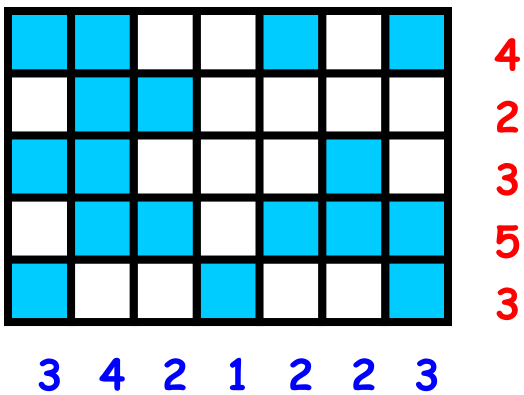


[Valiant '79] **#P-complete** for general (bipartite) graphs

Problems

Binary contingency tables



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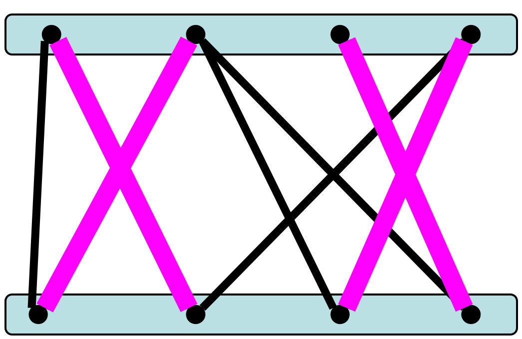

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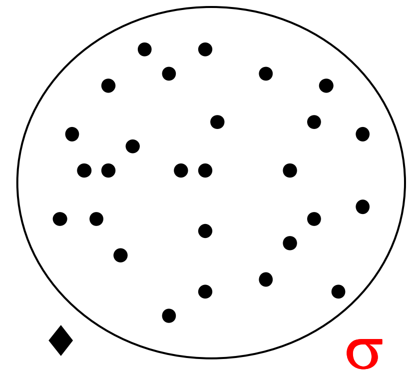
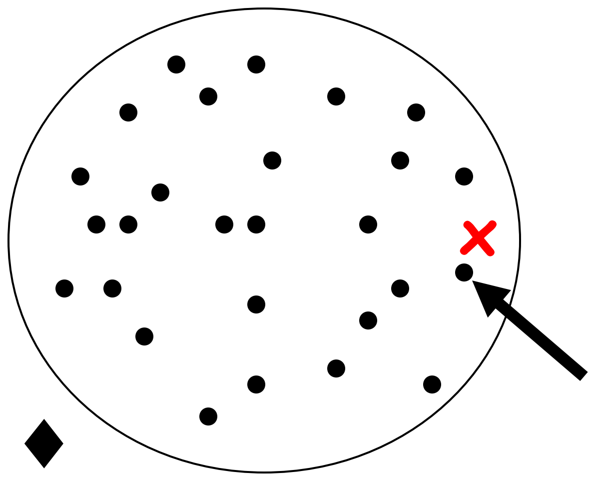


Simulated annealing

Importance Sampling for counting problems



Probability distribution σ

on the points + ♦

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

Random variable

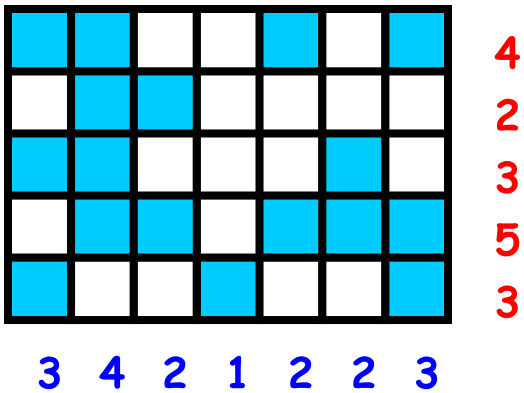
$$\eta(s) = \begin{cases} 1/\sigma(s) & \text{if s in the set} \\ 0 & \text{if s is ♦} \end{cases}$$

Unbiased estimator

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

Problems

Binary contingency tables



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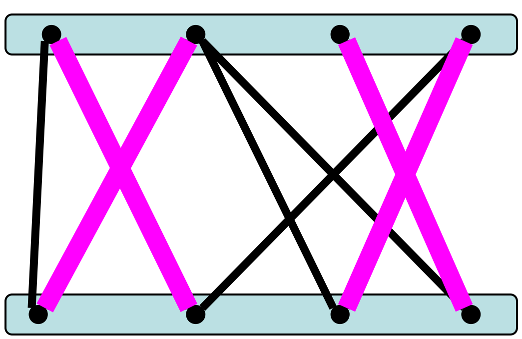

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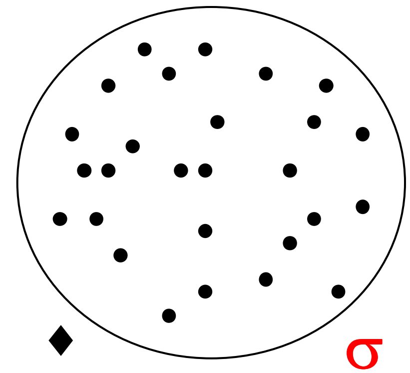


Simulated annealing

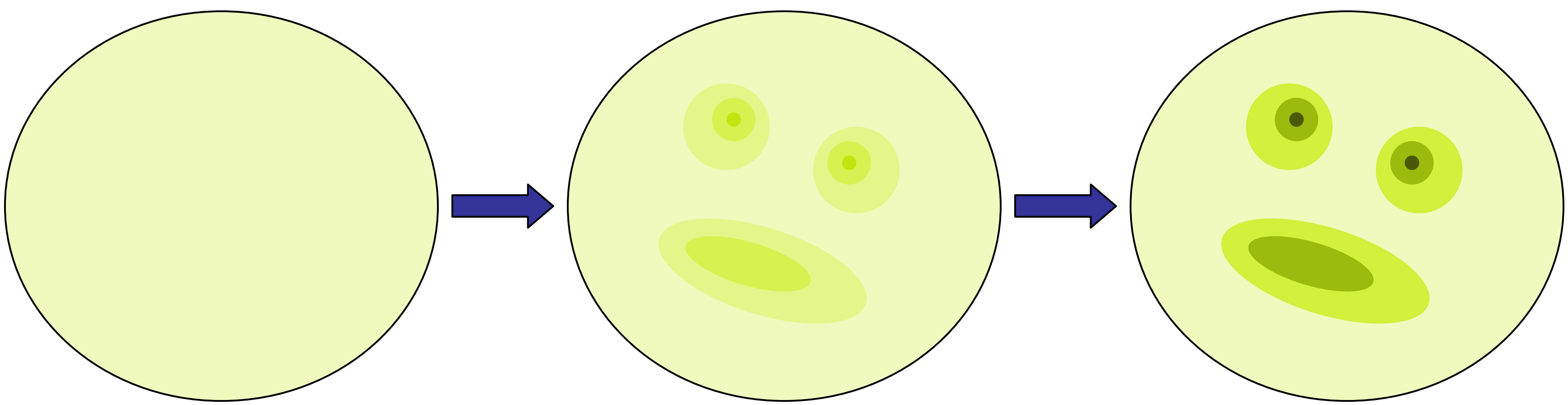
Simulated Annealing

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

Unordered state → Ordered state

(EASY) (DIFFICULT)

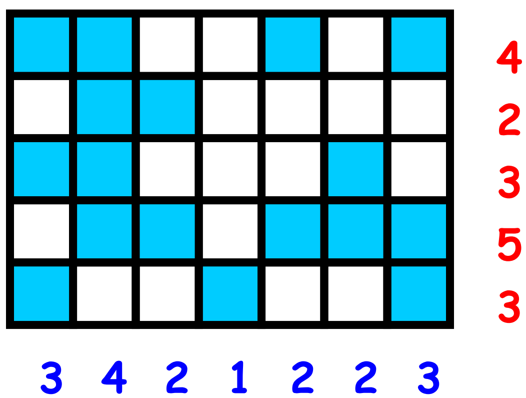
Cooling:



all equivalent differences more and more pronounced

Problems

Binary
contingency tables



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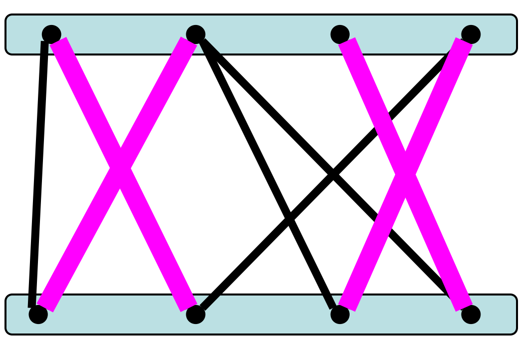

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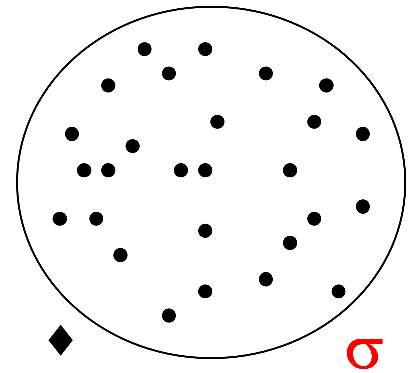

Simulated annealing

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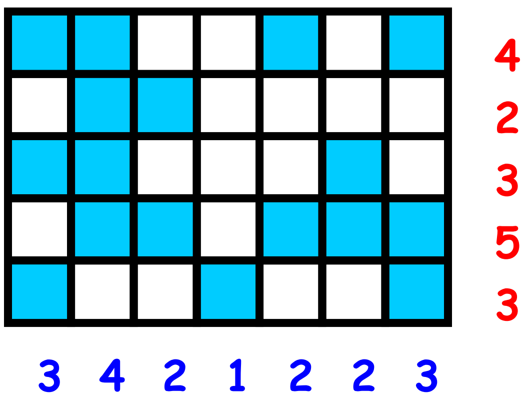

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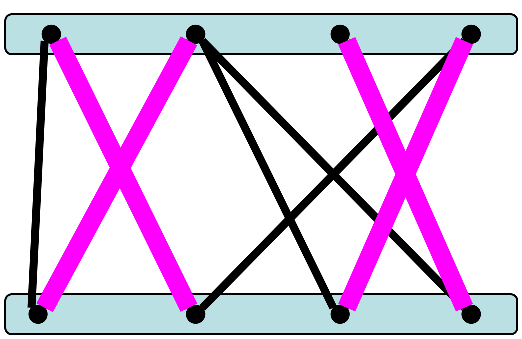

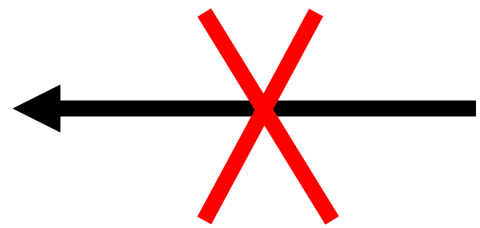

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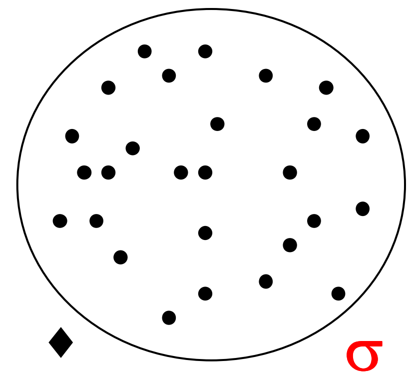

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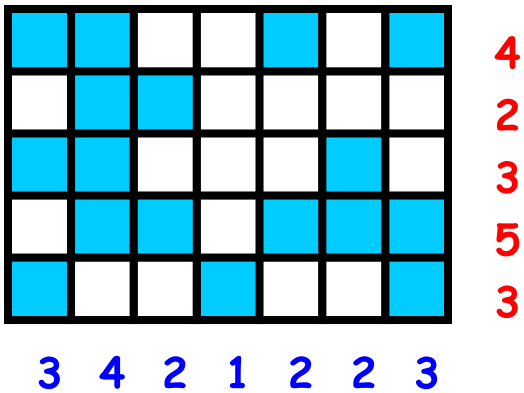

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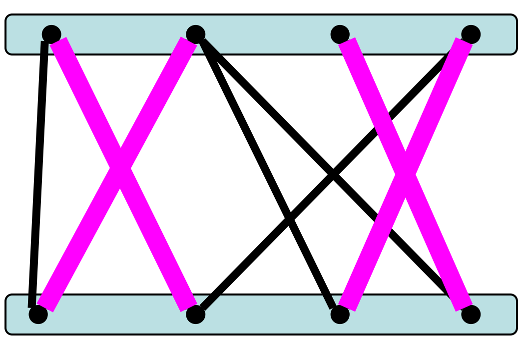

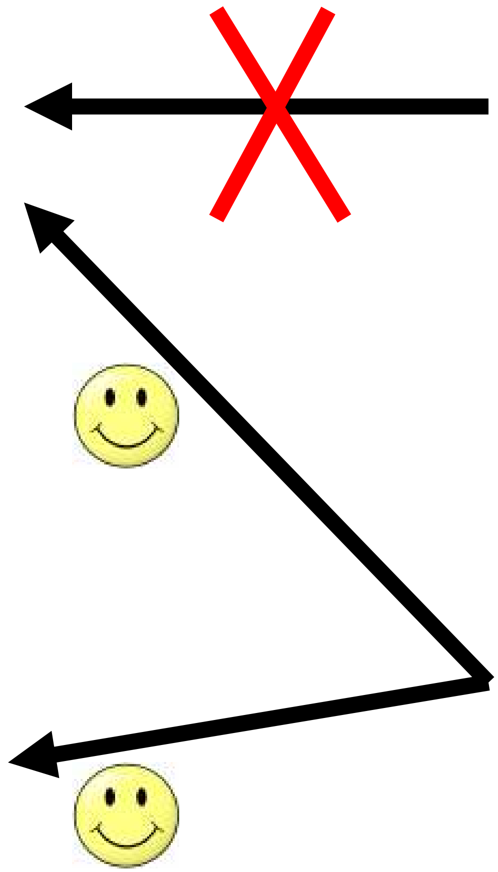

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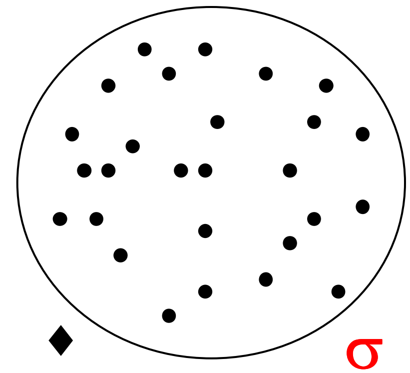

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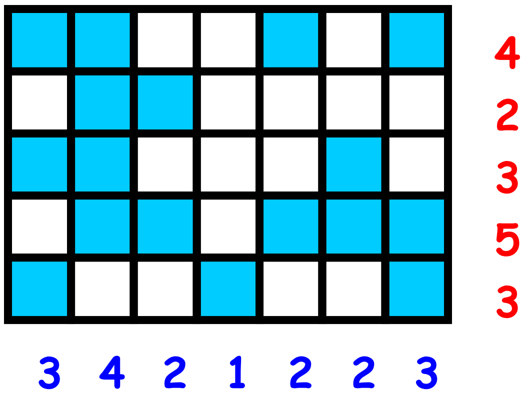

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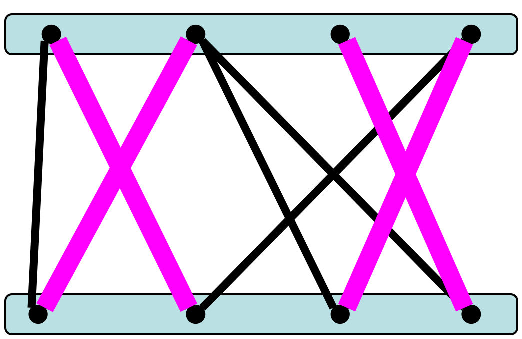

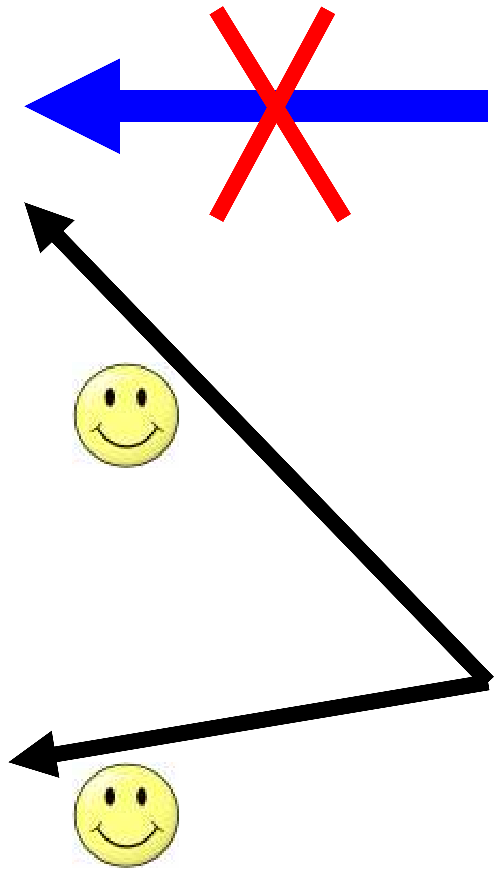

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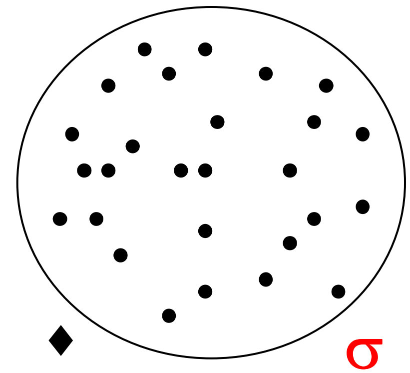

Simulated annealing

Sequential Importance Sampling for BCT

[Chen-Diaconis-Holmes-Liu '05]

a specific σ

- fill table column-by-column
- assign each column ignoring other column sums

							4
							2
							3
							5
							3
3	4	2	1	2	2	3	

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							4
							2
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4	3	3	2	2	2	1	

Sequential Importance Sampling for BCT

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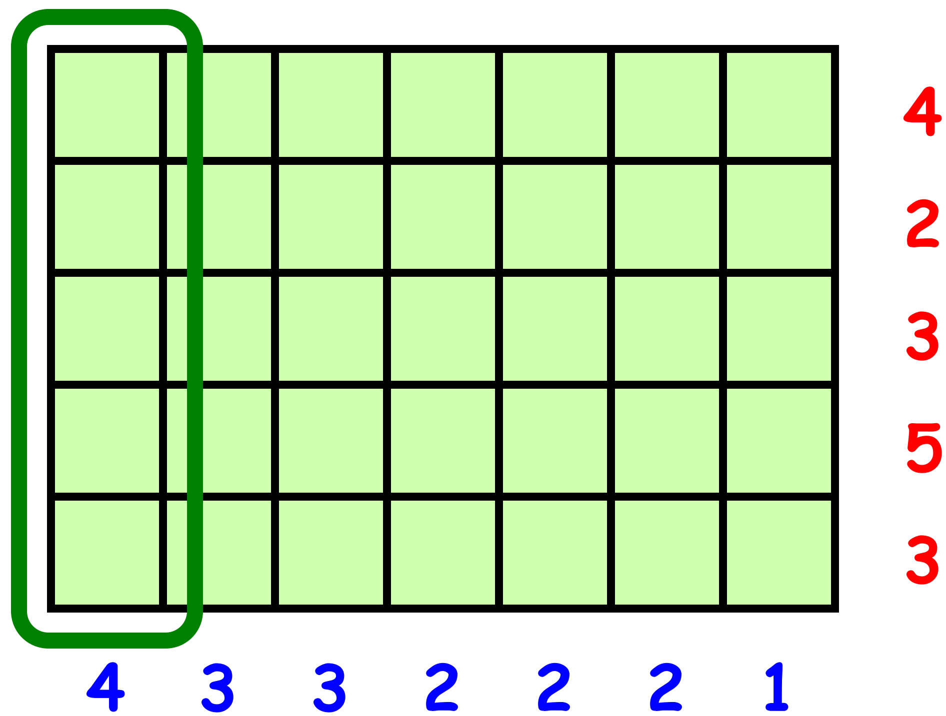

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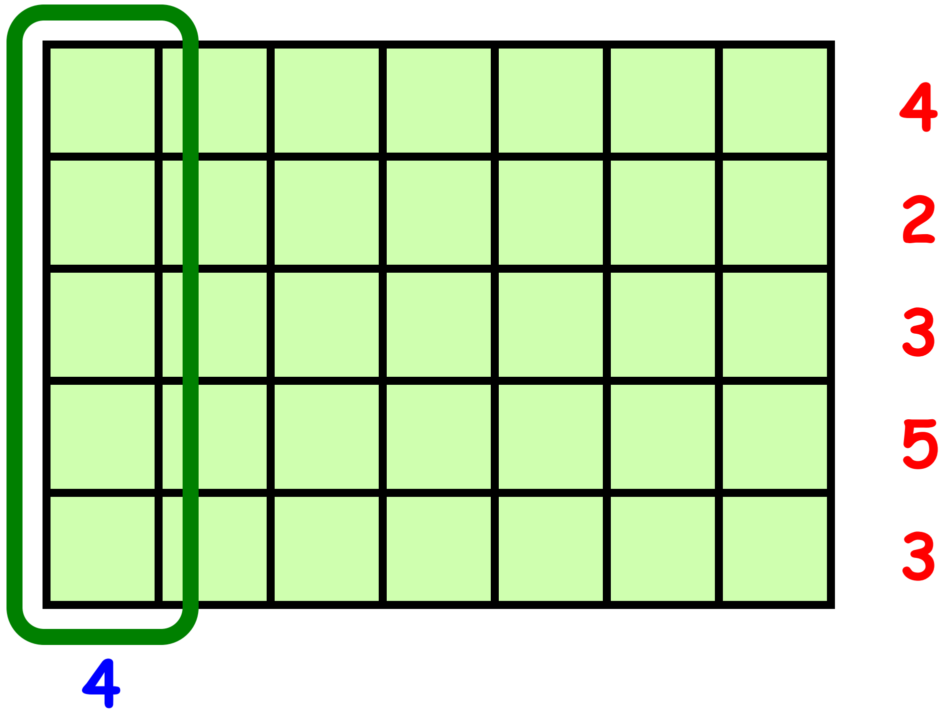

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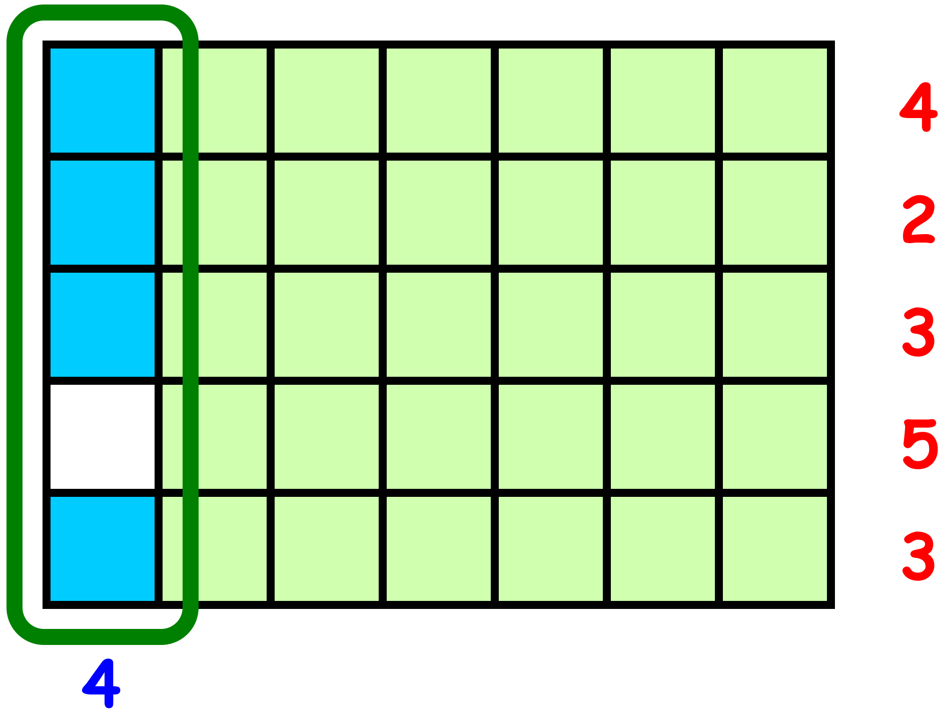

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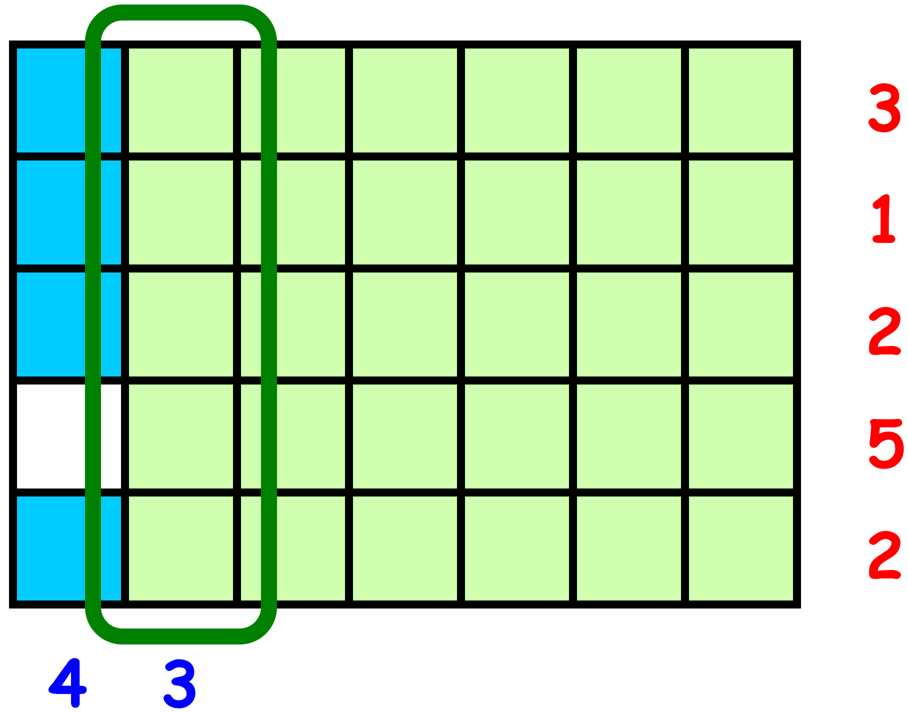

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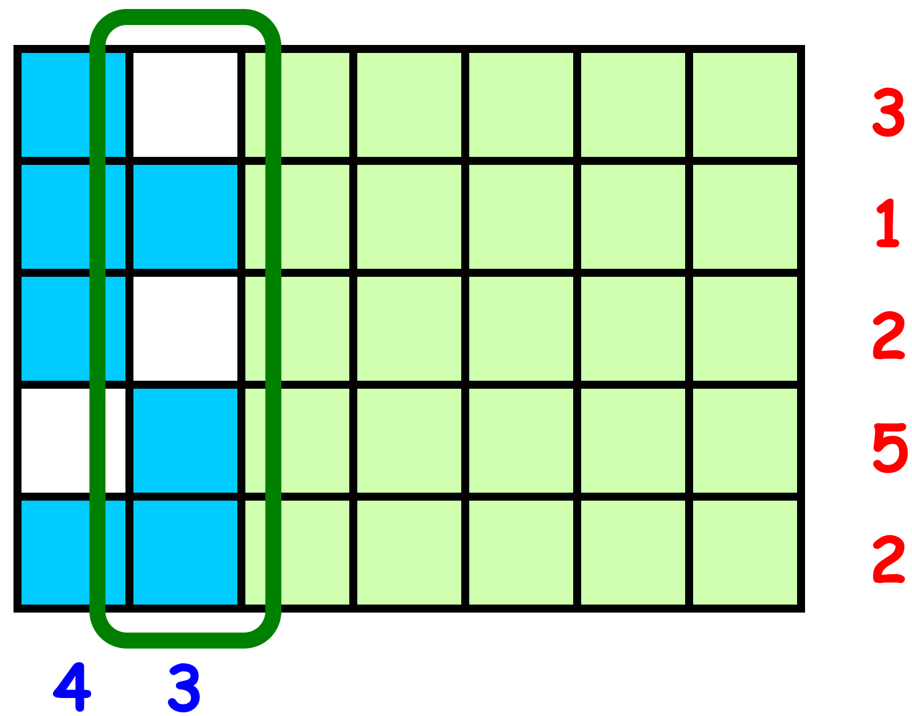

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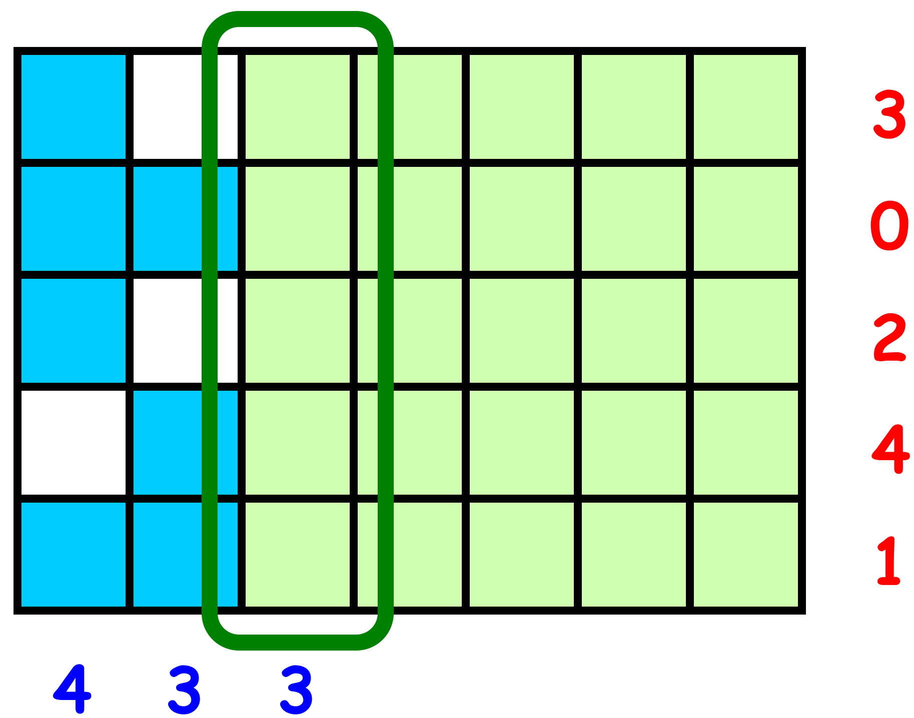

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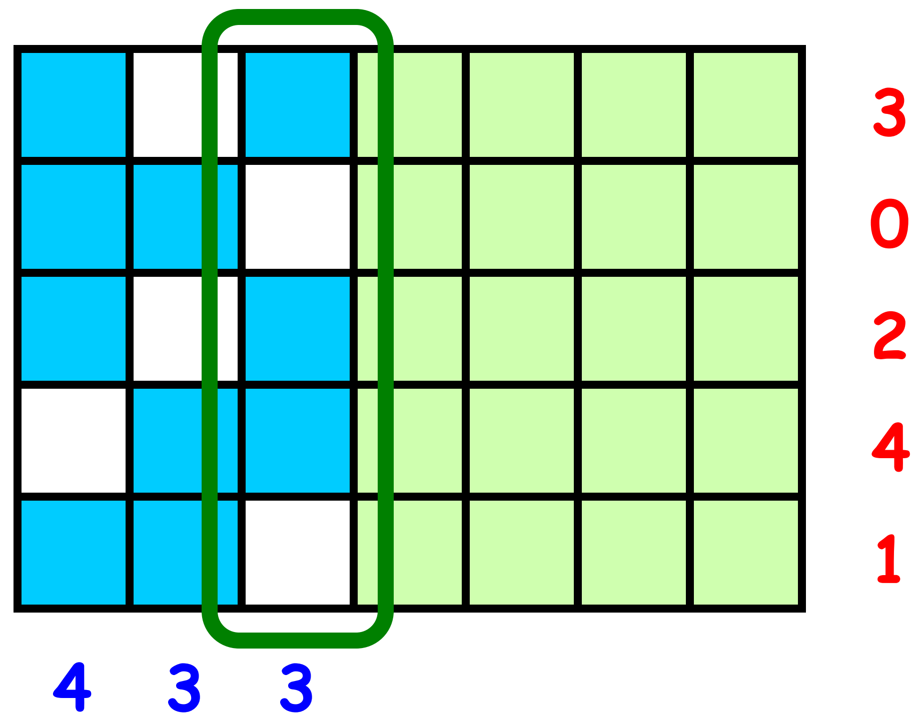

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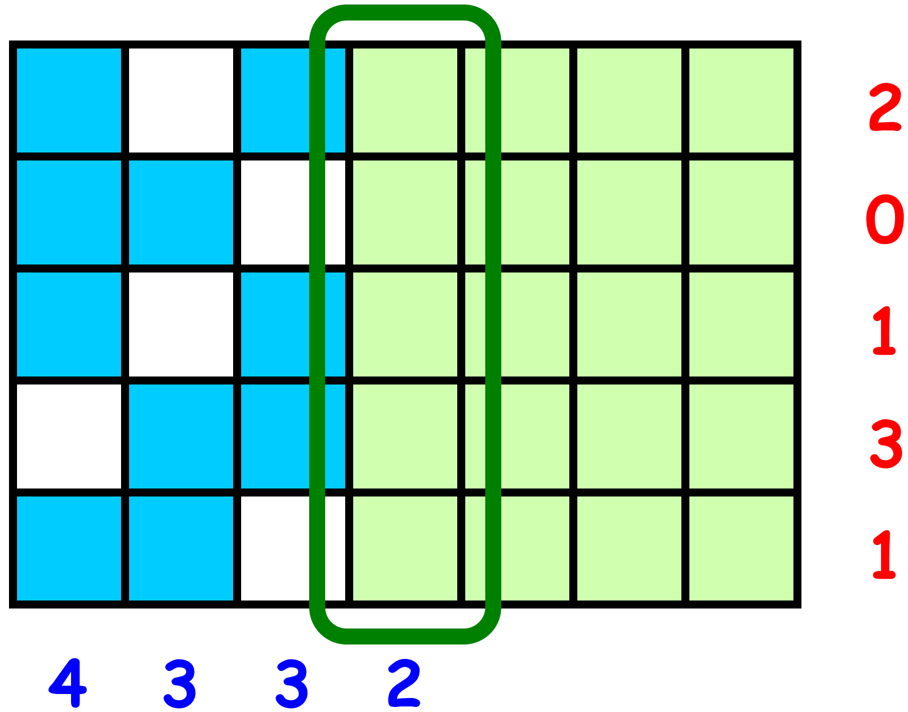

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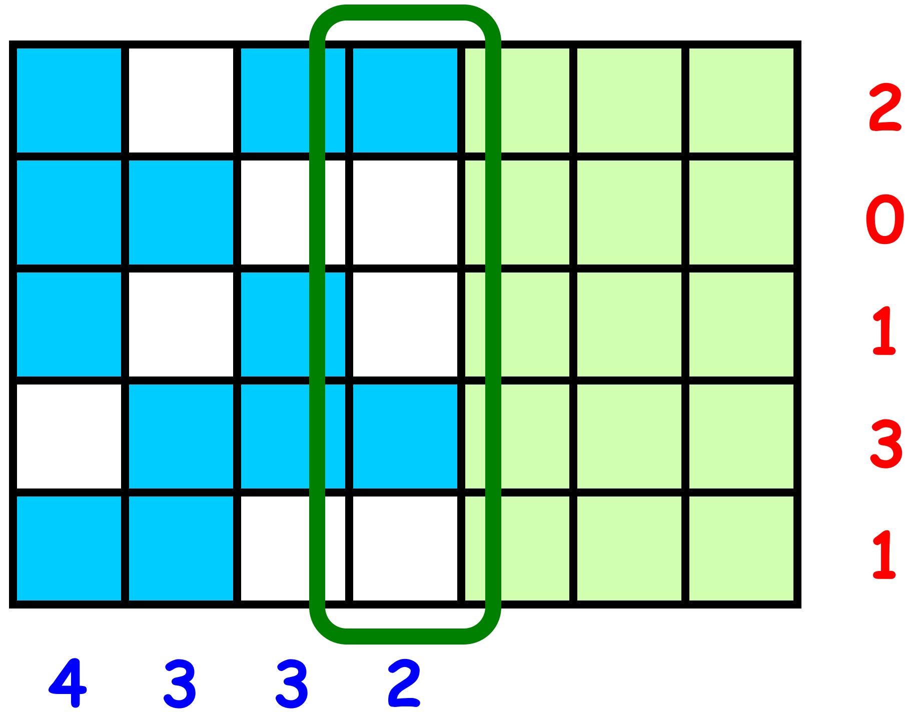

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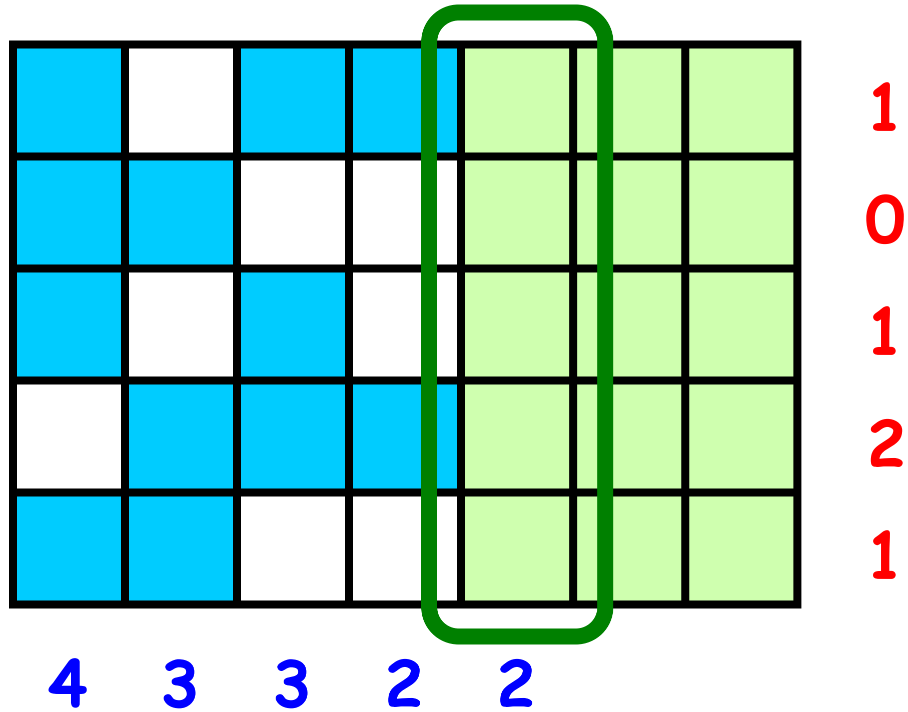

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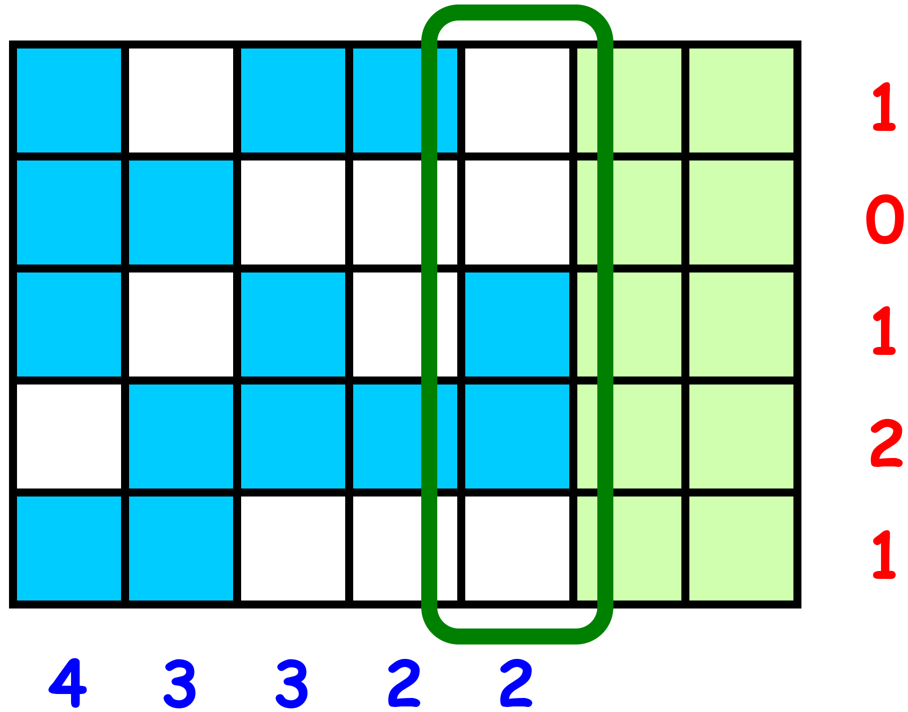

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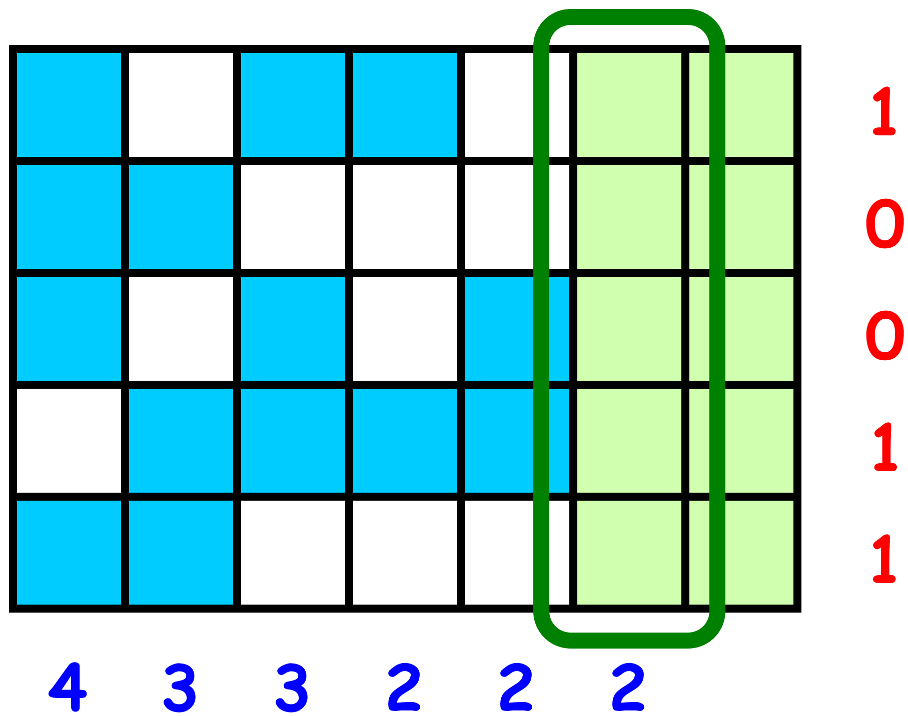

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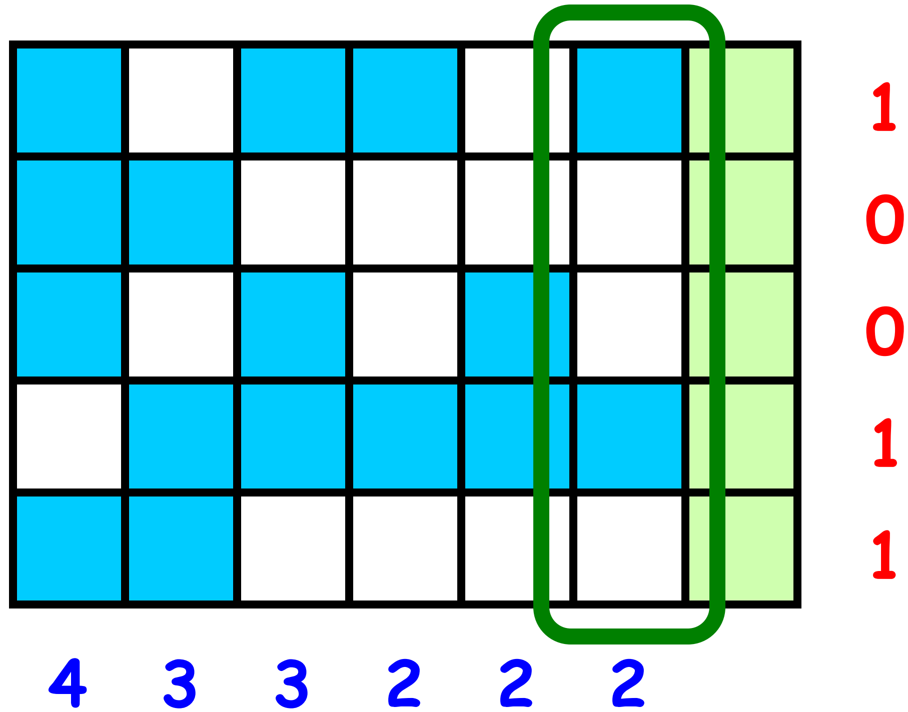

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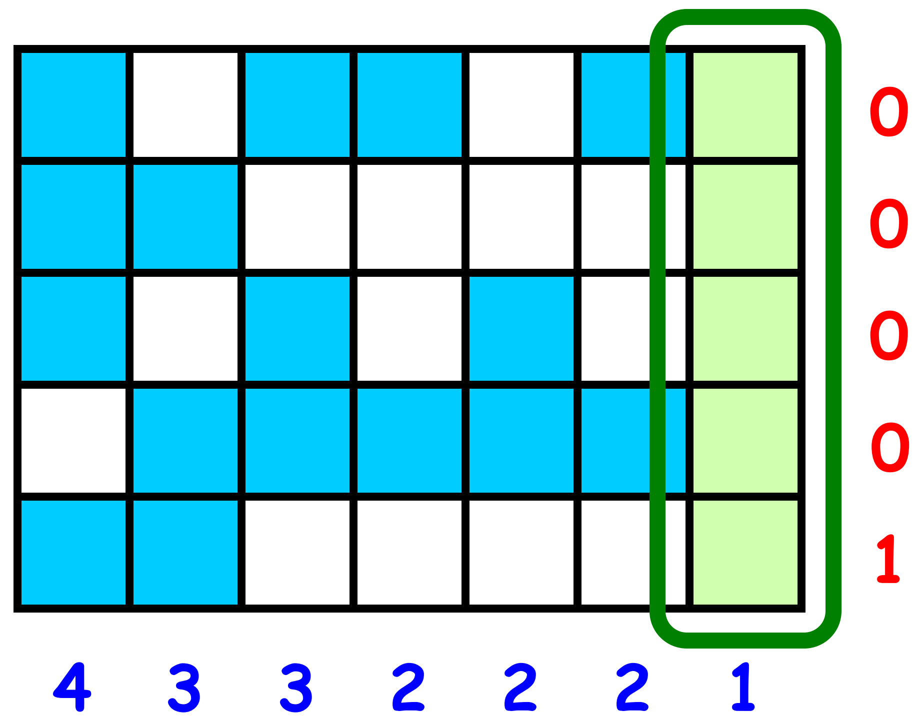

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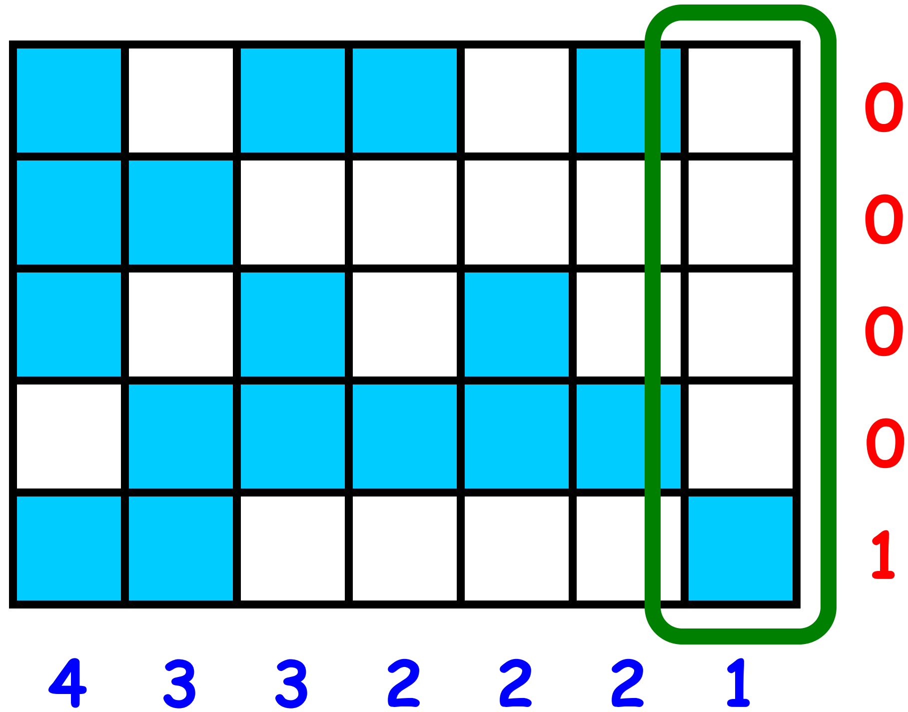

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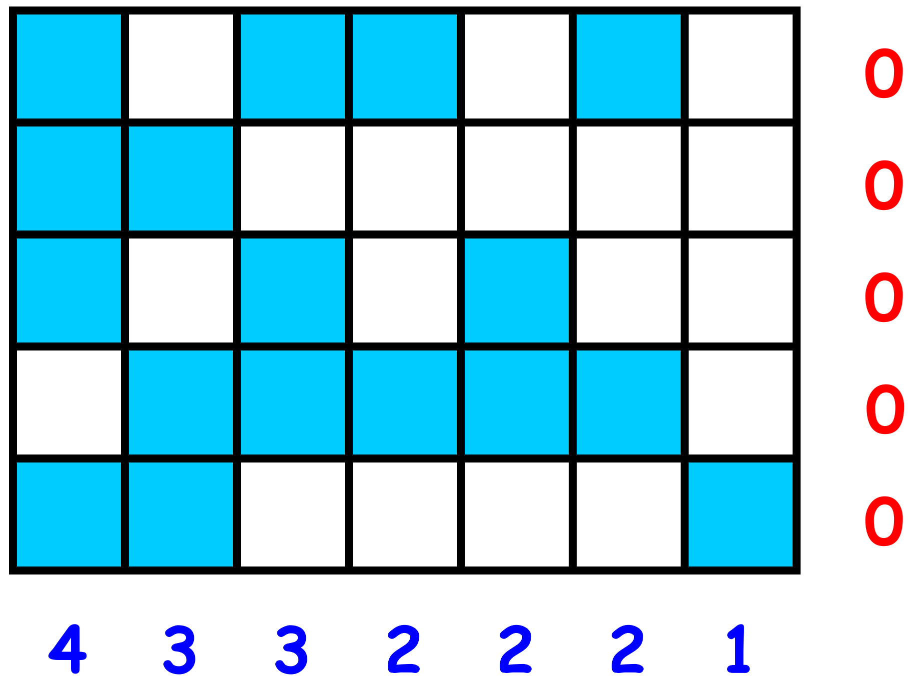

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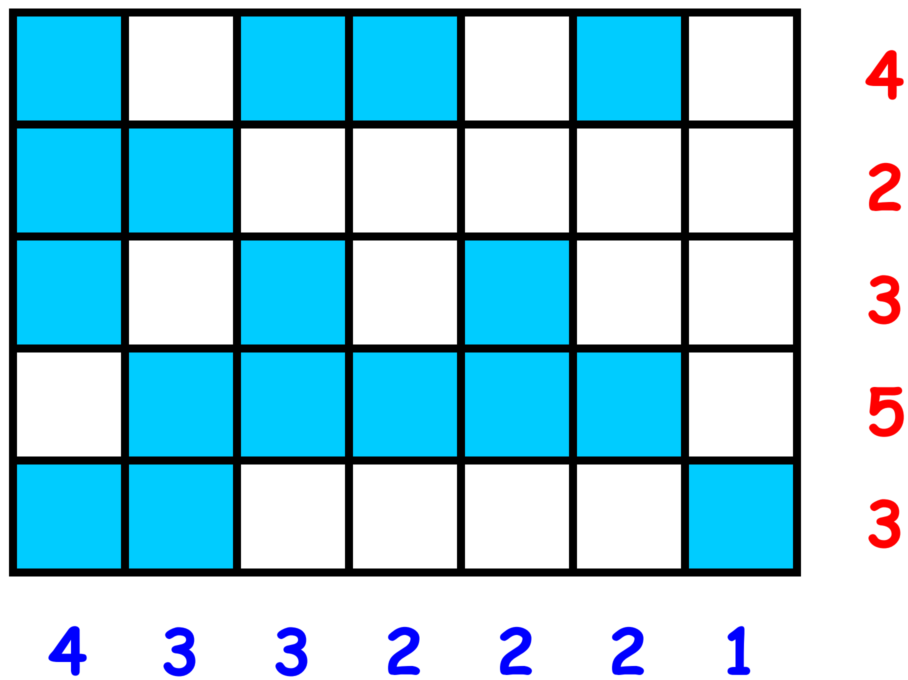
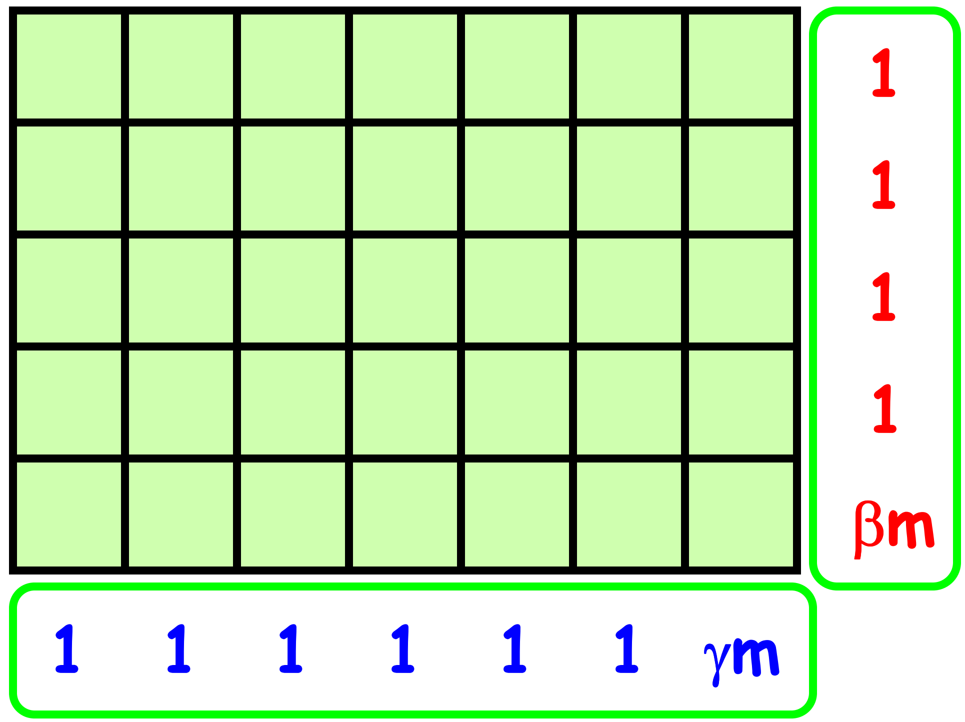


A Counterexample for SIS

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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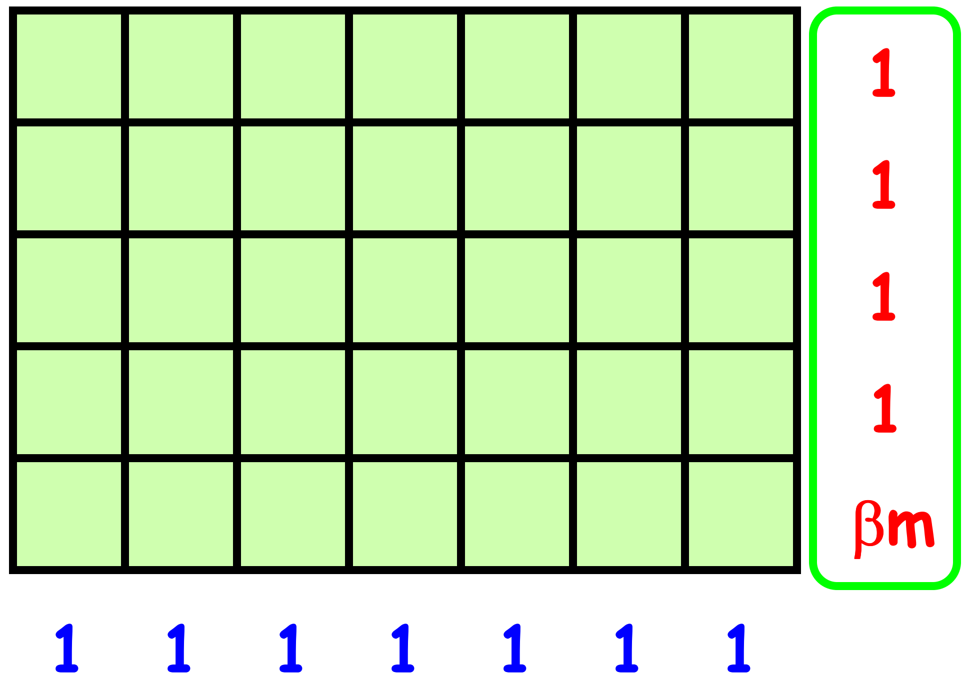

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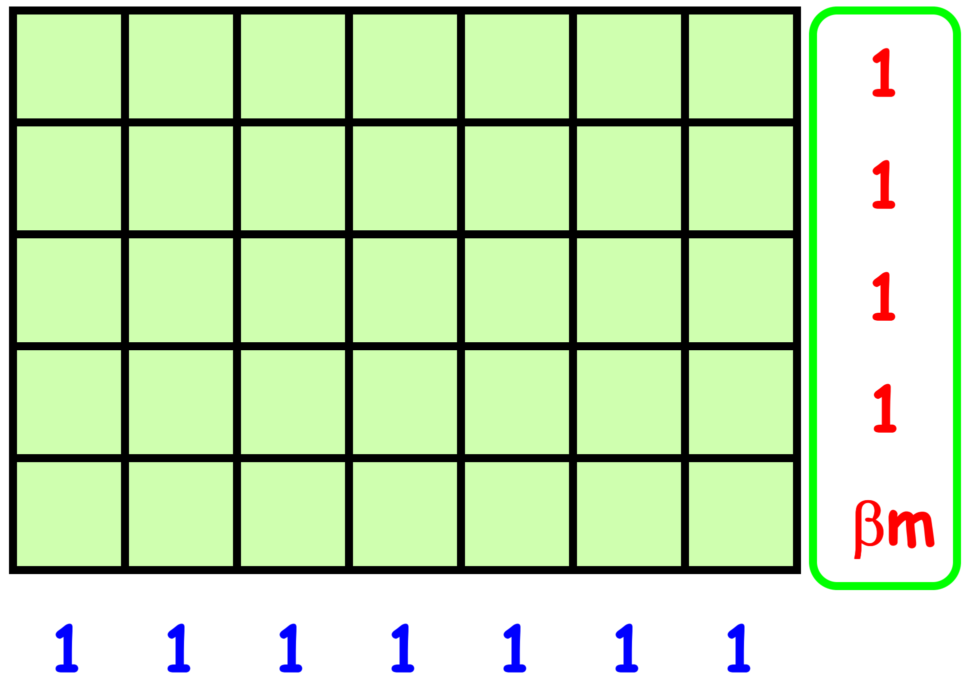

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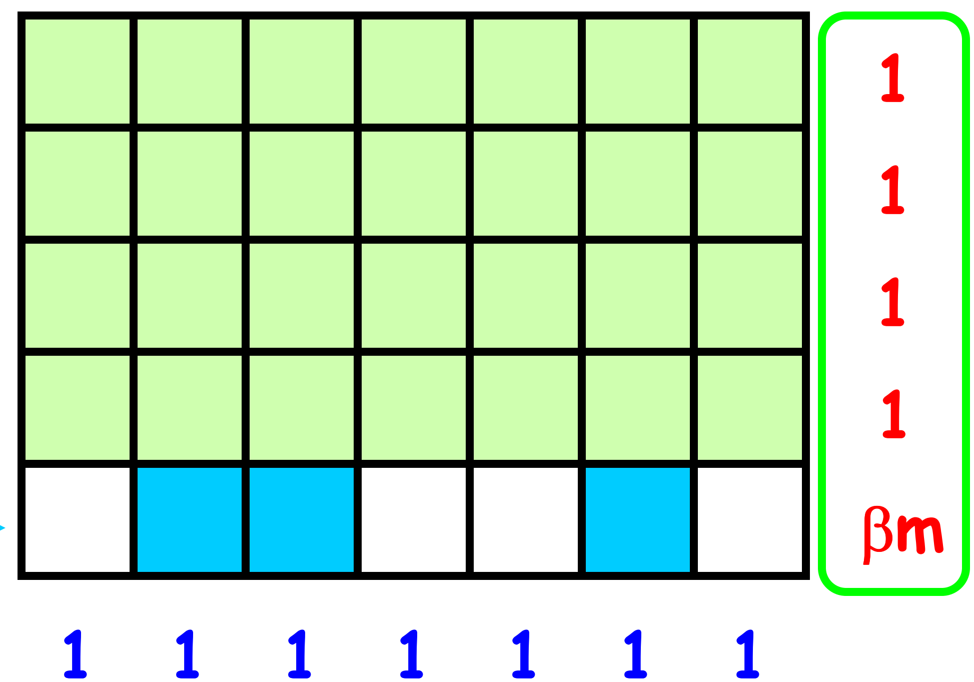

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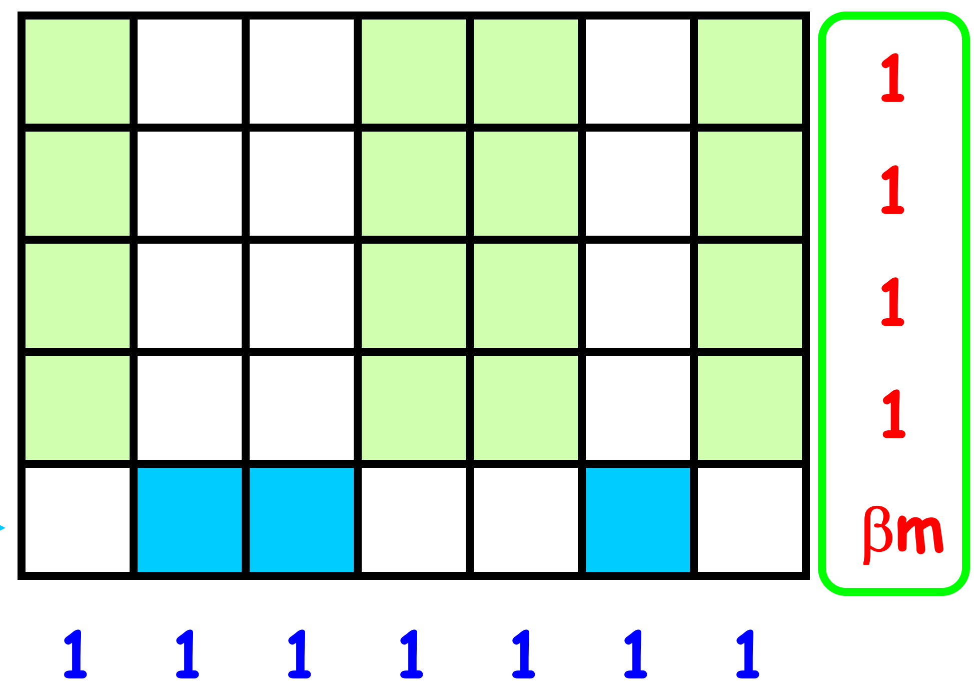

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SIS: asymptotically fewer

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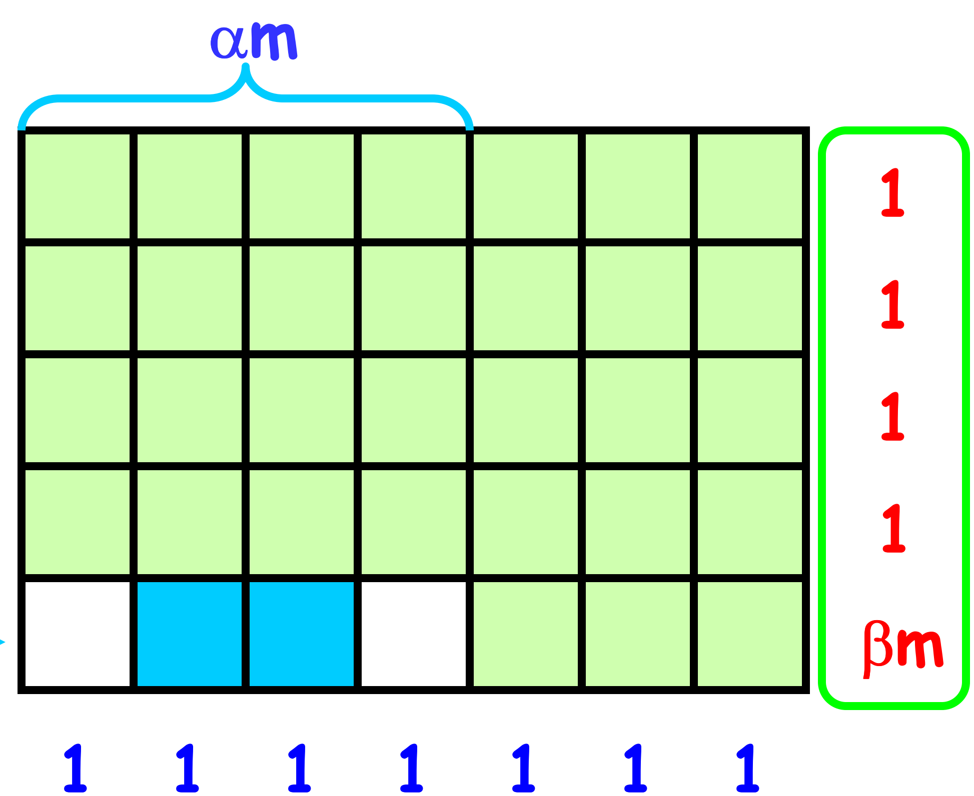

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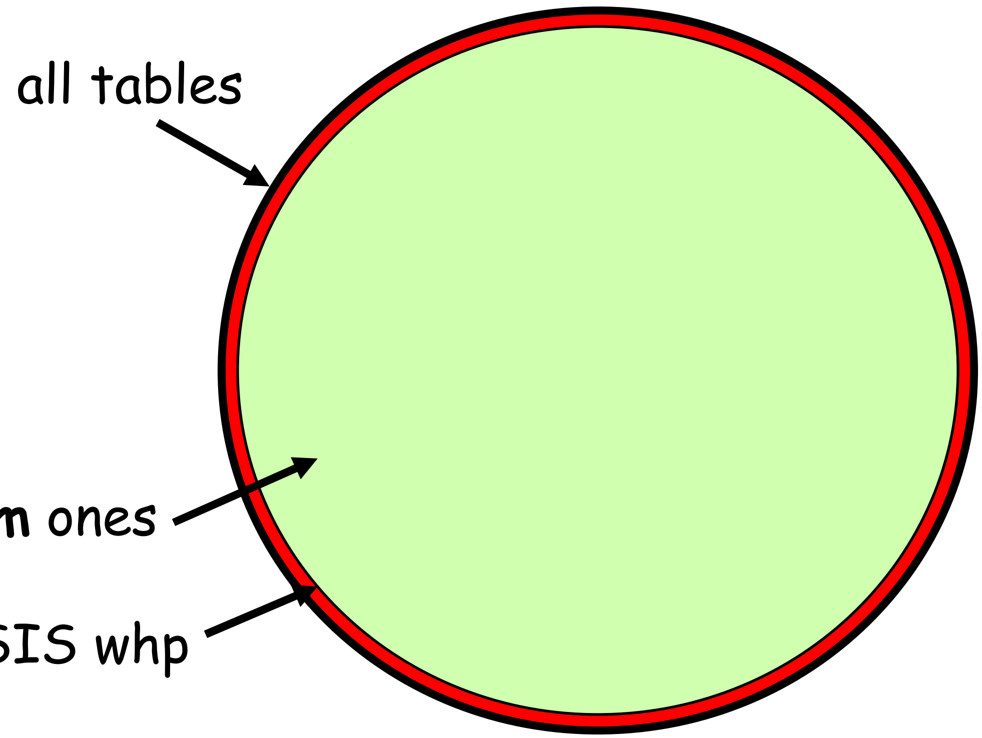
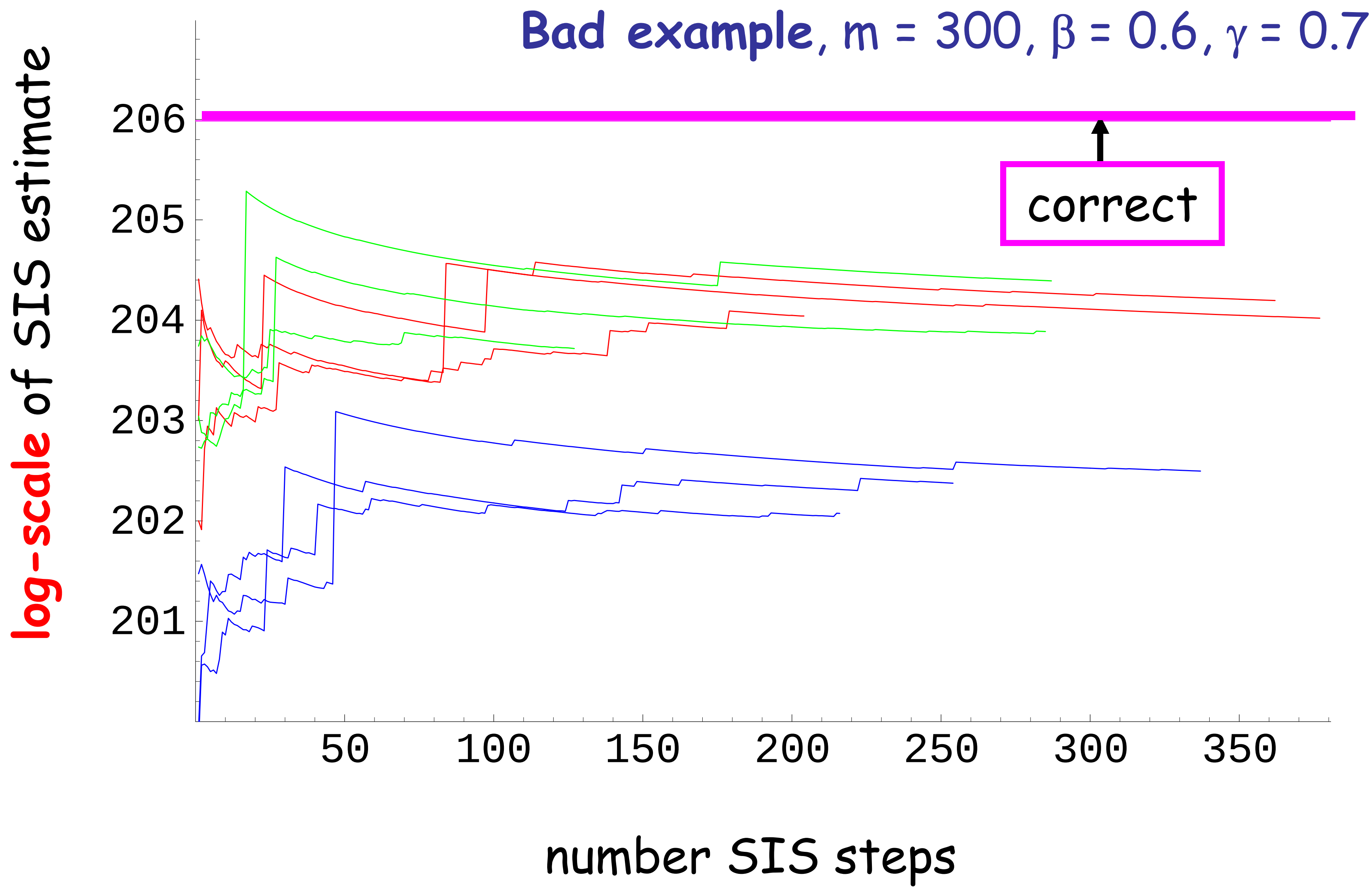


SIS - Experimental Results



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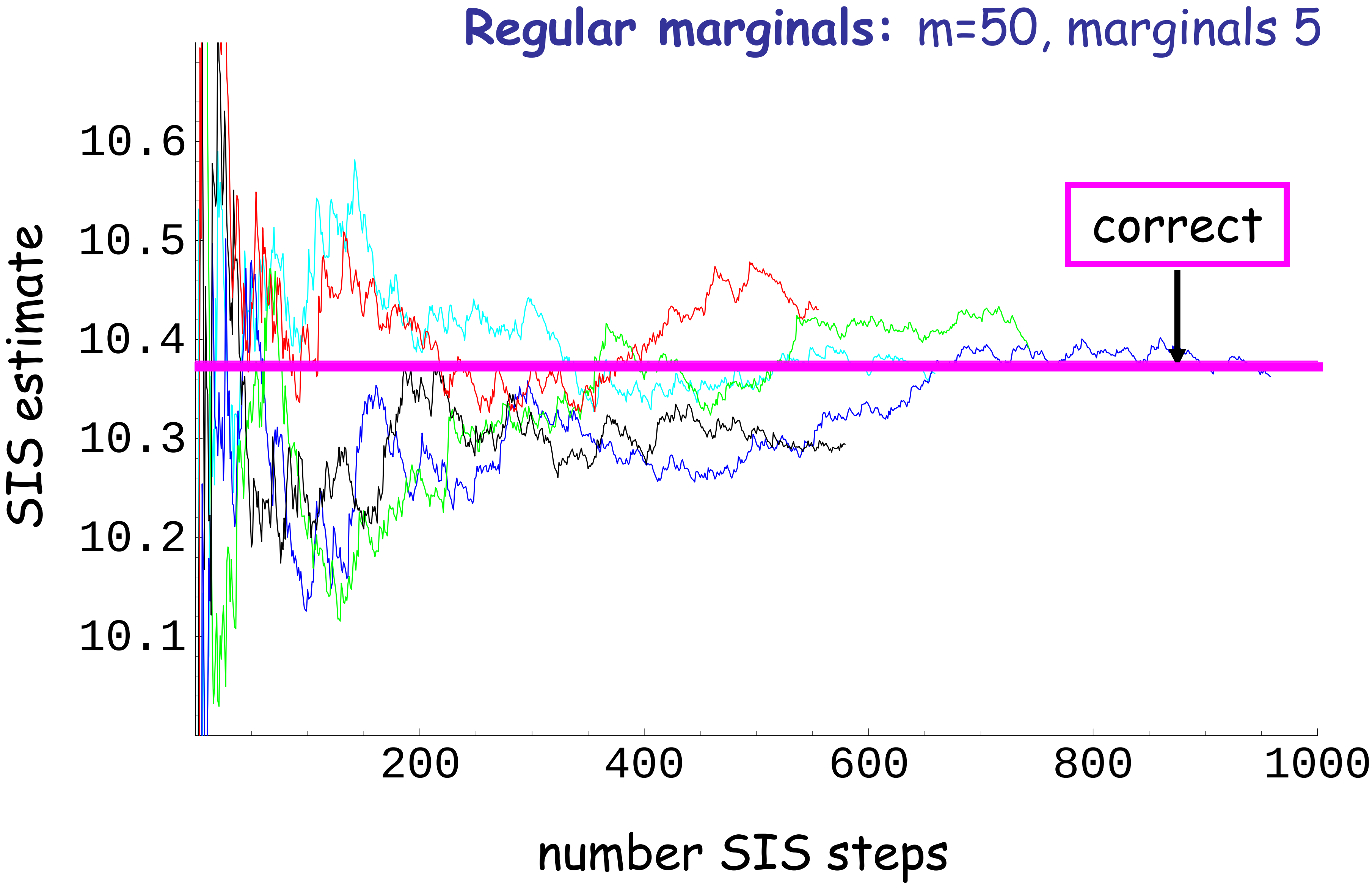
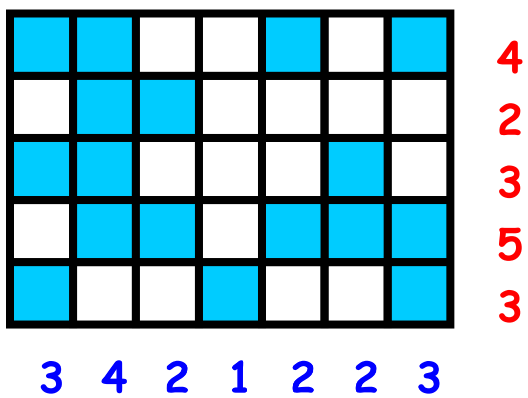
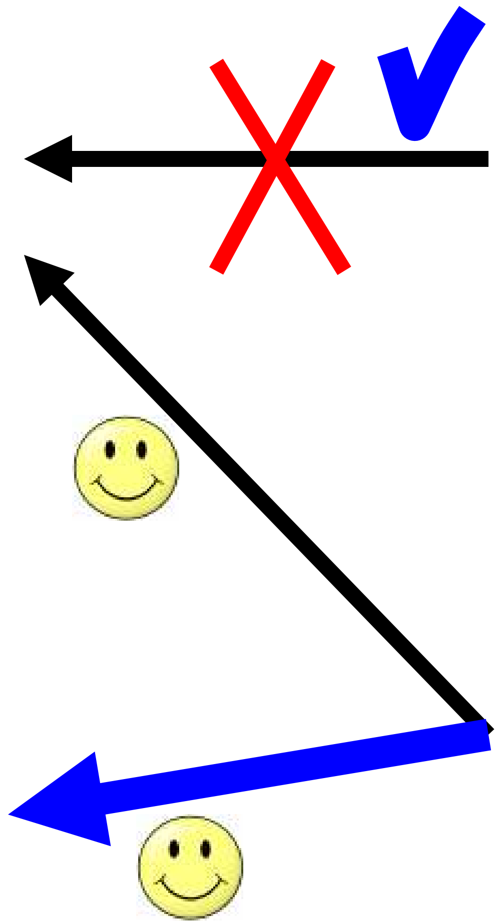


Problems

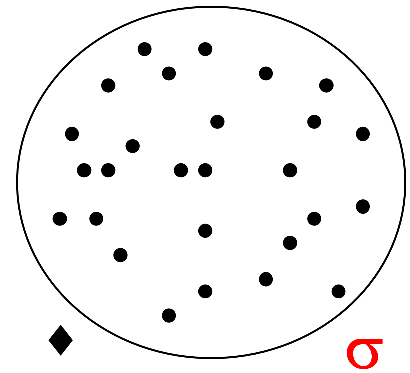
Heuristics

Binary contingency tables



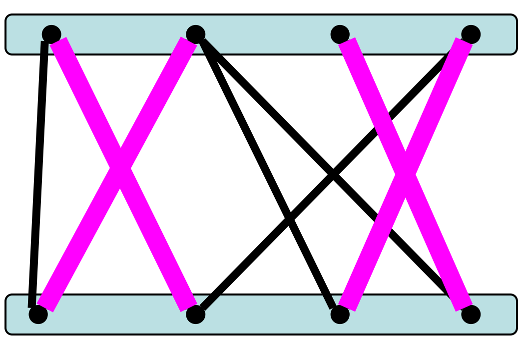


Importance sampling



Simulated annealing

Permanent

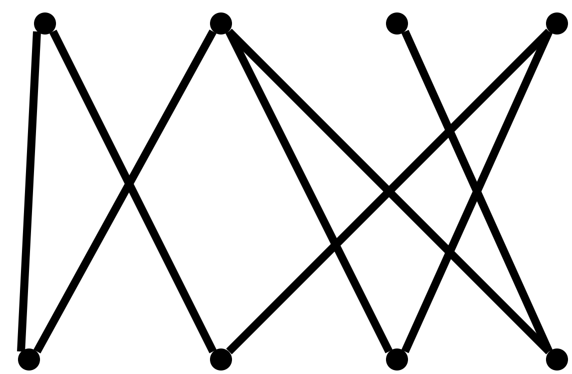


Broder Chain

[Broder '88]

What for: uniform sampling of perfect matchings

How: Markov chain on perfect + near-perfect matchings



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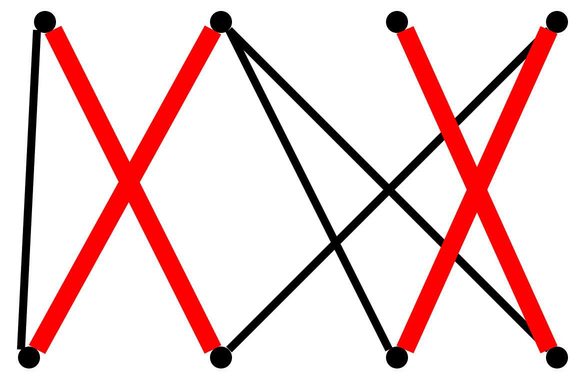

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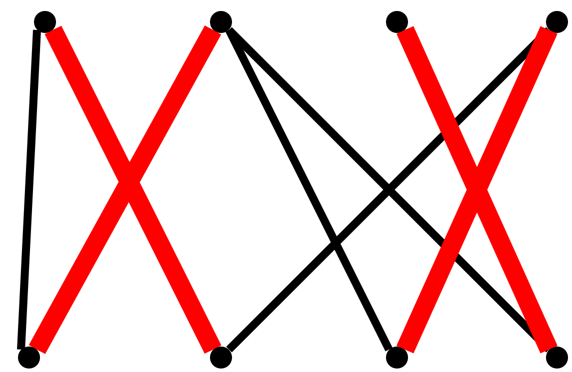

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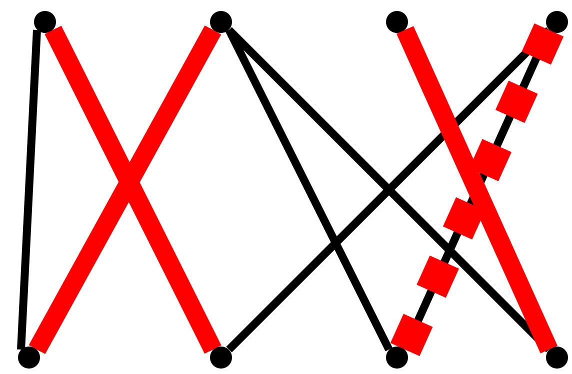

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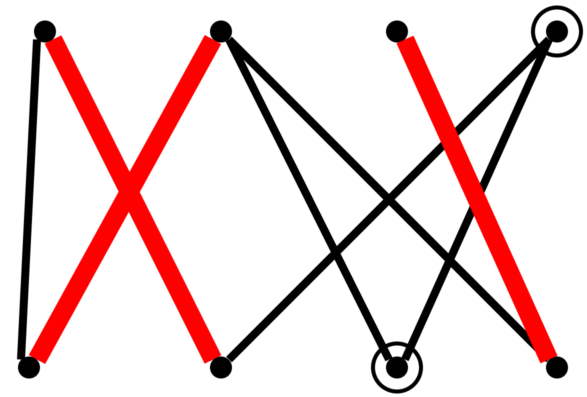

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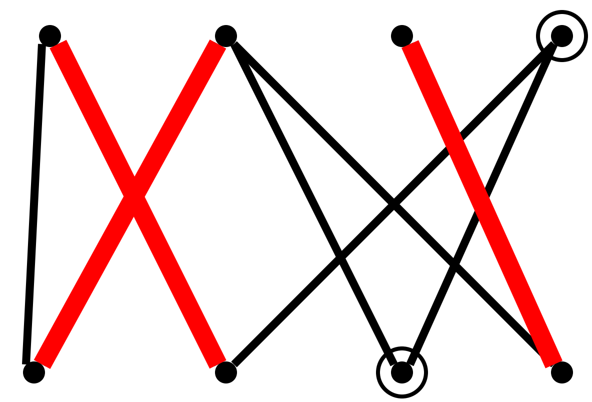

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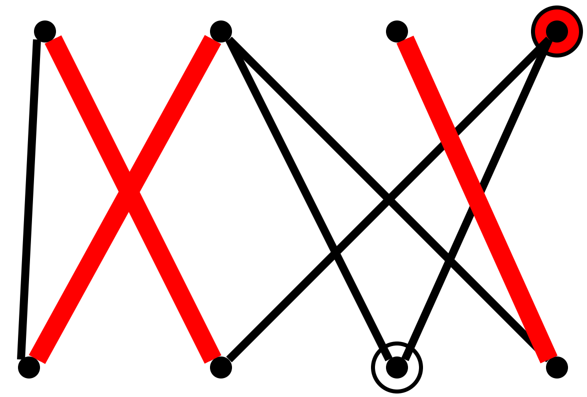

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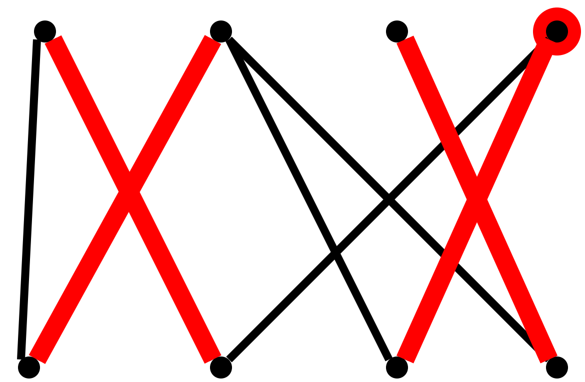

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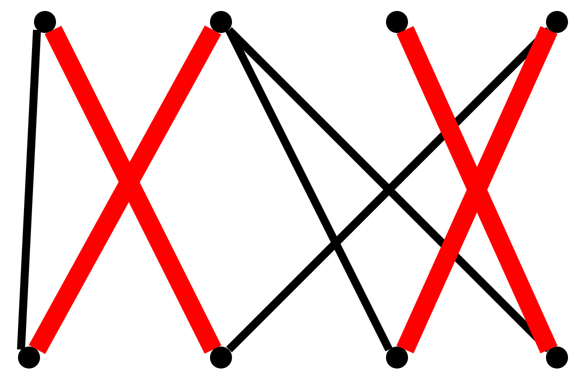

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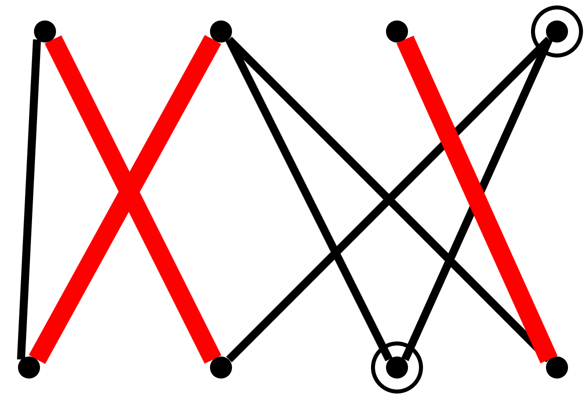

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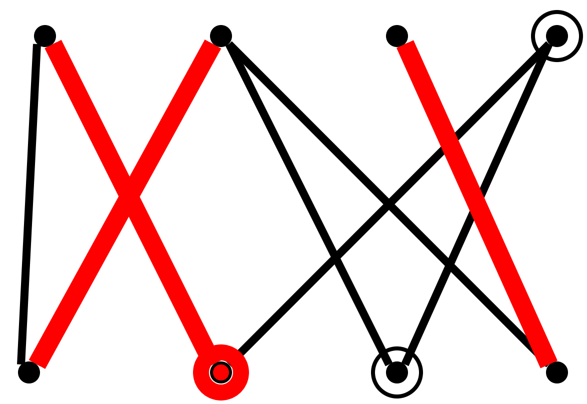

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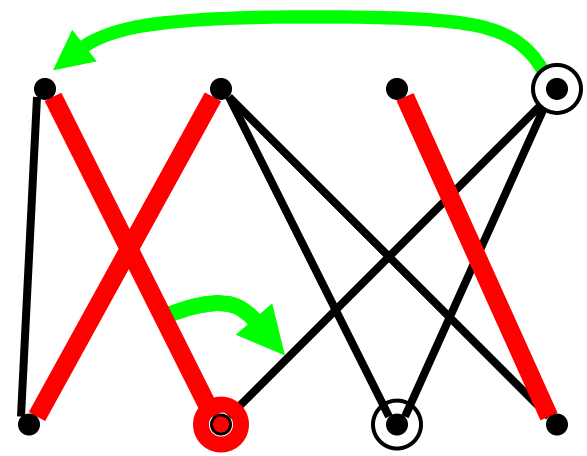

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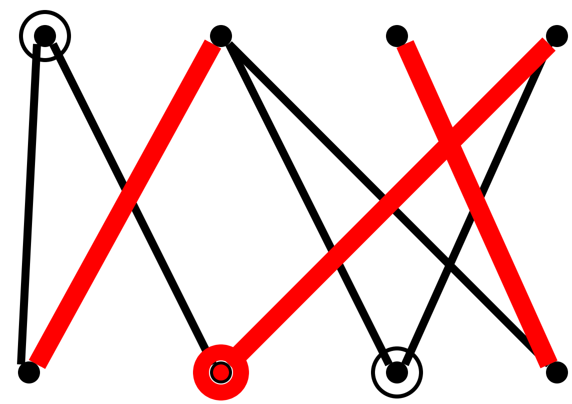

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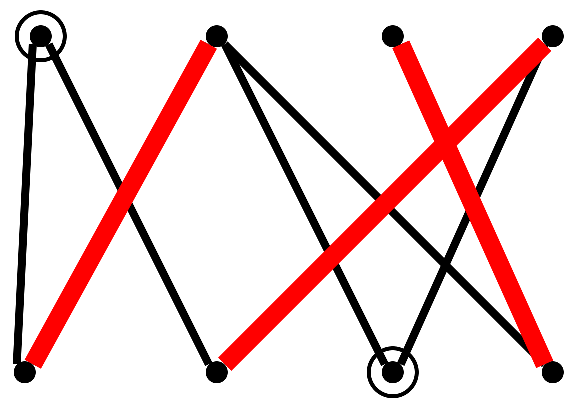

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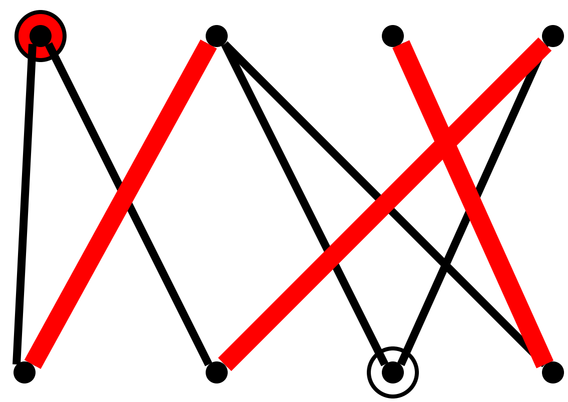

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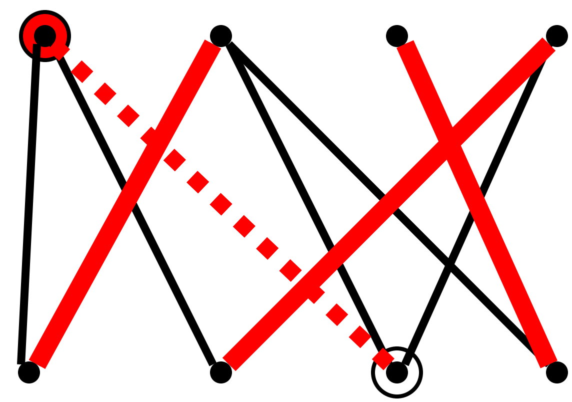

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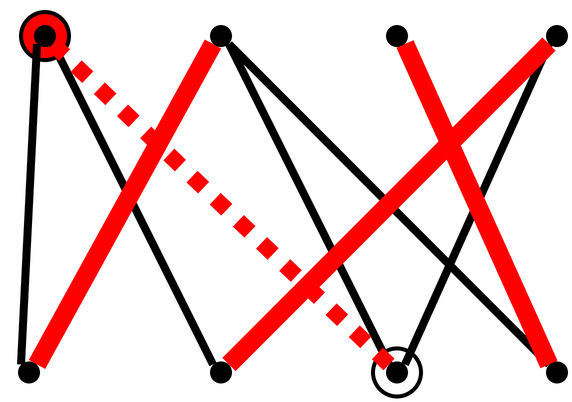

At a perfect matching:

- remove a random edge

At a near matching:

- choose a random vertex
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Broder Chain

[Broder '88]

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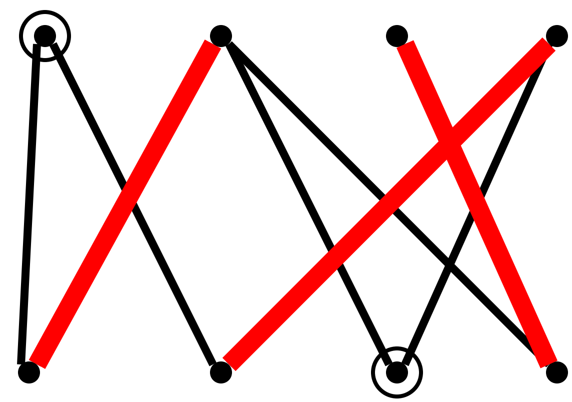

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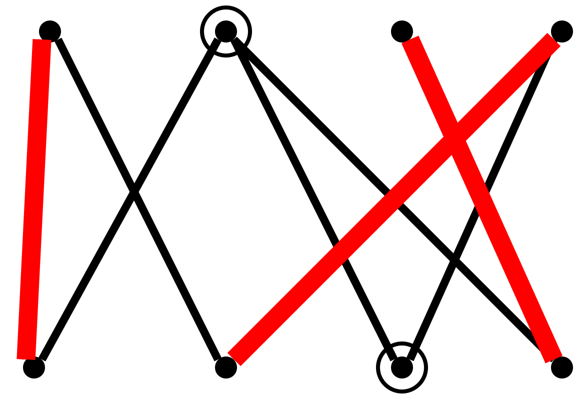

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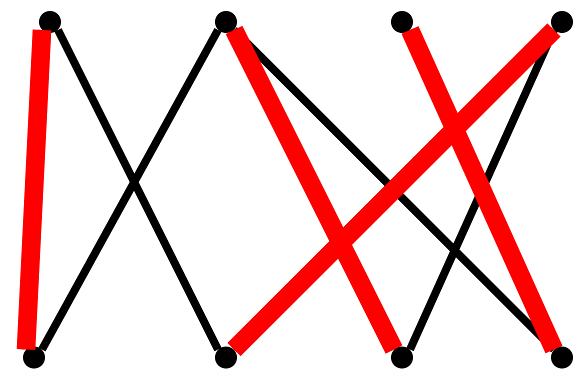

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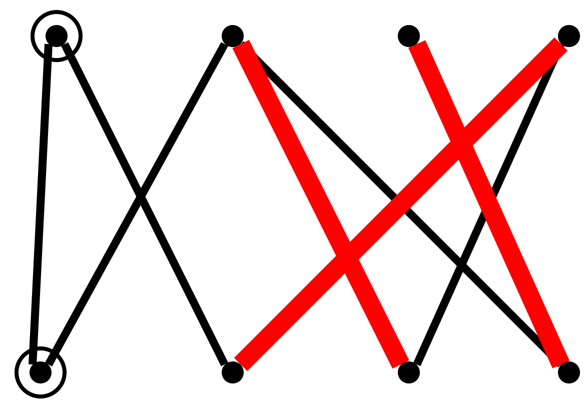

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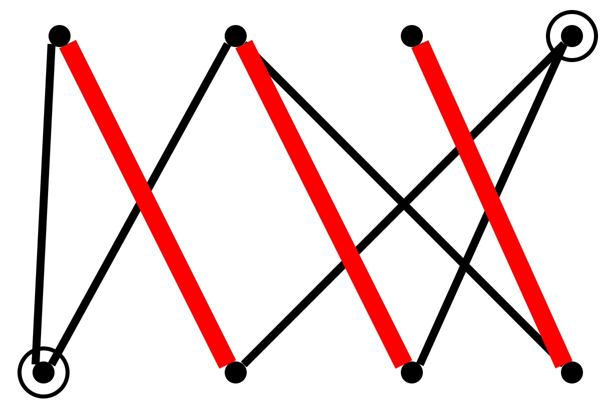

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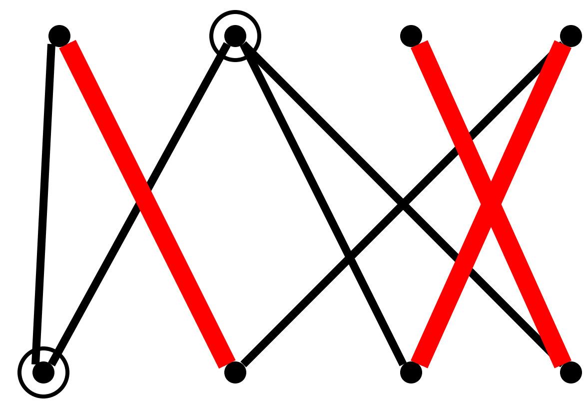

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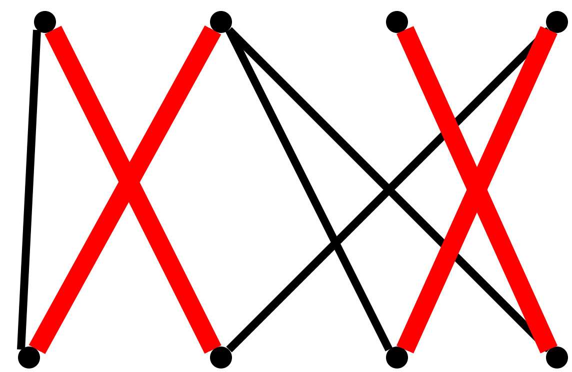

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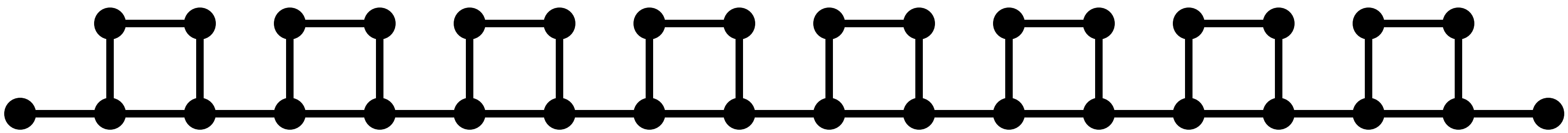
Mixes in polynomial time? Even if it did…



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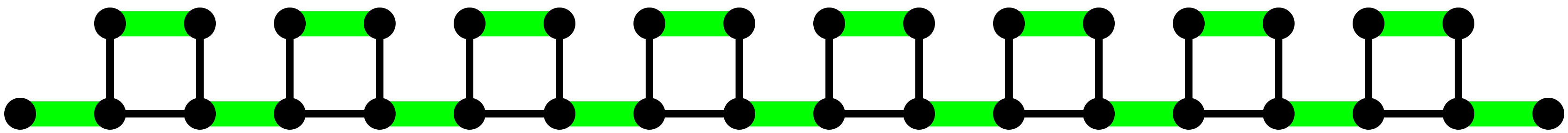

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Broder Chain

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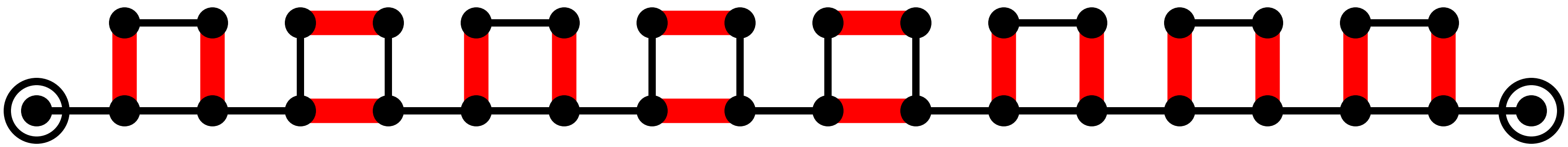
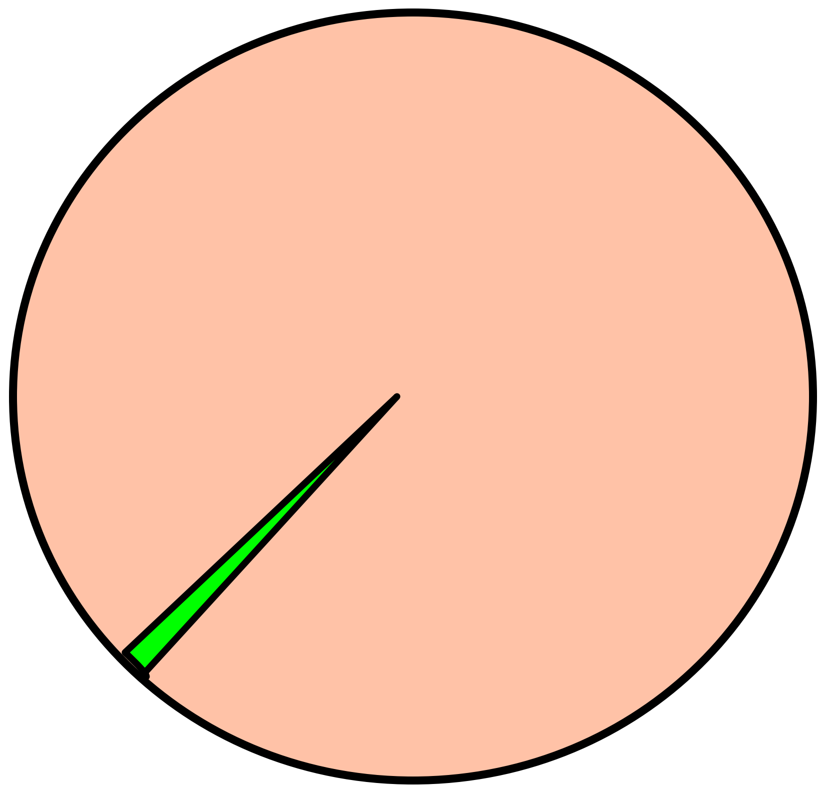


1 perfect matching

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



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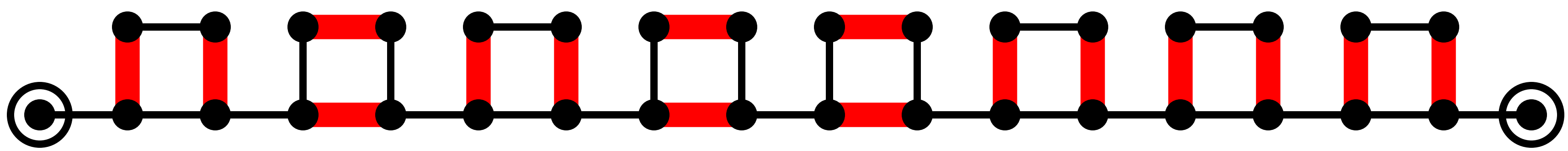

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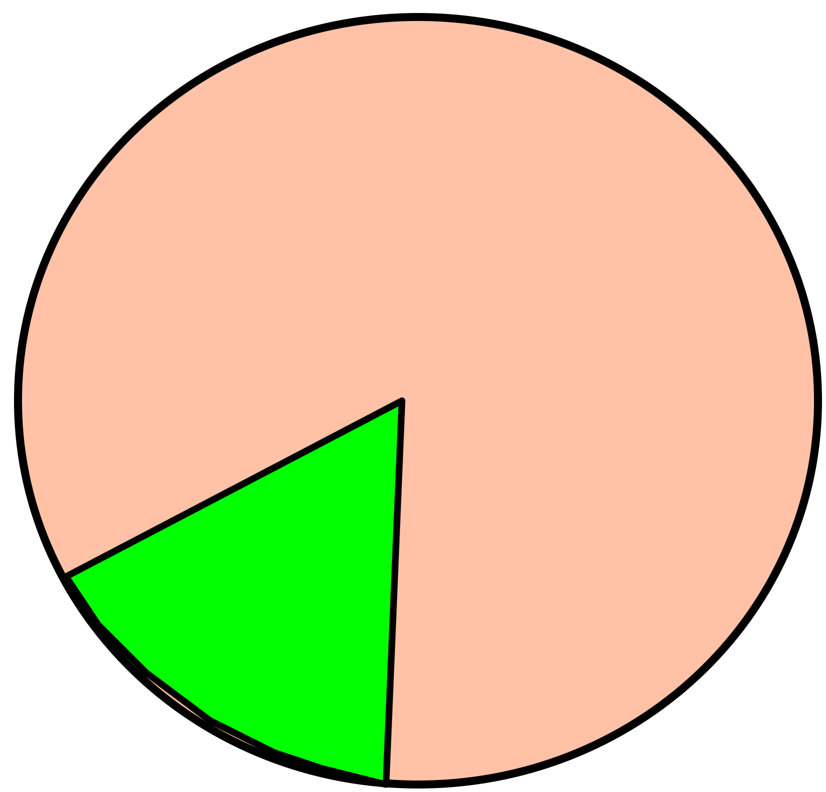


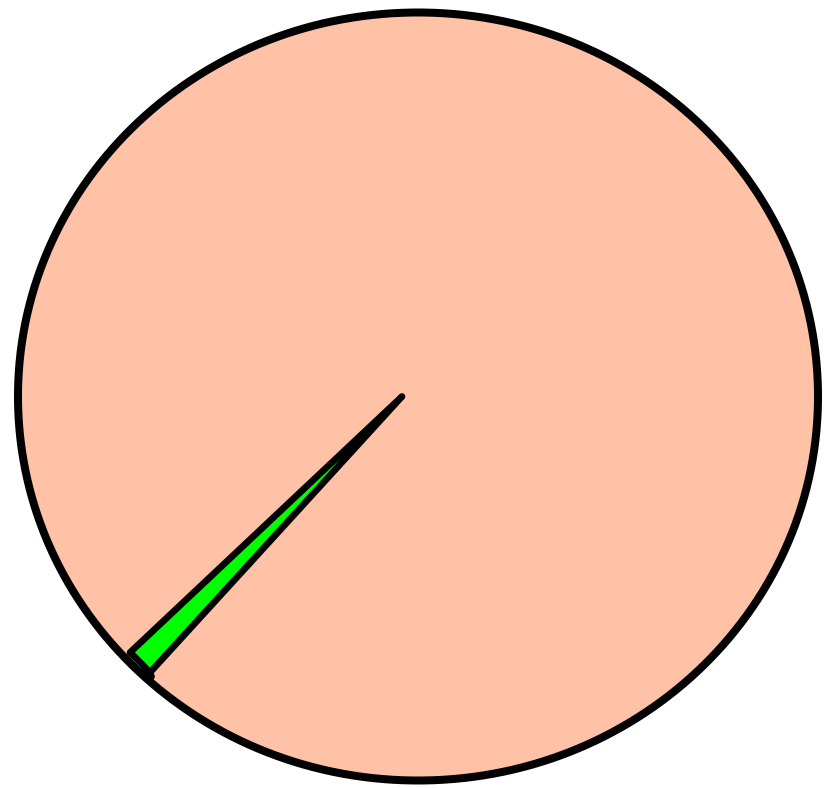
Thm [Jerrum-Sinclair '89]:

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.



Broder Chain

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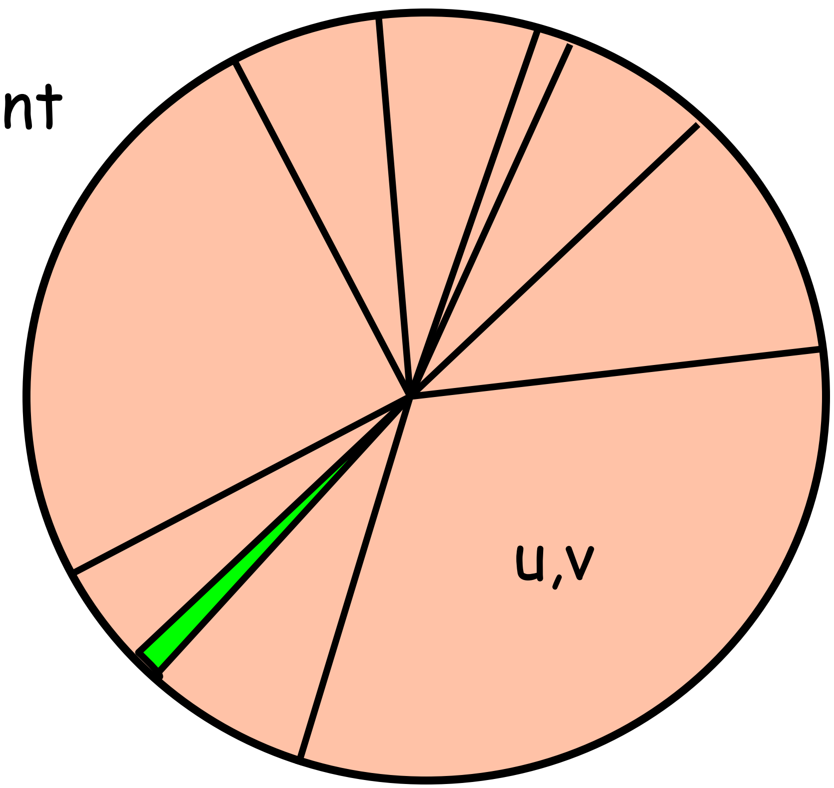
n^2+1 regions, very different size



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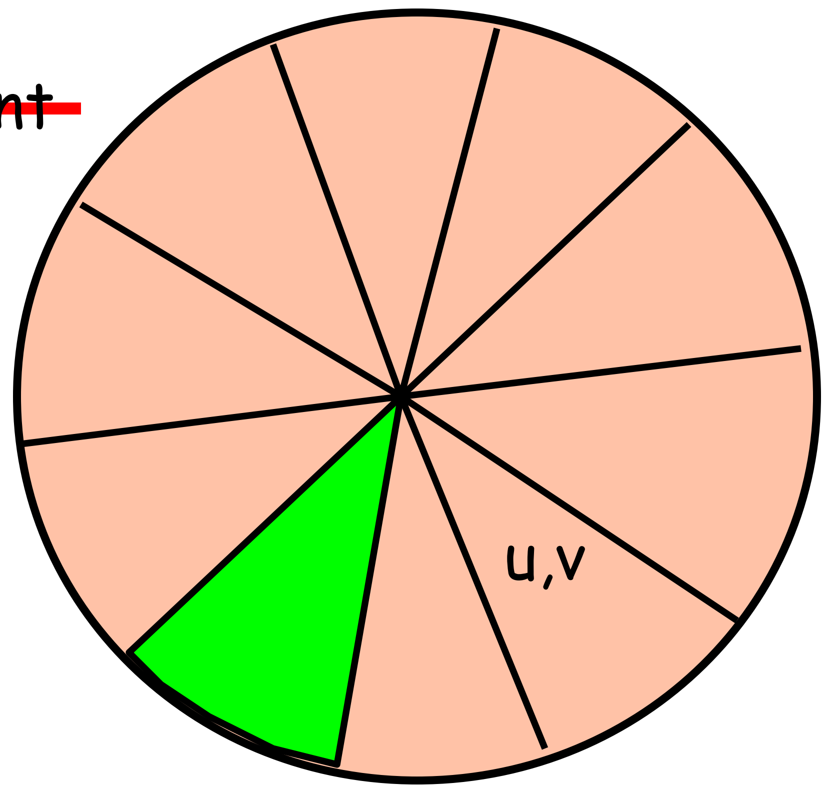

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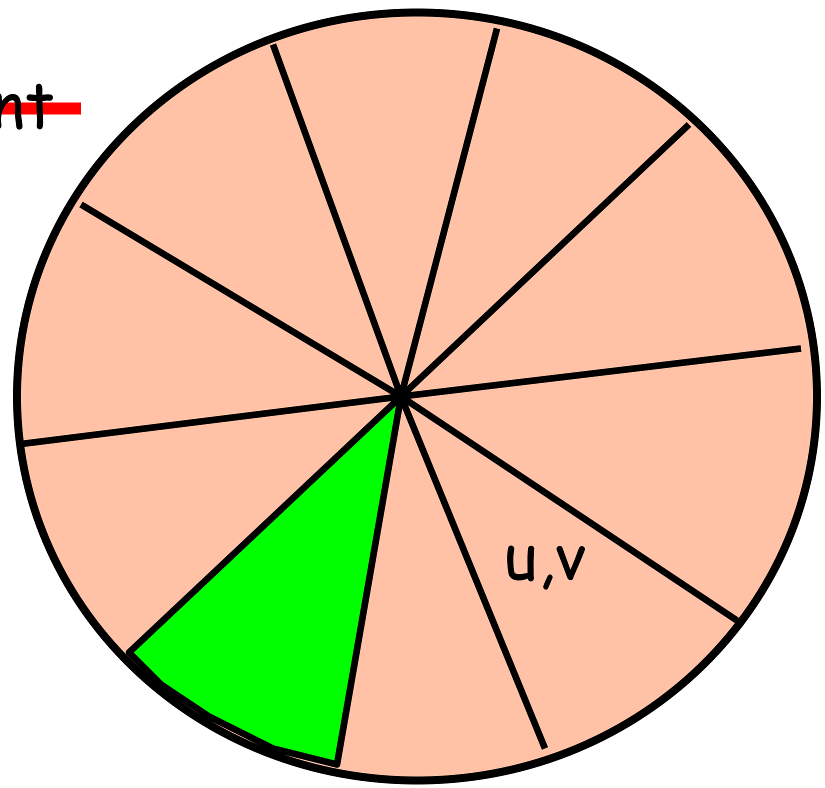

Ideal weights
(for a matching with holes u,v):

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

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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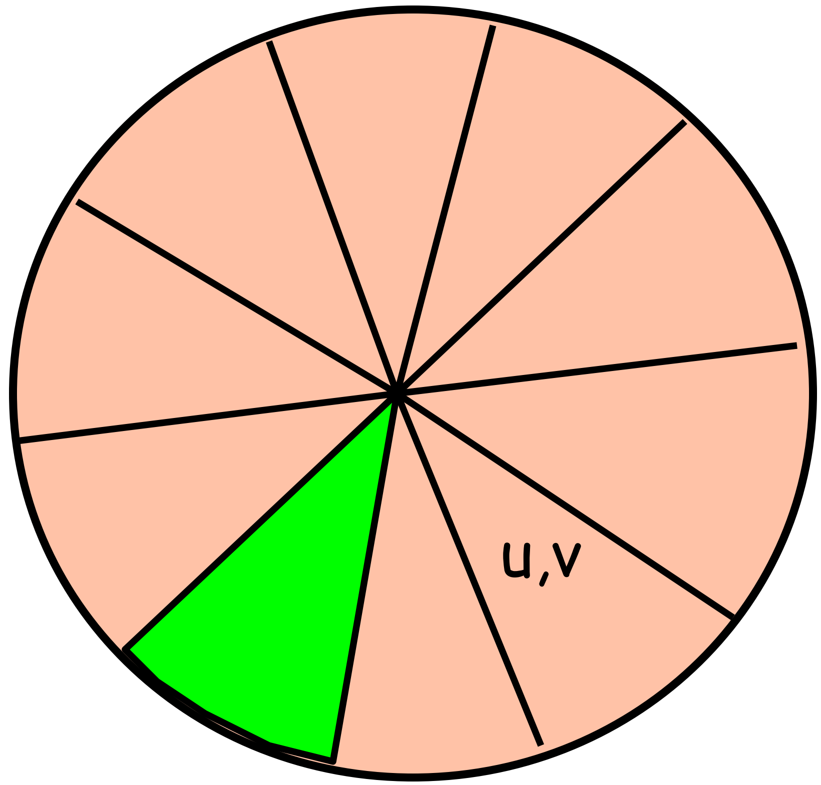

Simulated Annealing for Permanent

Unordered state → Ordered state

(EASY) (DIFFICULT)

$\boxed{G}$

Solution: **Approximate**

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Simulated Annealing for Permanent

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(EASY) (DIFFICULT)

$K_{n,n}$ → G

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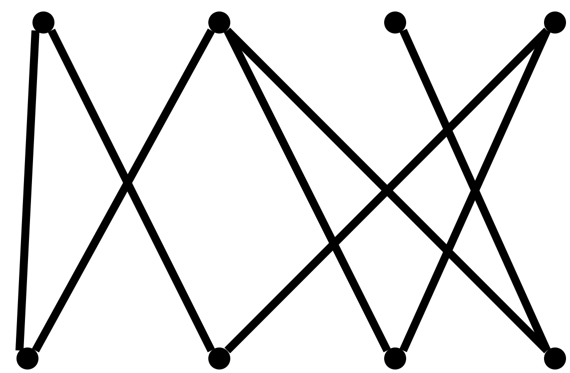

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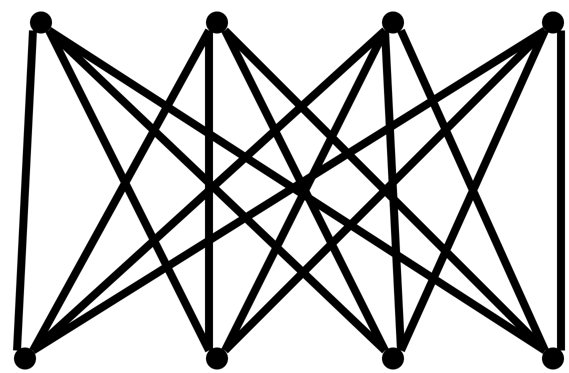

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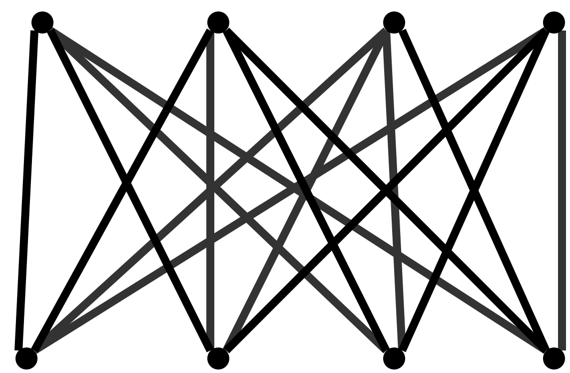

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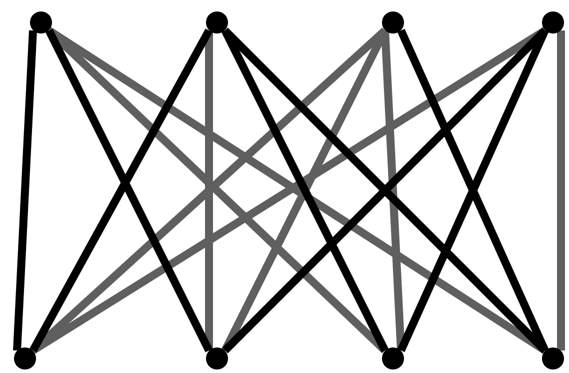

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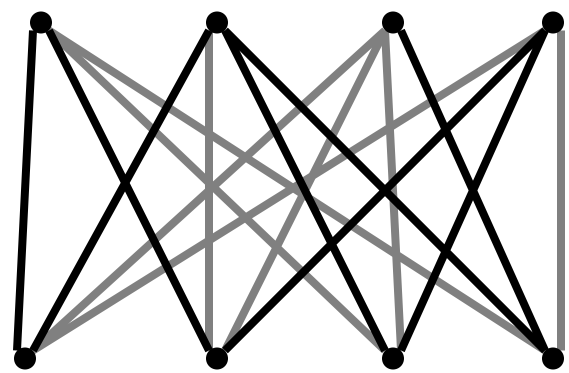

Simulated Annealing for Permanent

Unordered state → Ordered state

(EASY) (DIFFICULT)

$\boxed{K_{n,n}} \longrightarrow \boxed{G}$

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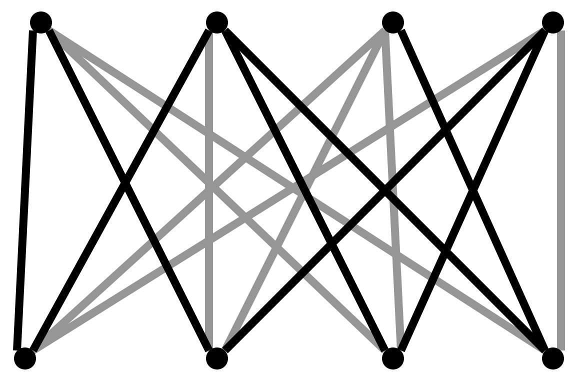

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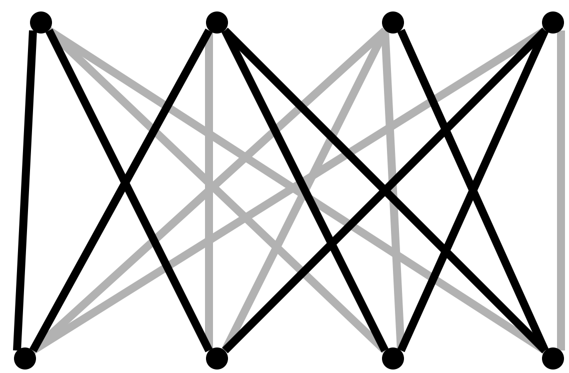

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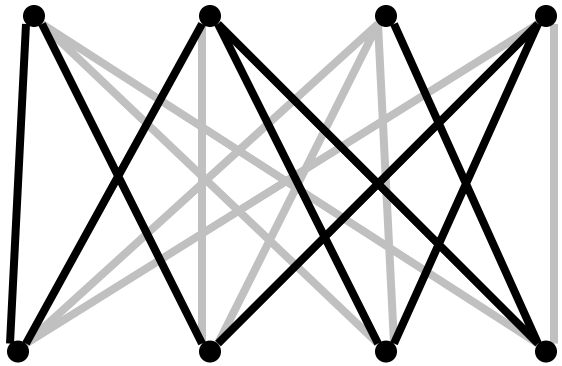

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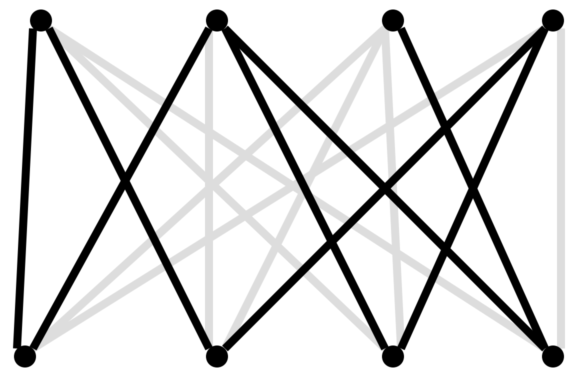

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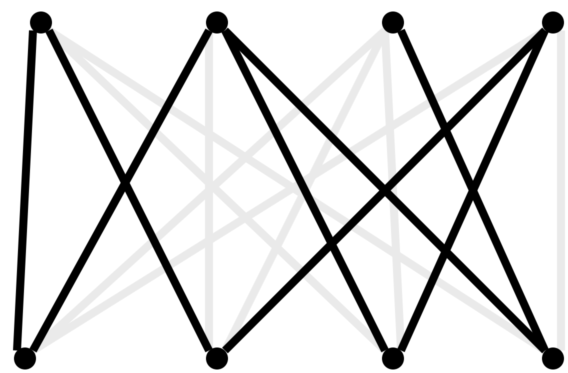

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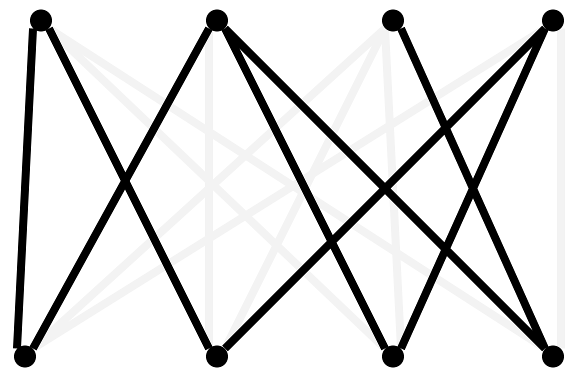

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(EASY) (DIFFICULT)

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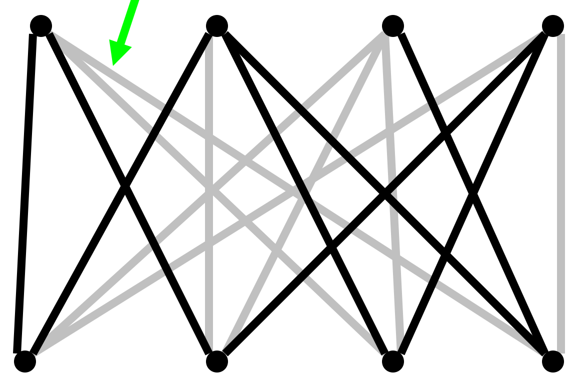
Solution: **Approximate**

$\boxed{\lambda}$ = 1 ... ~0



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New Cooling Schedule

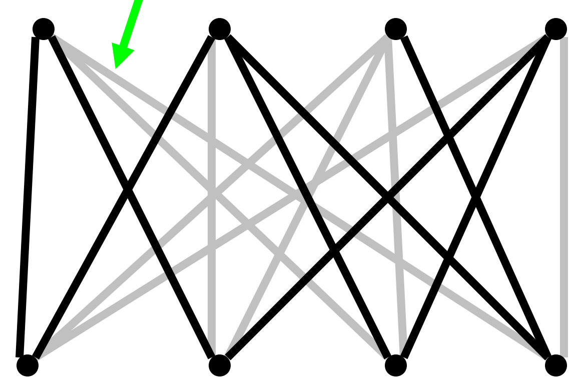
[Bezáková-Štefankovič-
Vazirani-Vigoda SODA '06]

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

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

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

$\boxed{\lambda}$ = 1 ... ~0



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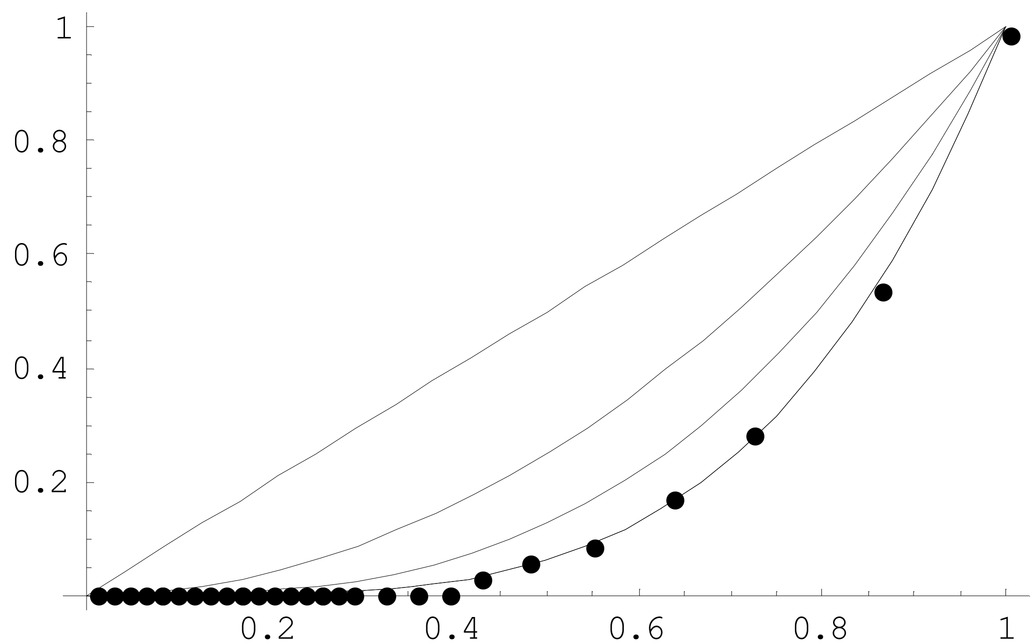

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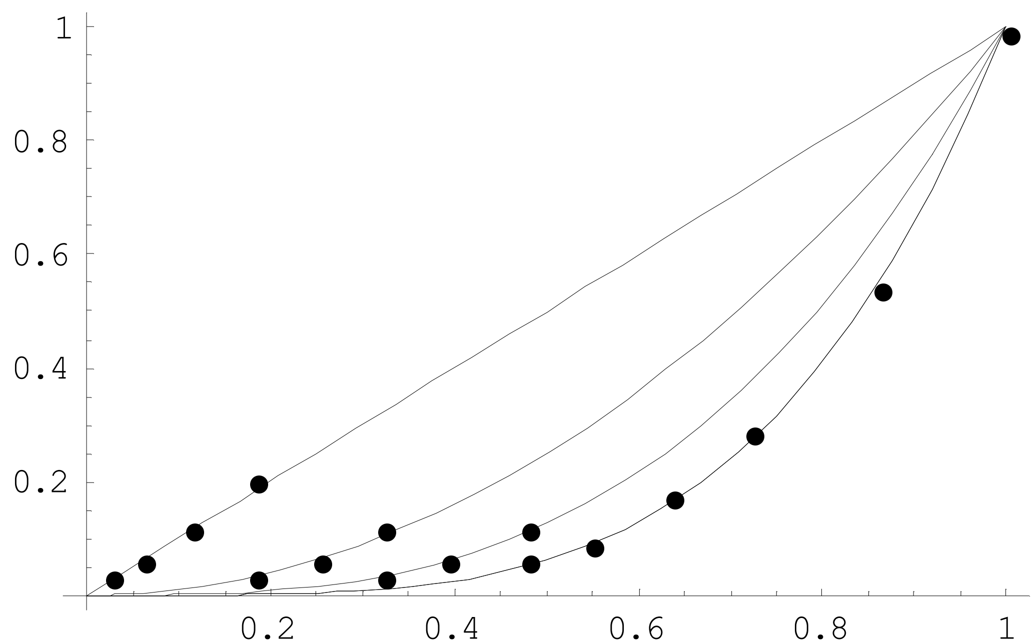
Idea: make use of low degrees.



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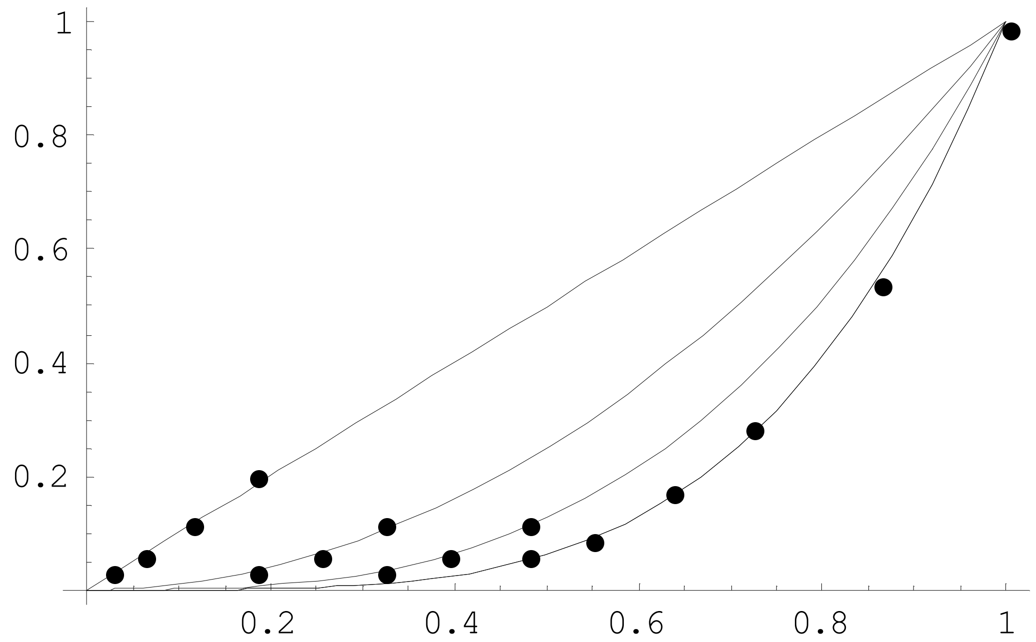
Thm [BŠVV '06]:

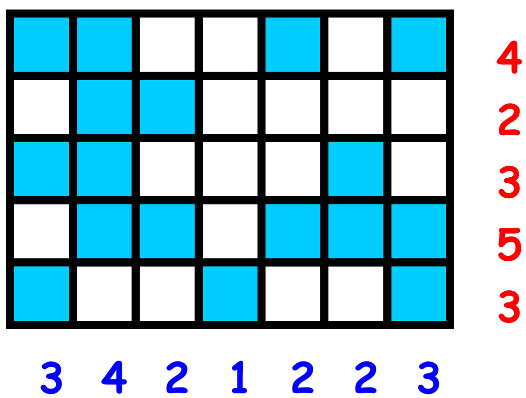
Permanent of nonnegative matrix in time **$O^*(n^7)$**.



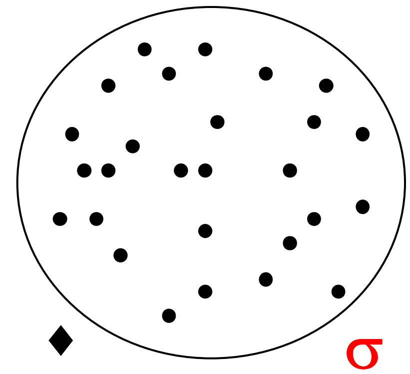
Problems

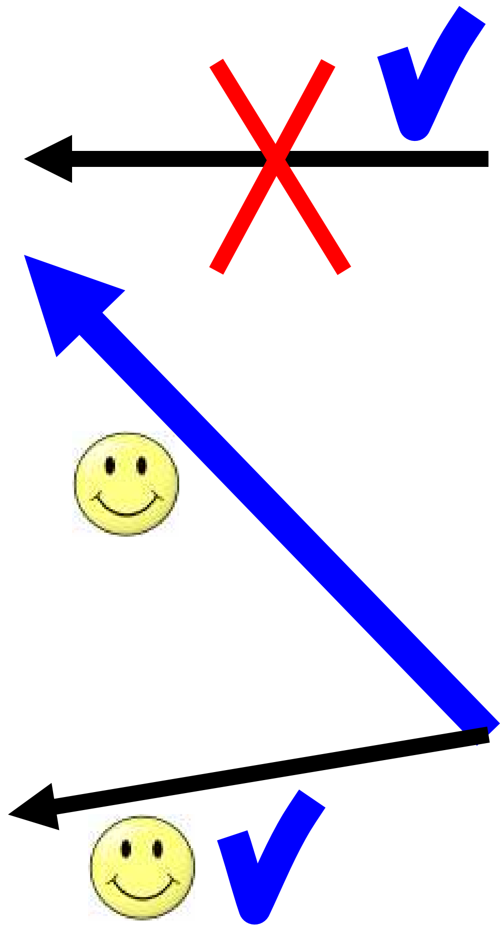
Heuristics

Binary contingency tables

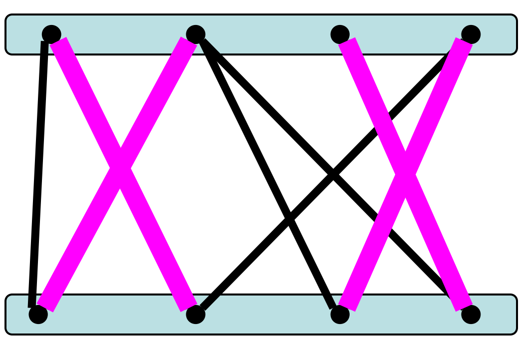


Importance sampling



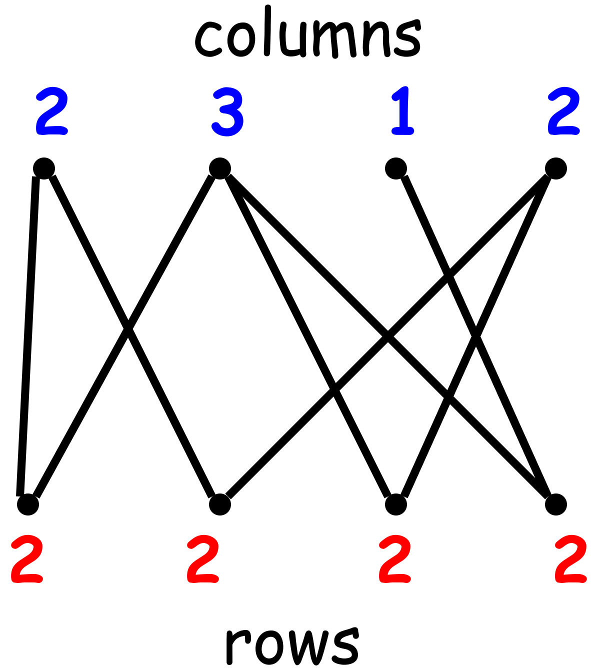


Permanent



Simulated annealing

BCT: Bipartite Graphs with Given Degrees



columns

rows					
	1	1	0	0	2
	1	0	0	1	2
	0	1	0	1	2
	0	1	1	0	2
	2	3	1	2	

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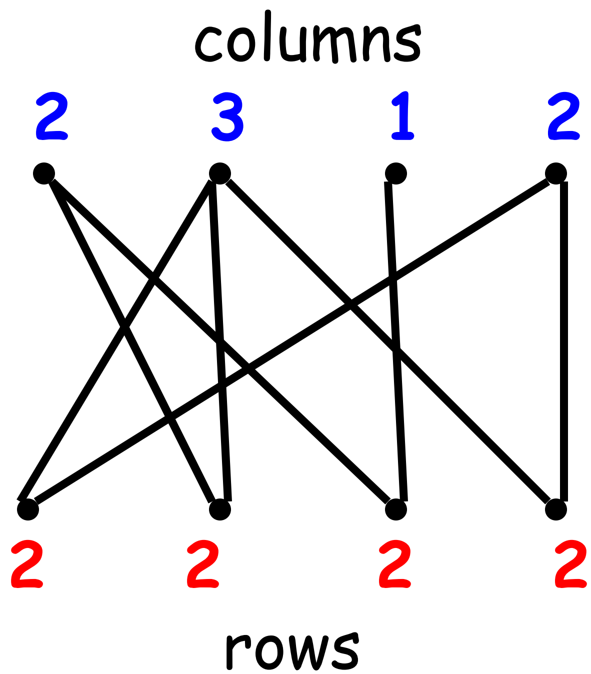

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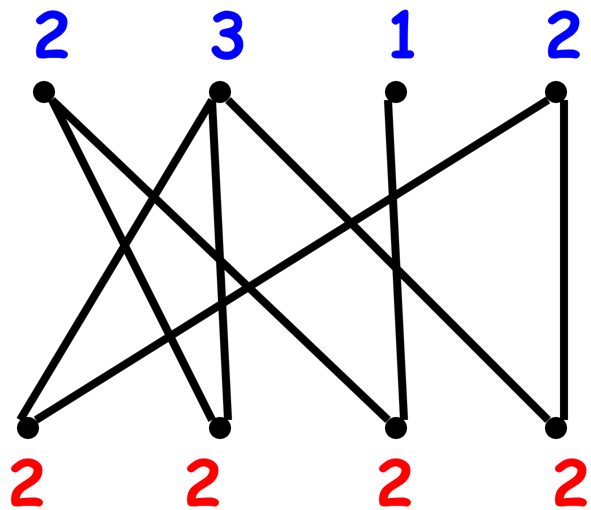

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"Sliding" Markov Chain on perfect and near tables

Perfect: remove a random edge

Near: slide edges or match

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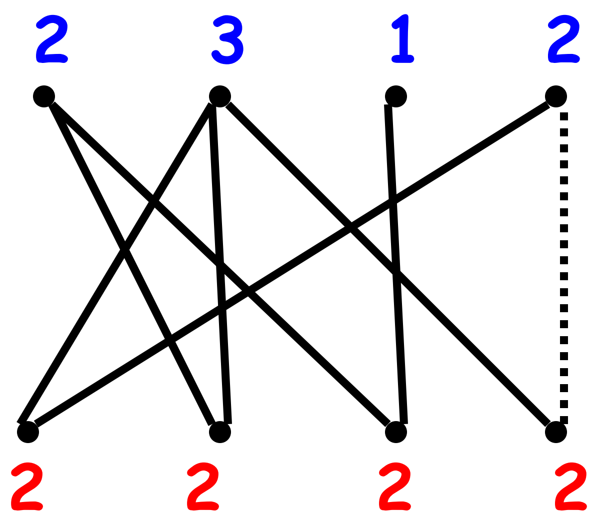

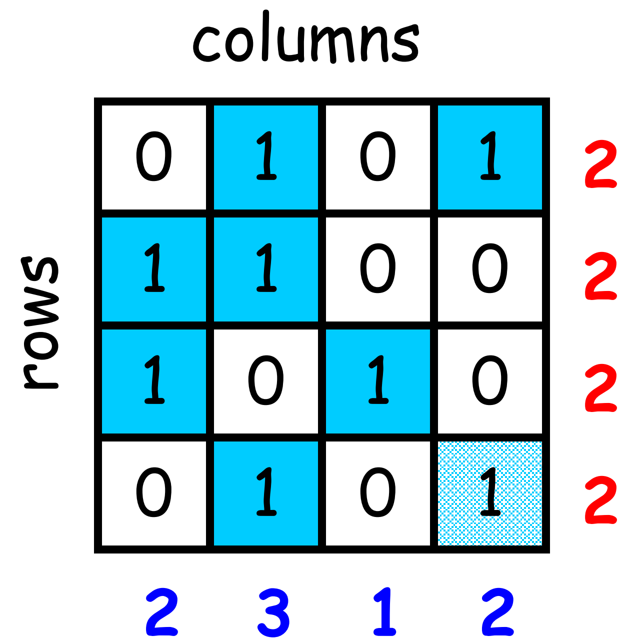

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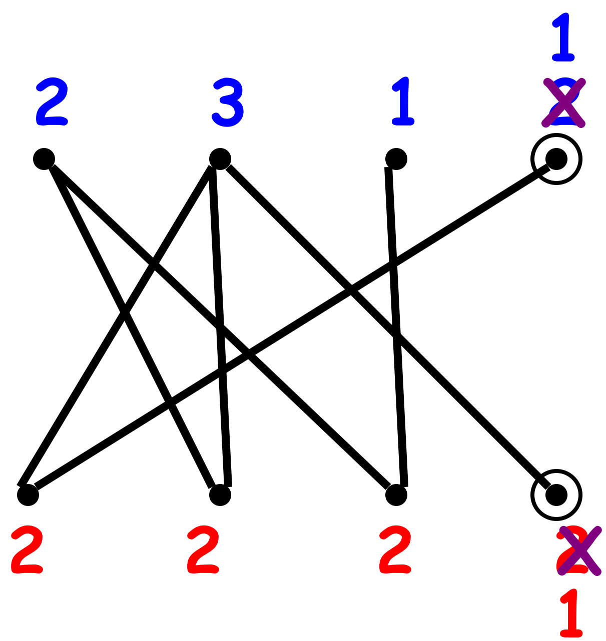

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rows

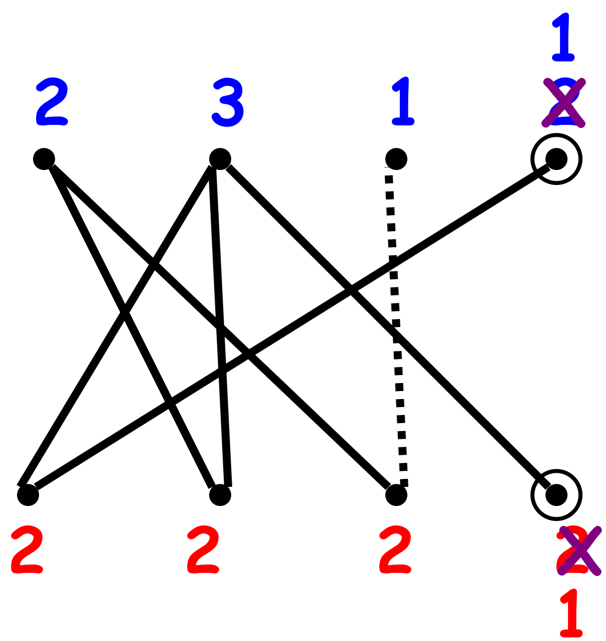
0	1	0	1	2
1	1	0	0	2
1	0	1	0	2
0	1	0	0	~~2~~ 1
2	3	1	~~2~~ 1	

"Sliding" Markov Chain on perfect and near tables

Perfect: remove a random edge

Near: slide edges or match

BCT: Bipartite Graphs with Given Degrees



columns

rows					
	0	1	0	1	2
	1	1	0	0	2
	1	0	1	0	2
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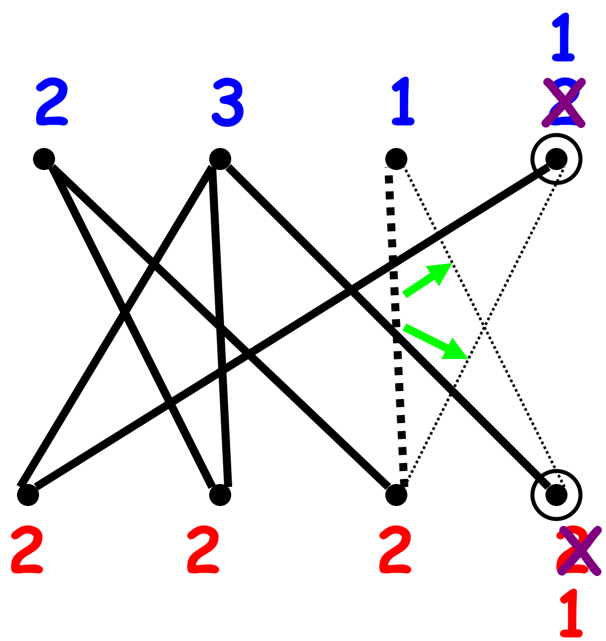

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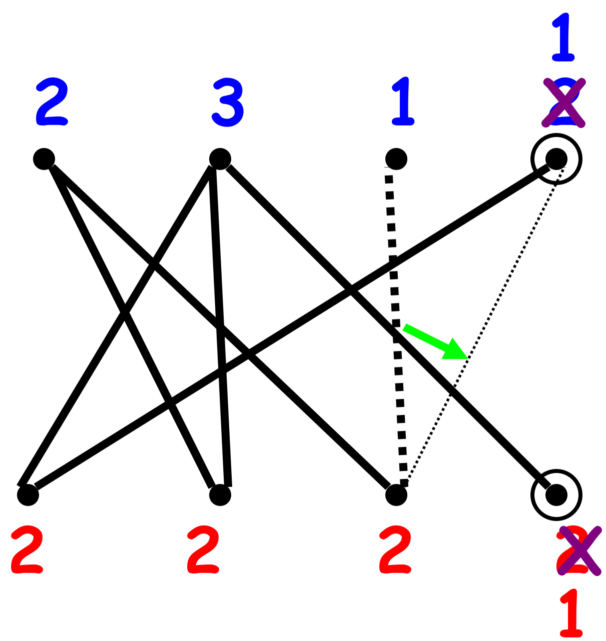

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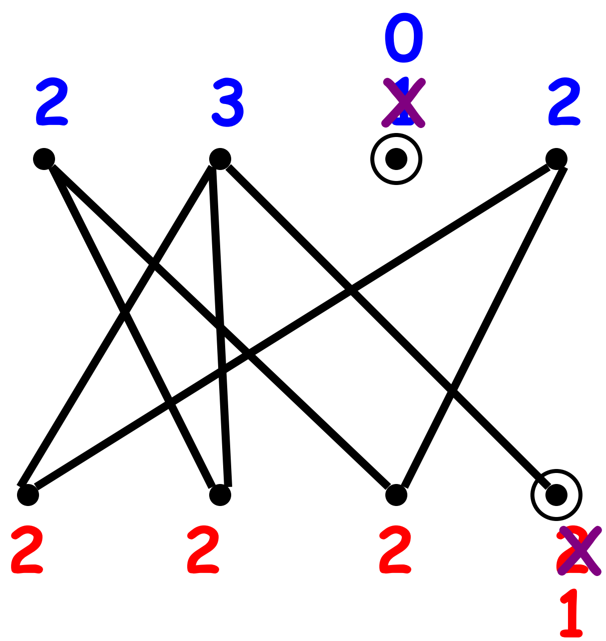

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rows

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1	1	0	0	2
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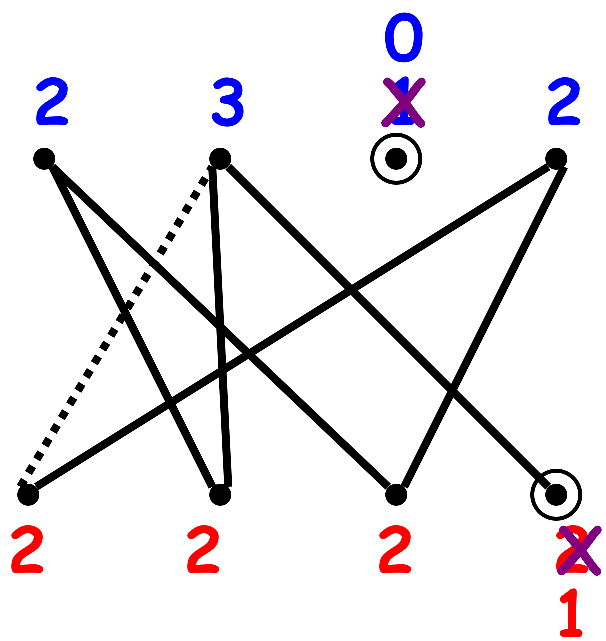

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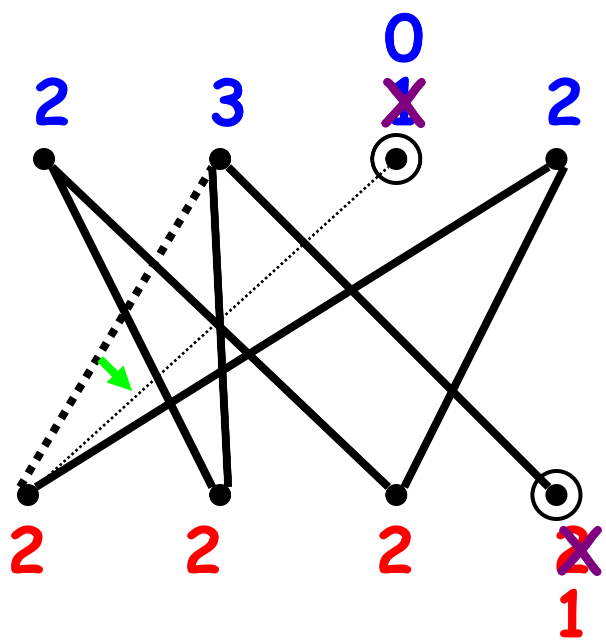

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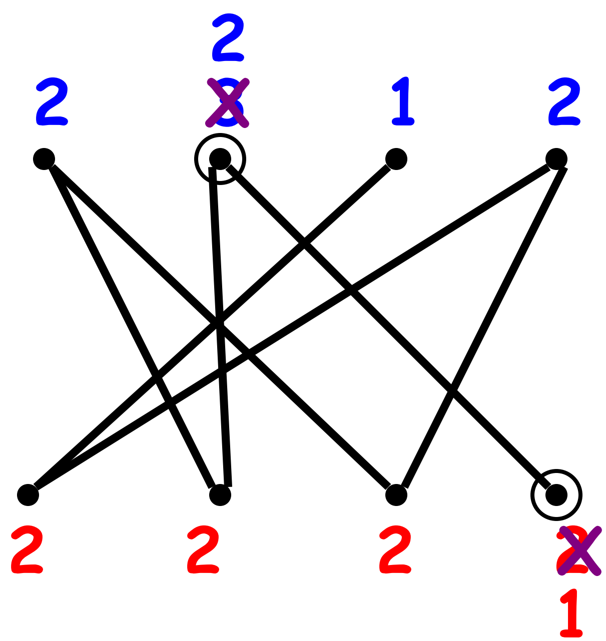

columns

rows	0	1	0	1	2
	1	0	1	0	2
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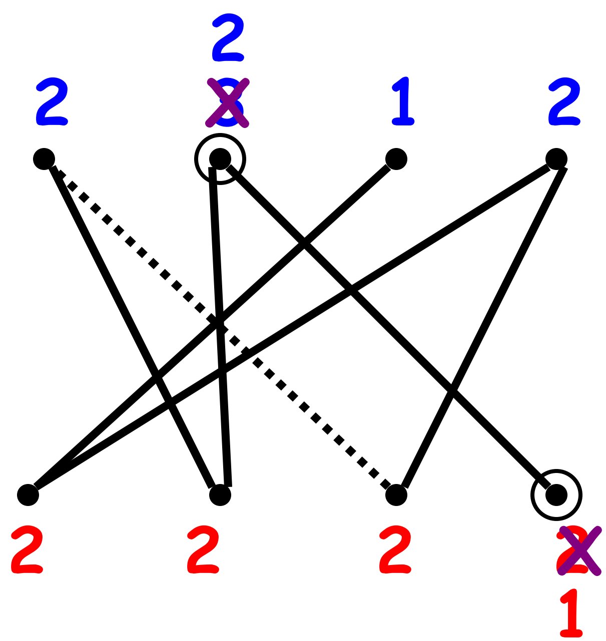

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1	0	1	0	2
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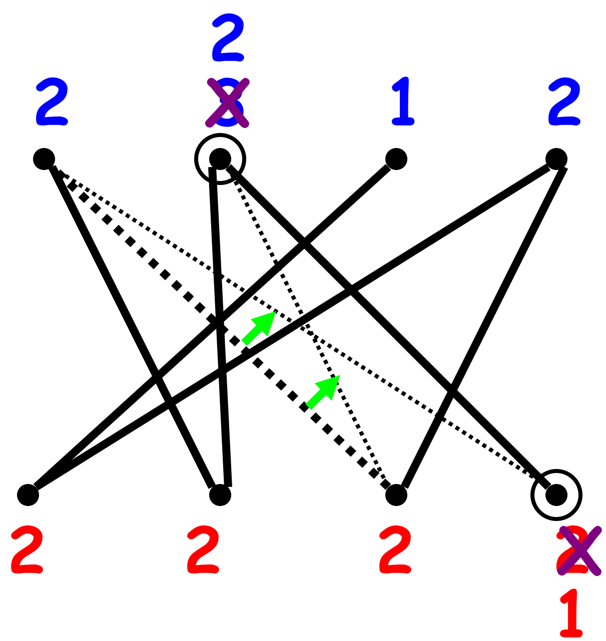

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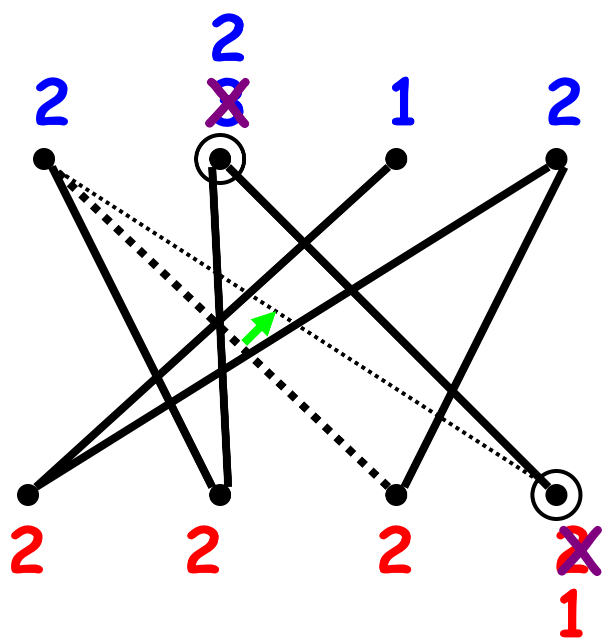

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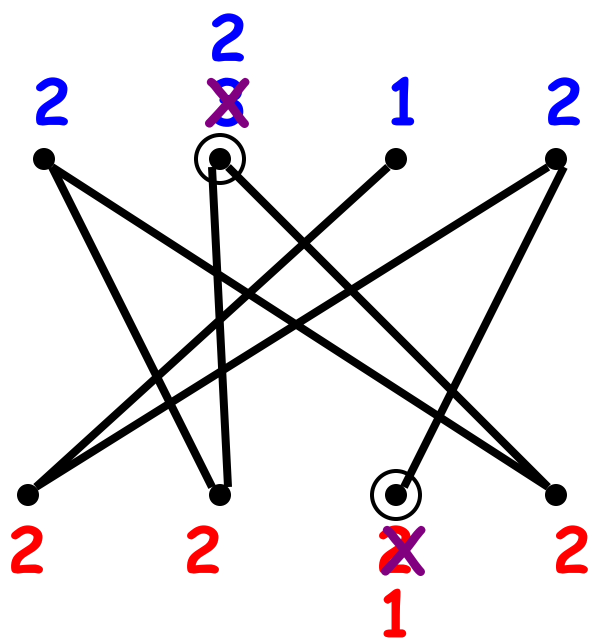

columns

$$\text{rows}\quad\begin{array}{|c|c|c|c|c}
\hline
0 & 1 & 0 & 1 & 2 \\
\hline
1 & 0 & 1 & 0 & 2 \\
\hline
0 & 0 & 0 & 1 & \cancel{2}\ 1 \\
\hline
1 & 1 & 0 & 0 & 2 \\
\hline
\multicolumn{1}{c}{2} & \multicolumn{1}{c}{\cancel{3}\ 2} & \multicolumn{1}{c}{1} & \multicolumn{1}{c}{2} &
\end{array}$$

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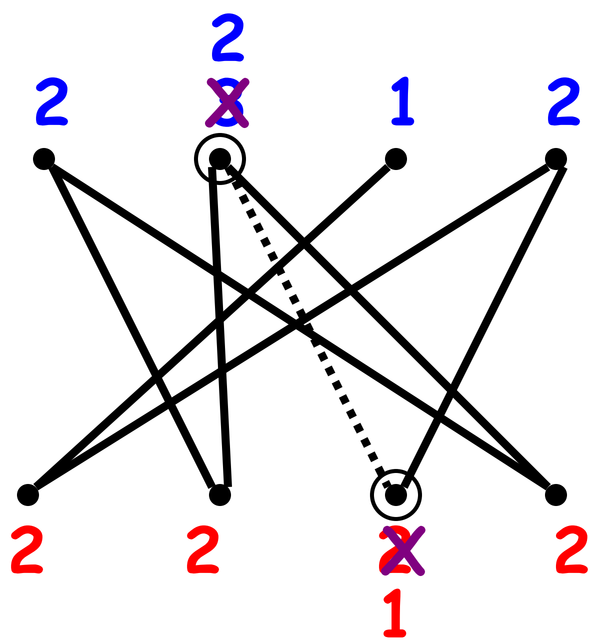

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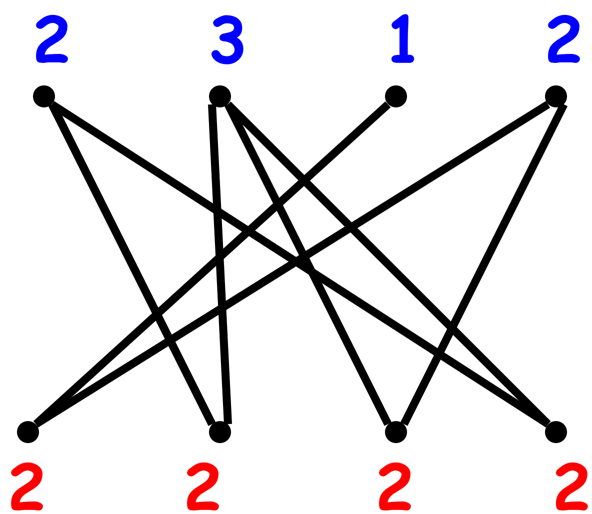

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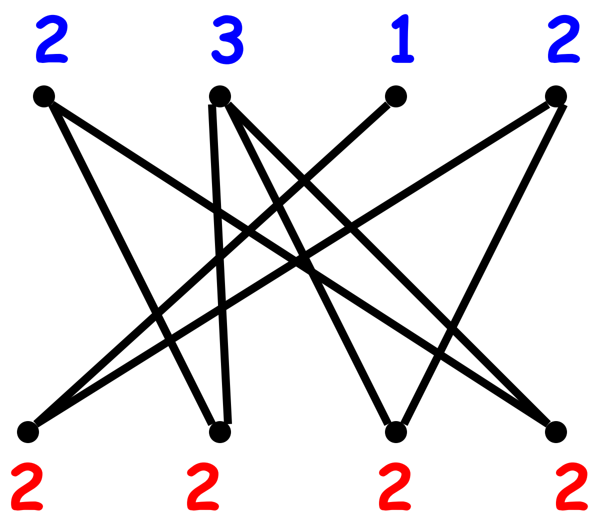
Simulated Annealing for BCT ?

[Bezáková-Bhatnagar-Vigoda SODA '06]



Ideal weights

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

Unordered state → Ordered state

(EASY) (DIFFICULT)

? → 2 3 1 2 / 2 2 2 2

Simulated Annealing for BCT ?

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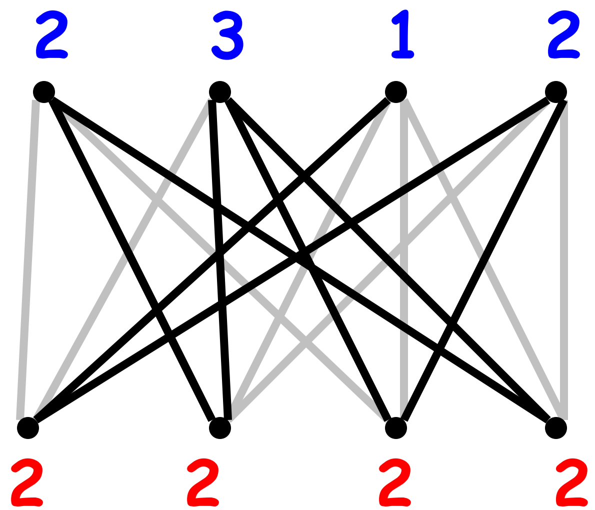


Ideal weights

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

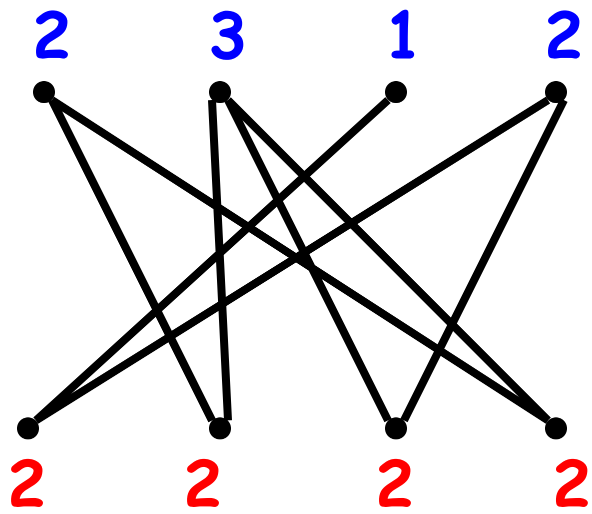
Unordered state → Ordered state

(EASY) (DIFFICULT)

? → 2 3 1 2 / 2 2 2 2 on $K_{n,n}$

Simulated Annealing for BCT ?

[Bezáková-Bhatnagar-Vigoda SODA '06]



Ideal weights

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

Unordered state → Ordered state

(EASY)

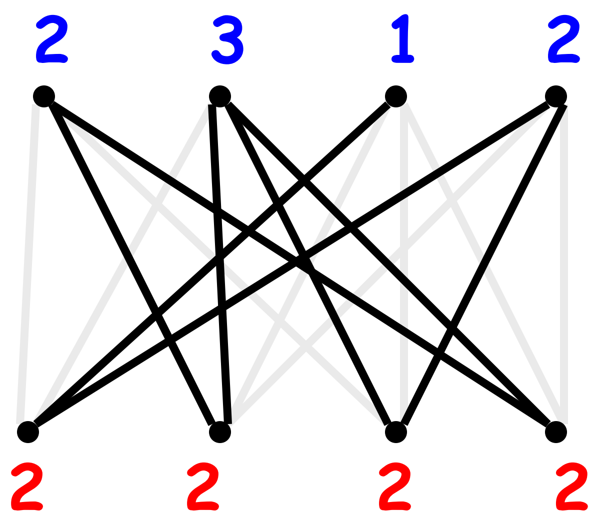
2 3 1 2
2 2 2 2
on G^*

(DIFFICULT)

2 3 1 2
2 2 2 2
on $K_{n,n}$

Simulated Annealing for BCT ?

[Bezáková-Bhatnagar-Vigoda SODA '06]



Thm [BBV '06]:

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

Unordered state → Ordered state

(EASY) (DIFFICULT)

2 3 1 2 2 2 2 2 on *G**	2 3 1 2 2 2 2 2 on $K_{n,n}$

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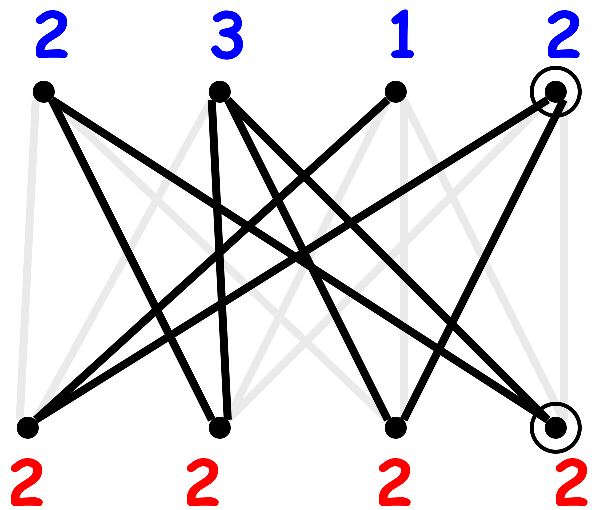

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Unordered state → Ordered state

(EASY)

2 3 1 2
2 2 2 2
on ***G****

(DIFFICULT)

2 3 1 2
2 2 2 2
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Simulated Annealing for BCT ?

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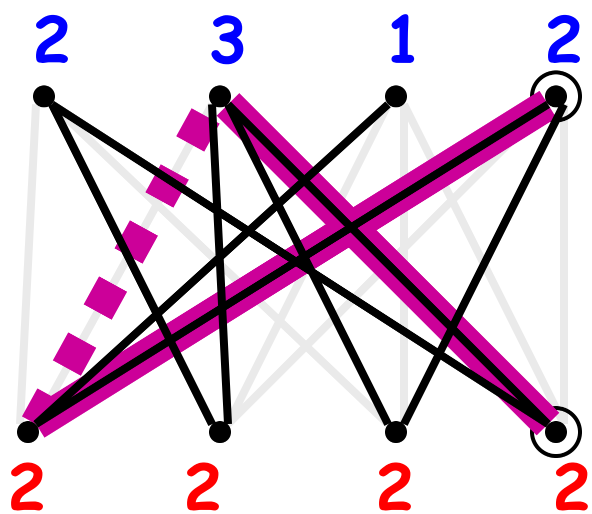

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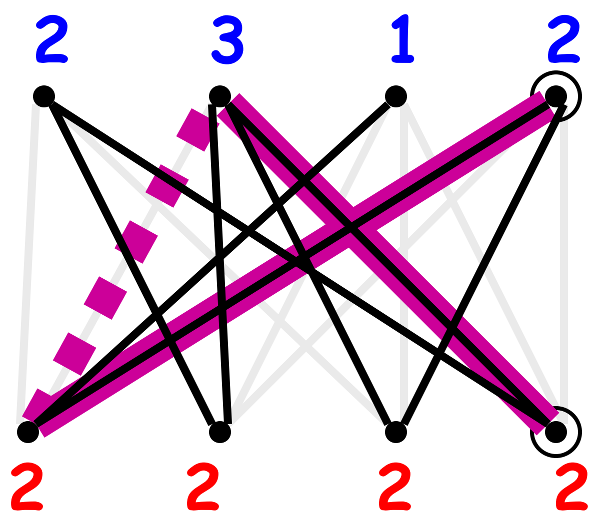

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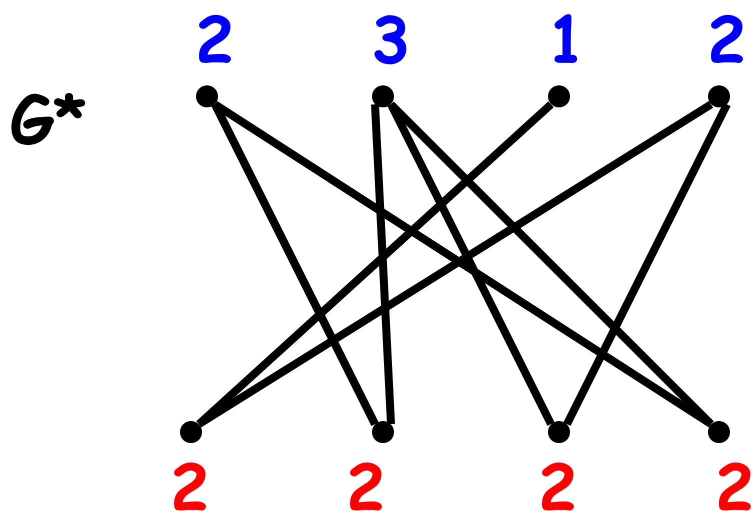
Counting **subgraphs** (of a bipartite graph) **with given degrees** in poly-time.

Simulated Annealing for BCT ?

[Bezáková-Bhatnagar-Vigoda SODA '06]



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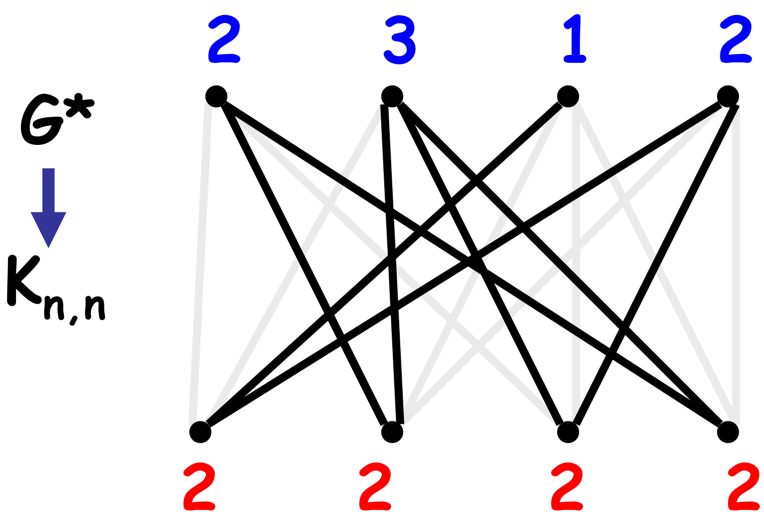

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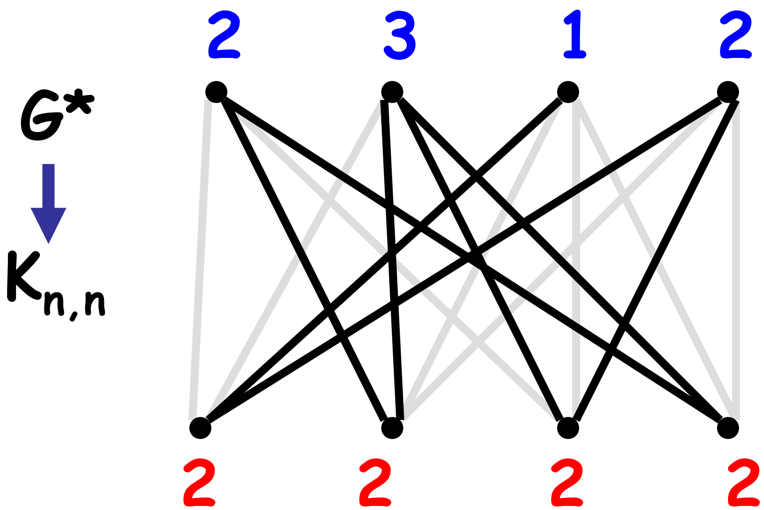

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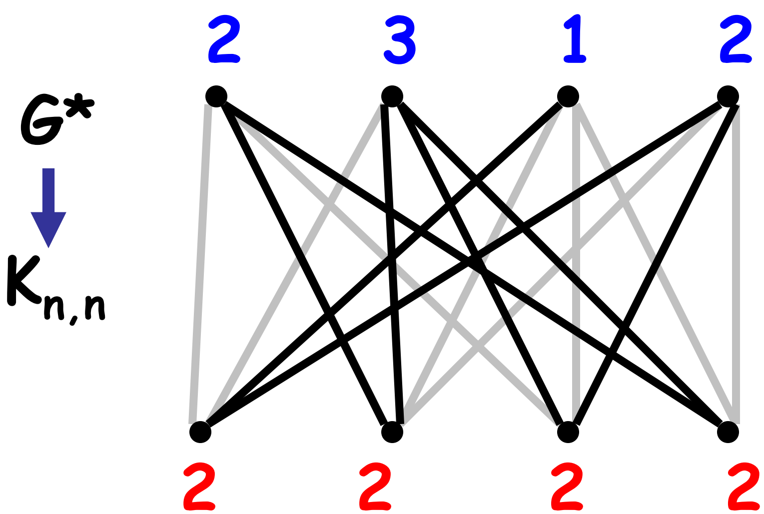

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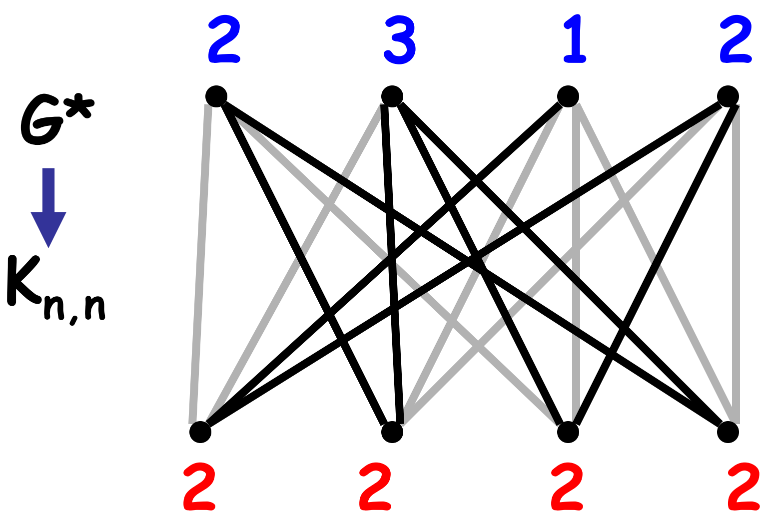

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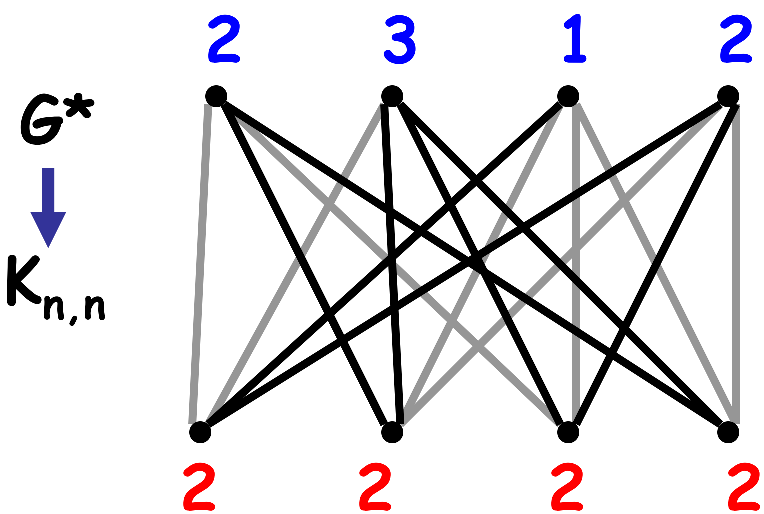

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Simulated Annealing for BCT ?

[Bezáková-
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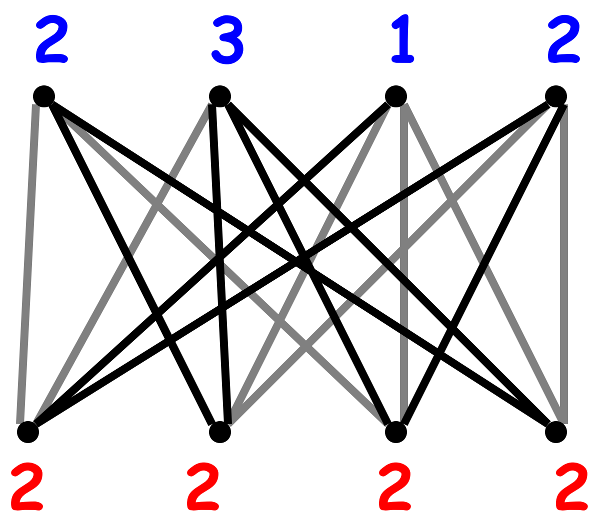
G^*

$K_{n,n}$



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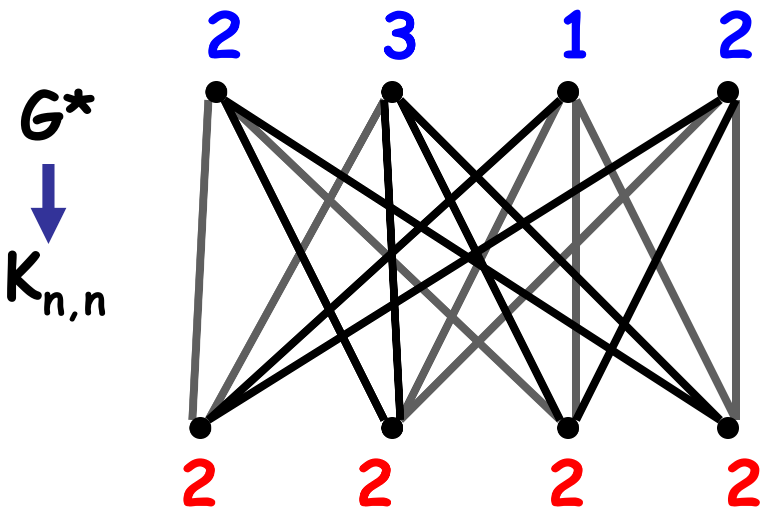

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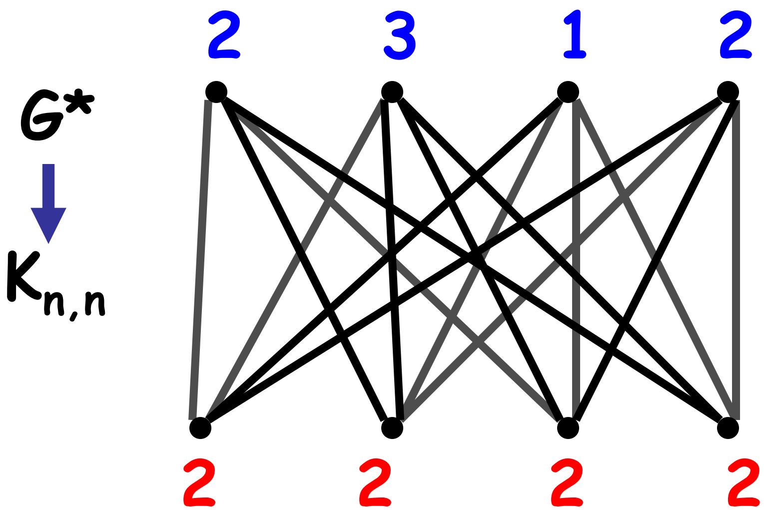

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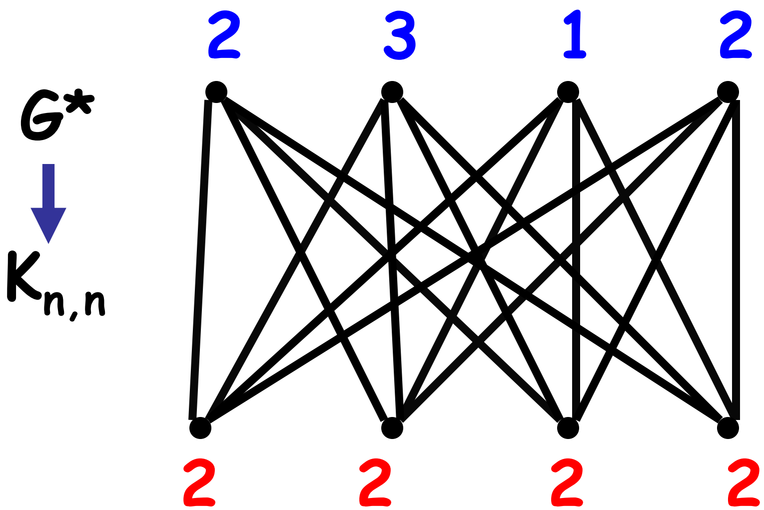

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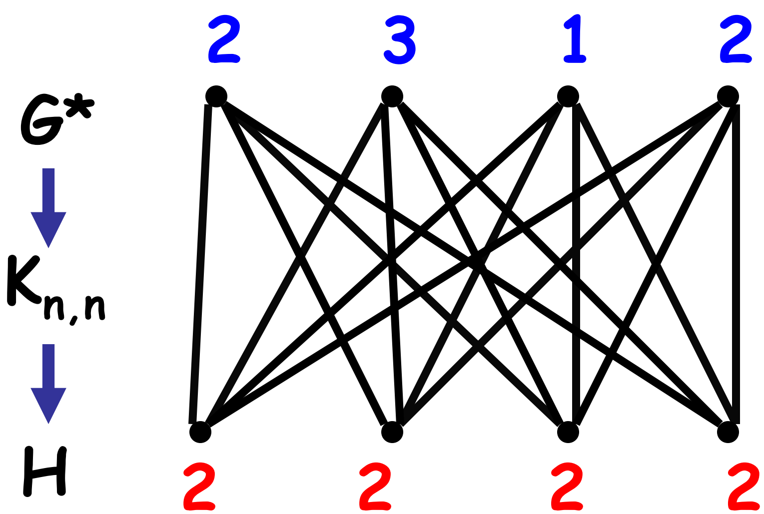

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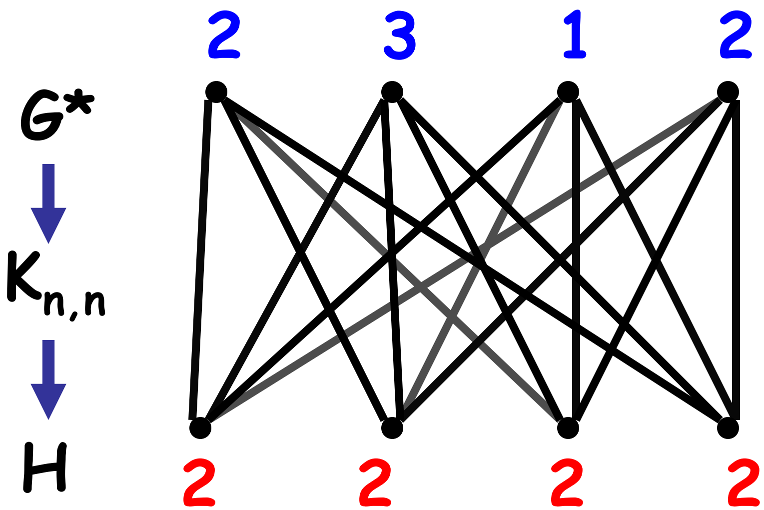

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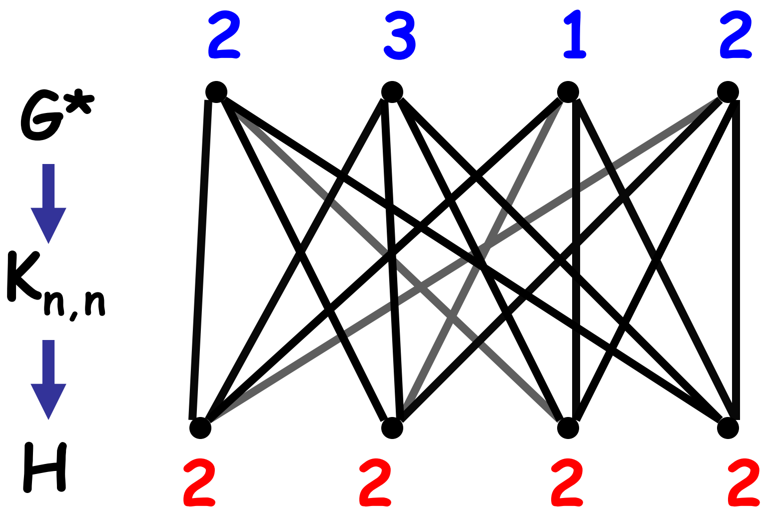

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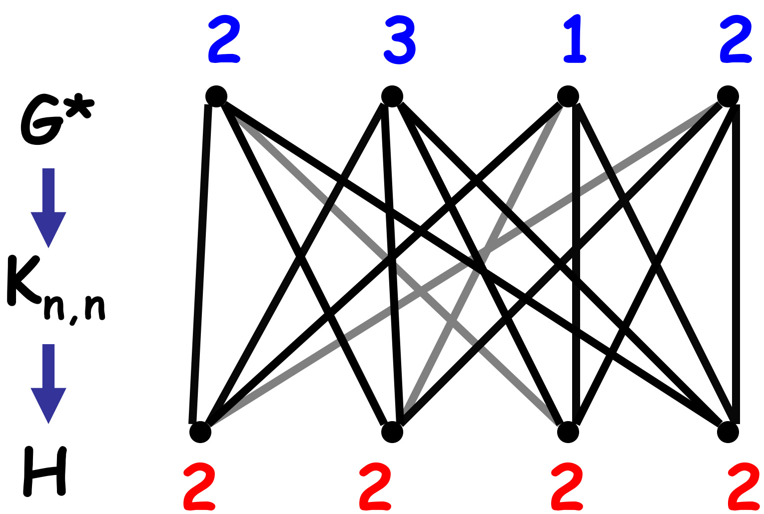

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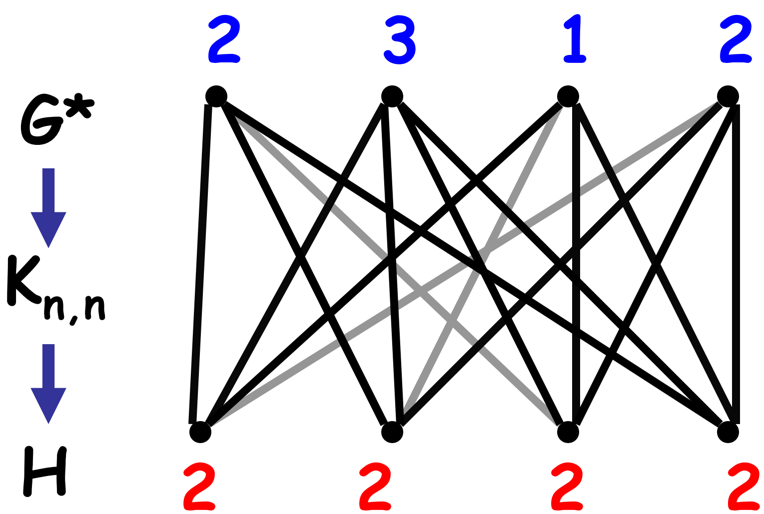

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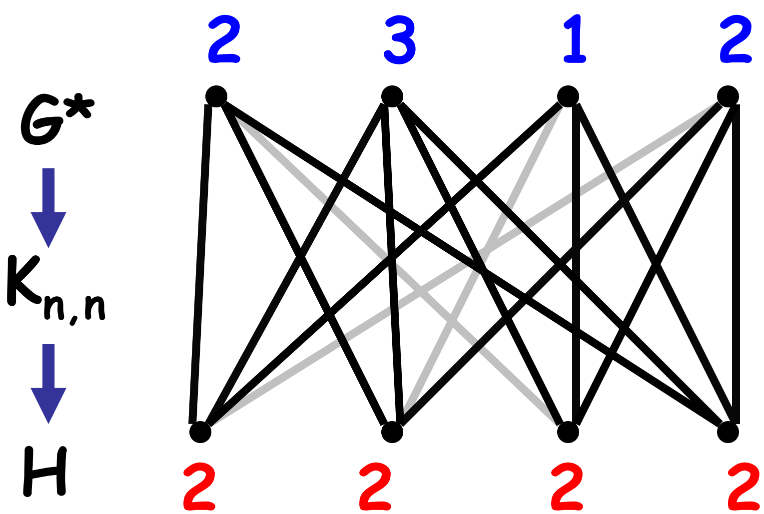

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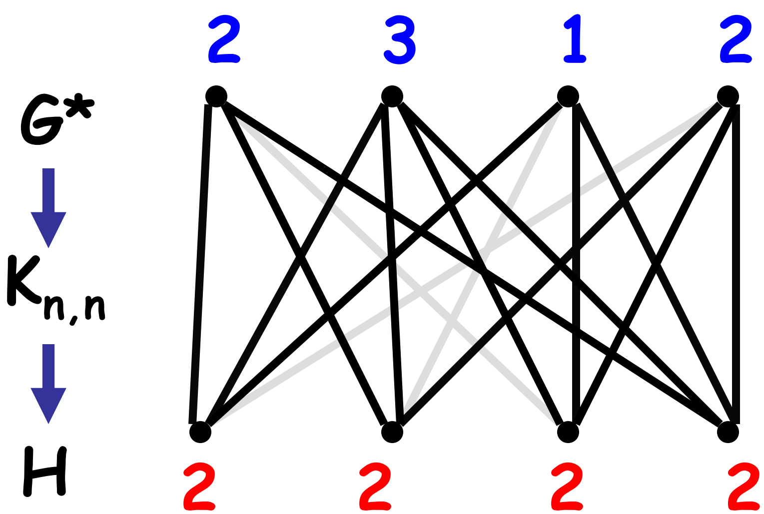
[Bezáková-Bhatnagar-Vigoda SODA '06]



Thm [BBV '06]:

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

Note: some graphs force linear length paths.

Thm [BBV '06]:

$\boxed{H}$

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

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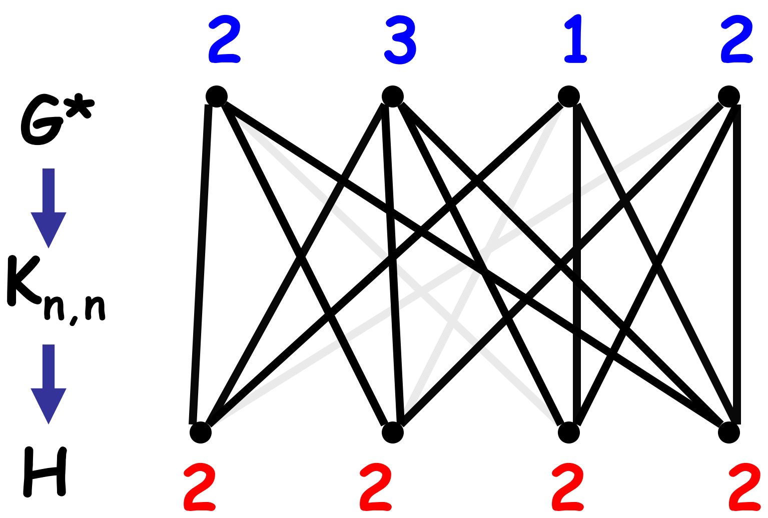

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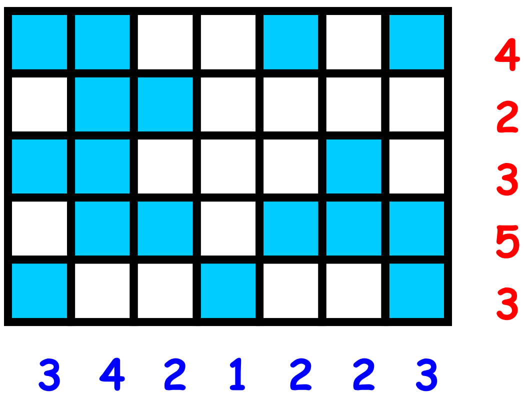
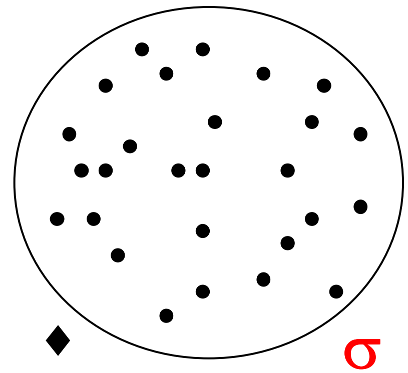
Problems

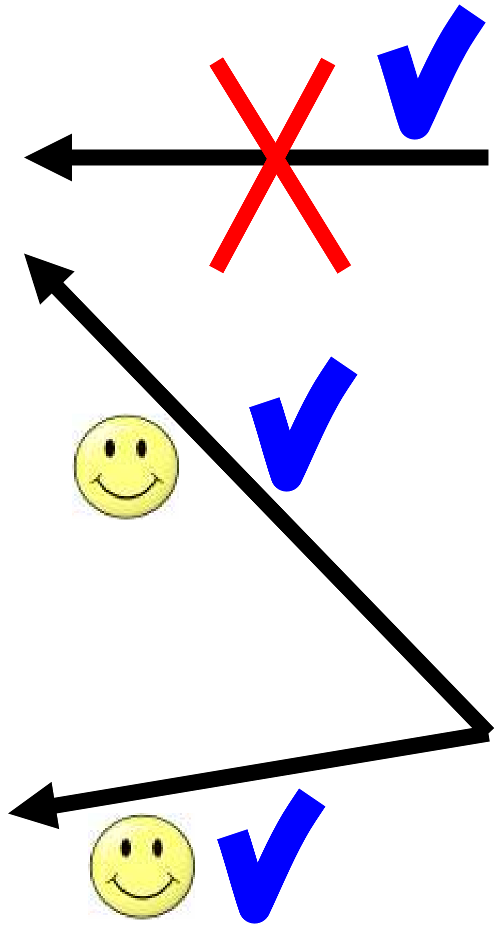
Heuristics

Binary contingency tables



Importance sampling





Simulated annealing

Permanent