Binary Contingency Tables in Theory and Practice

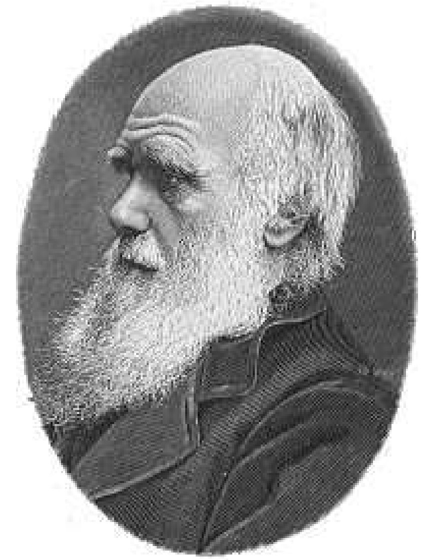
Ivona Bezáková

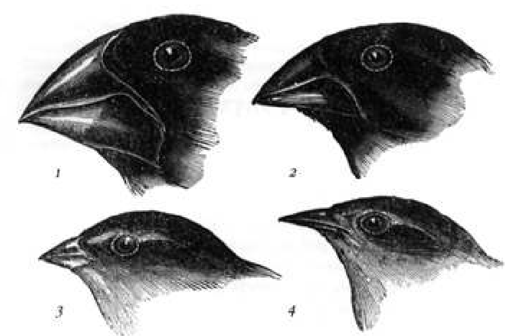
(Rochester Institute of Technology)

Based on joint works with Nayantara Bhatnagar, Alistair Sinclair, Daniel Štefankovič, and Eric Vigoda.

DIMACS Workshop on Markov Chain Monte Carlo: Synthesizing Theory and Practice June 5th, 2007

Darwin's Finches





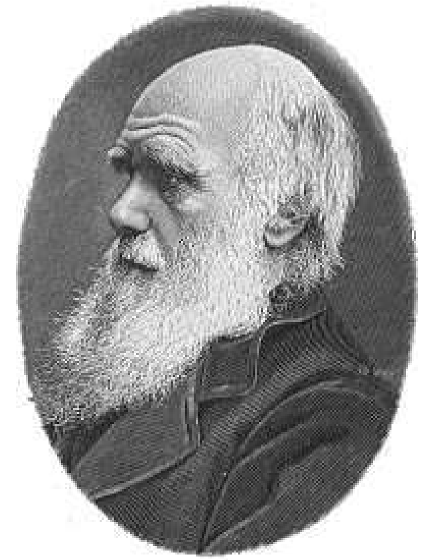
The Voyage of the Beagle

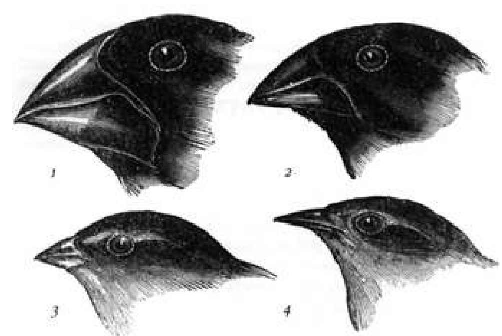
Galápagos archipelago (1835)

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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Mangrove Finch							●	●		
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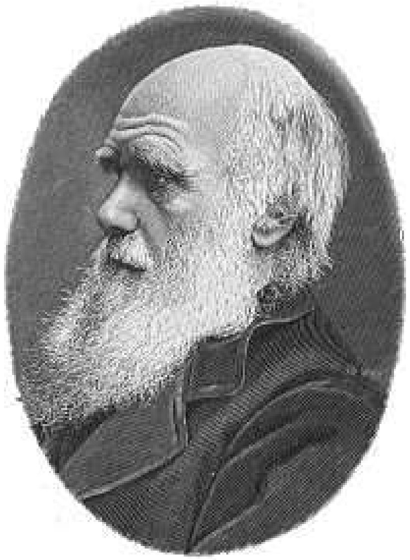
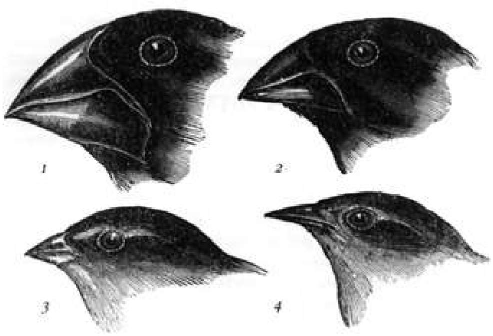
8

10





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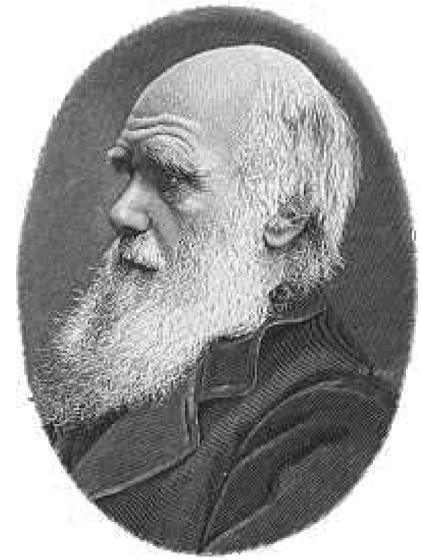
Distribution of Darwin's Finches on Visitor Islands

	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

Input: marginals
(row sums $r_1, r_2, \ldots, r_m$, column sums $c_1, c_2, \ldots, c_n$)

Sample space: 0/1 tables satisfying the marginals

Goal: count / sample

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

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

Different Approaches

Theory (Markov chain Monte Carlo with simulated annealing)

- Jerrum-Sinclair-Vigoda '01: approximate permanent in $O^*(n^{10})$, yields $O^*((mn)^{10})$ algorithm for m x n binary contingency tables
- Bezáková-Bhatnagar-Vigoda '06: $O^*((mn)^3(m+n)^5)$

Practice (sequential importance sampling, Chen-Diaconis-Holmes-Liu '05)

- Bezáková-Sinclair-Štefankovič-Vigoda '06: negative example
- Jose Blanchet '06: SIS works if marginals $O(n^{1/4})$
- Bayati-Kim-Saberi '07: alternative importance sampling method, works if marginals $O(n^{1/4})$

Practice (the switching Markov chain, Diaconis-Gangolli '94)

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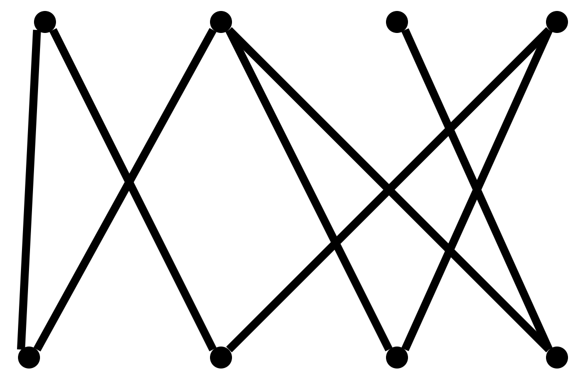
Permanent: Broder Chain

[Broder '88]

What for: uniform sampling of perfect matchings

How: Markov chain on perfect + near-perfect matchings



Perfect matching:

subset of vertex-disjoint edges covering all vertices

Permanent:

number of all perfect matchings

Permanent: Broder Chain

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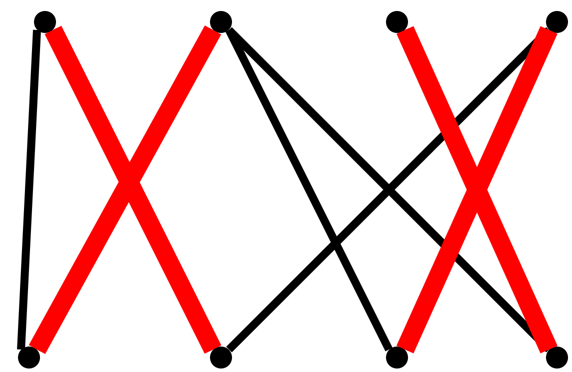

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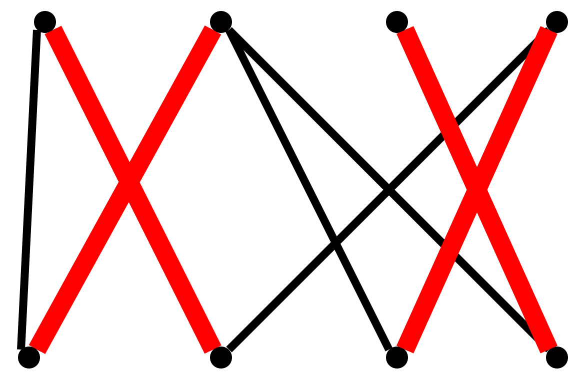

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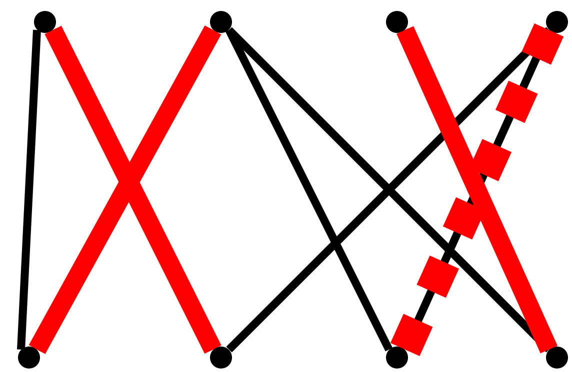

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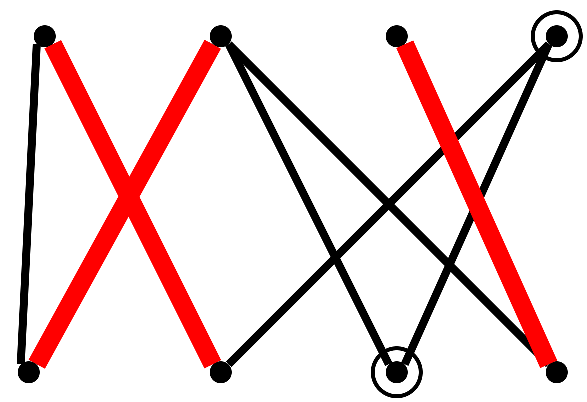

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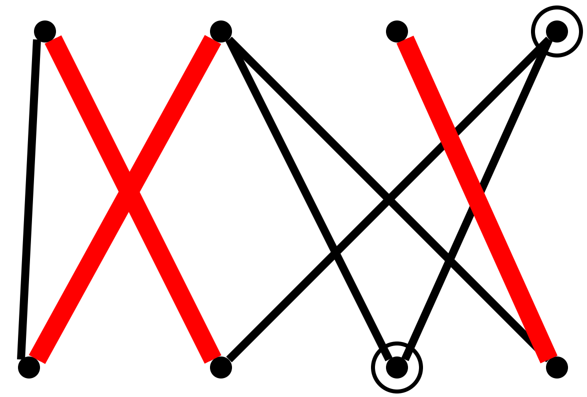

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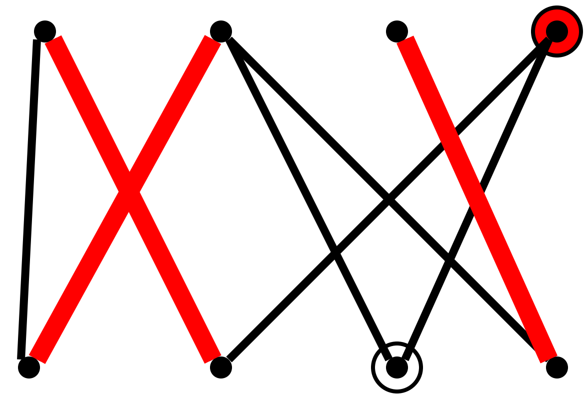

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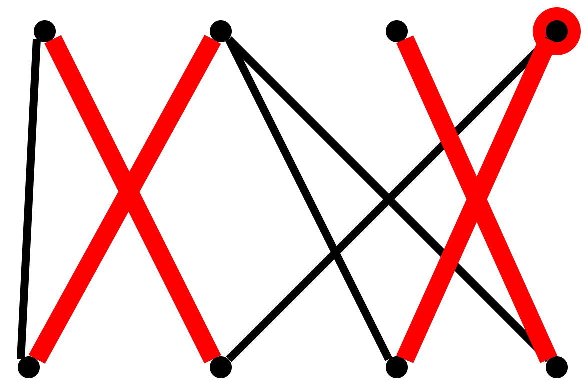

At a near matching:

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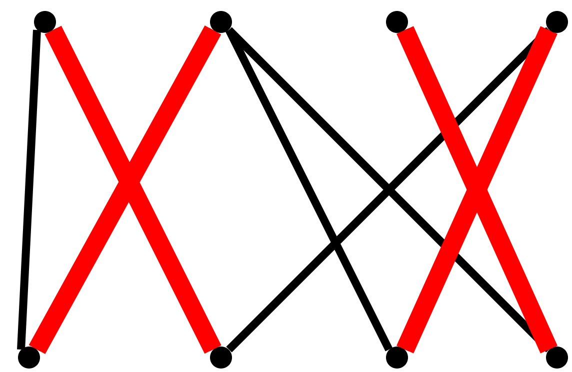

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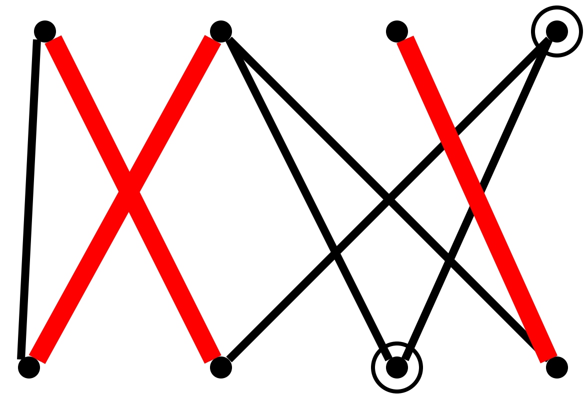

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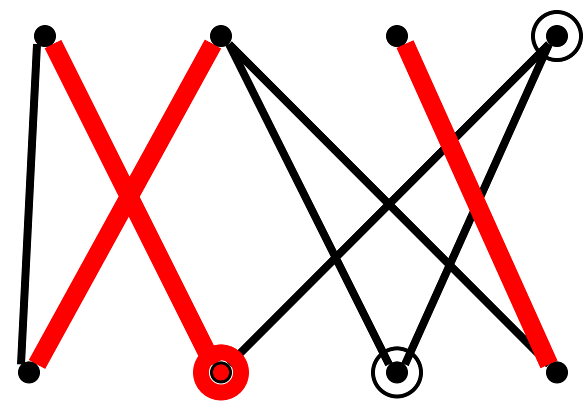

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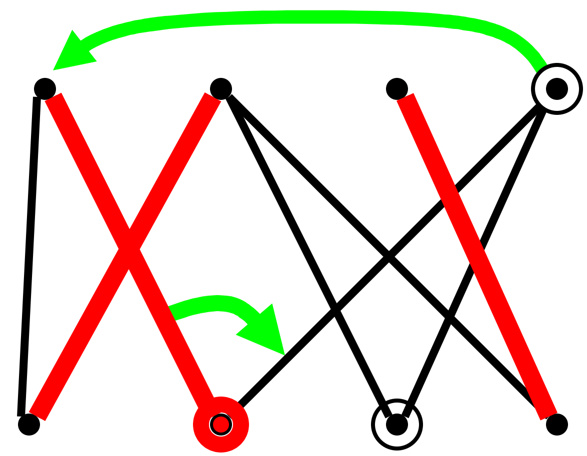

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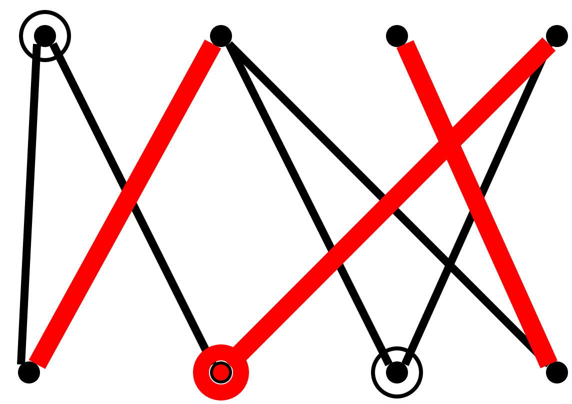

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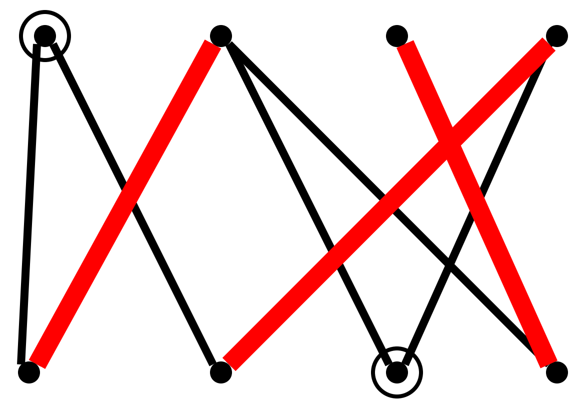

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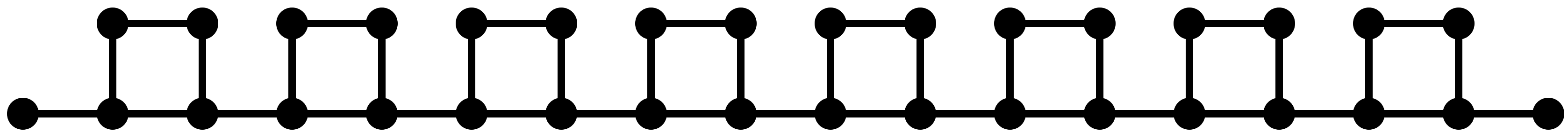
Mixes in polynomial time? Even if it did…



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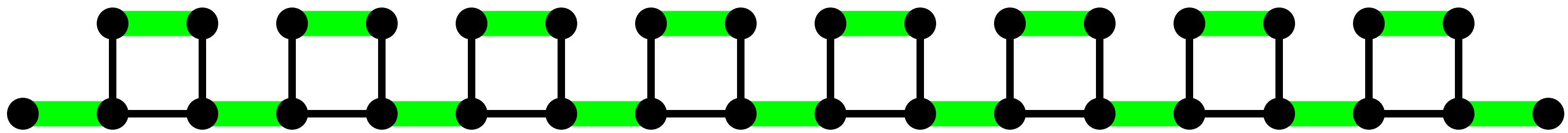

1 perfect matching

Broder Chain

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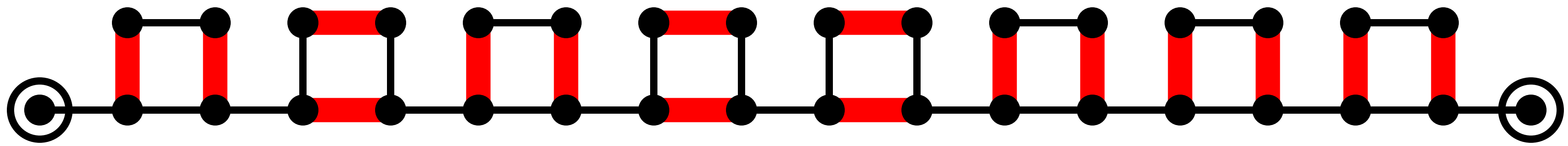
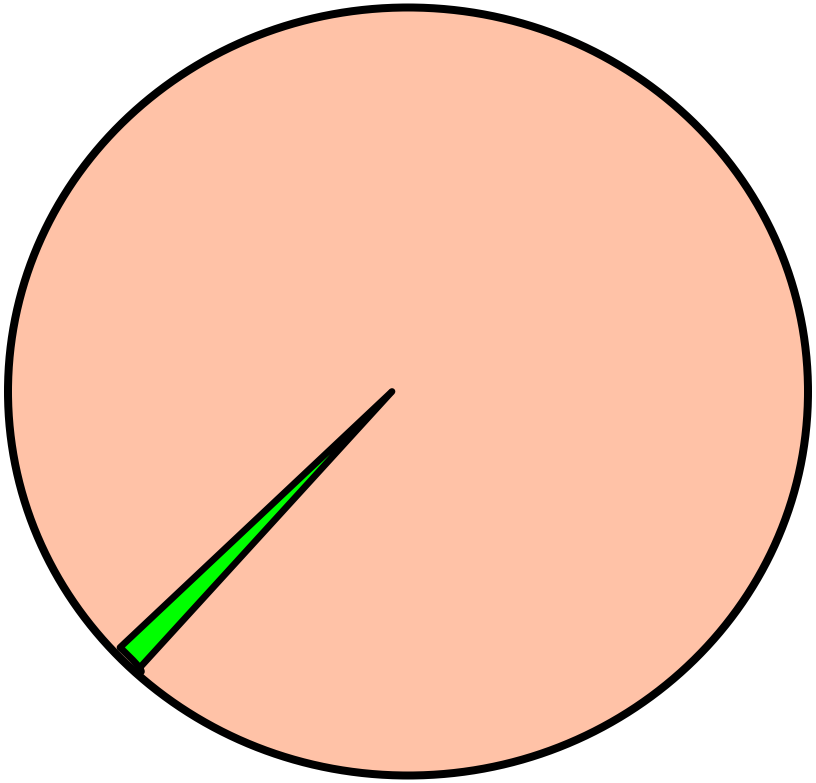


1 perfect matching

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



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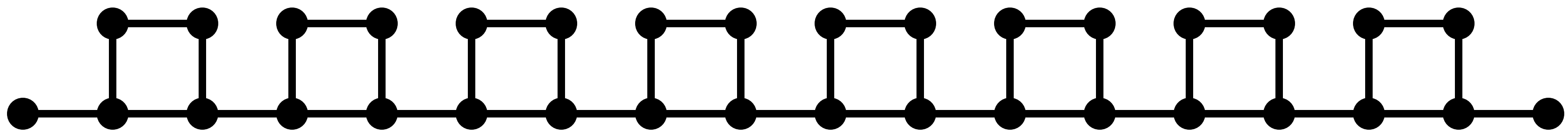

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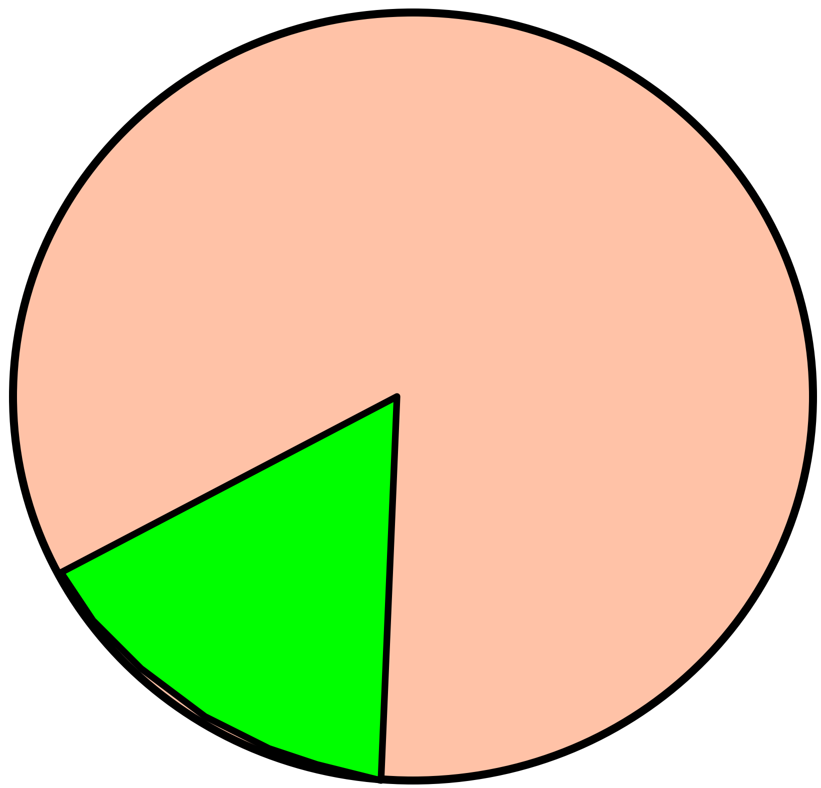


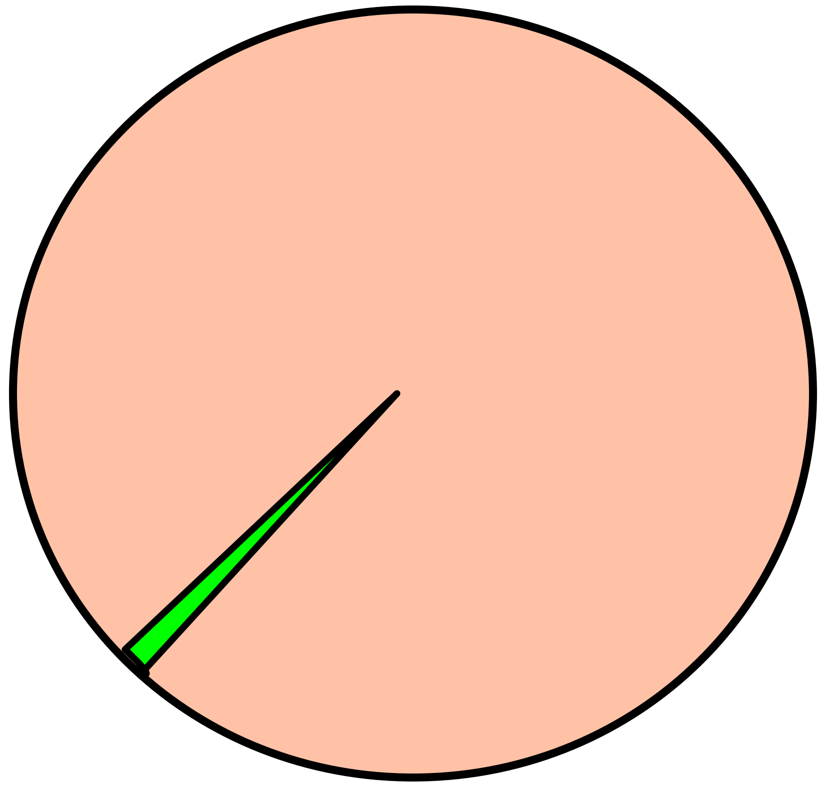
Thm [Jerrum-Sinclair '89]:

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

Simulated Annealing for Permanent

Jerrum-Sinclair-Vigoda '01:

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



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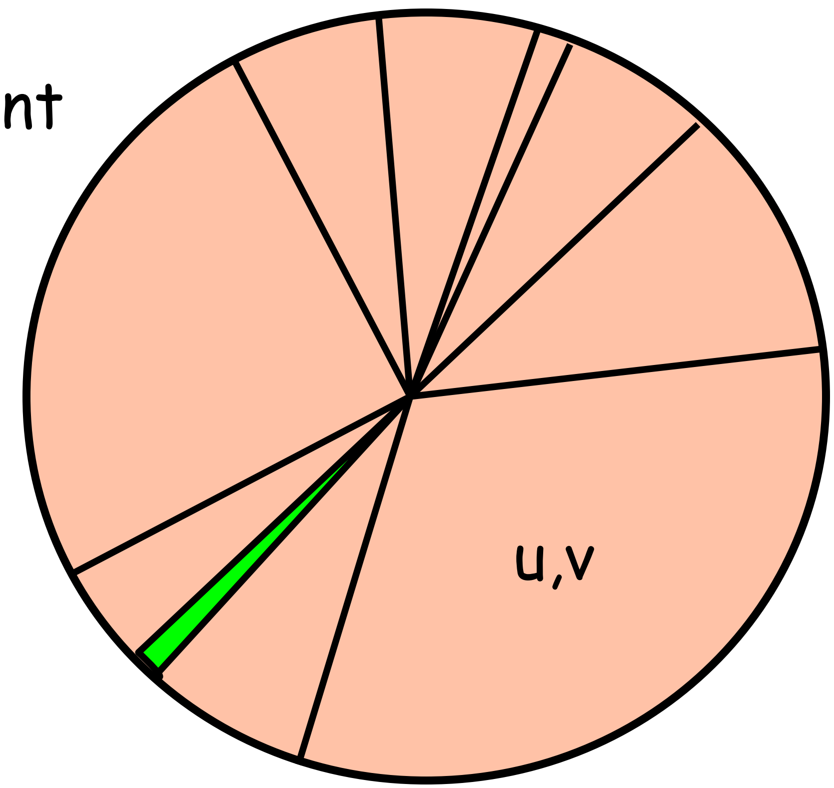
Originally: n^2+1 regions, very different size



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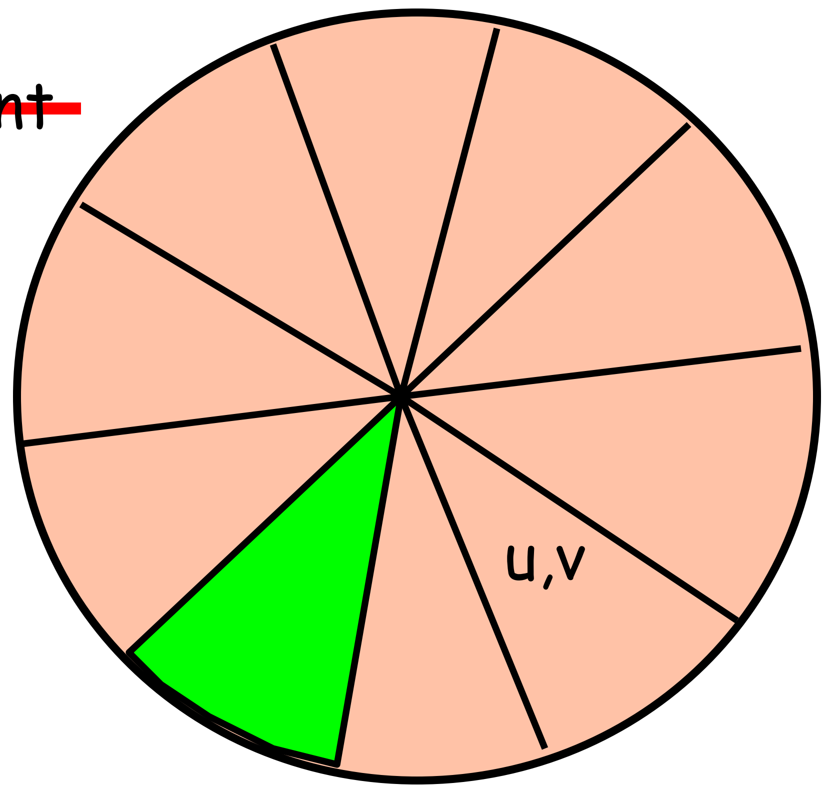
Want: n^2+1 regions, ~~very different~~

the same size



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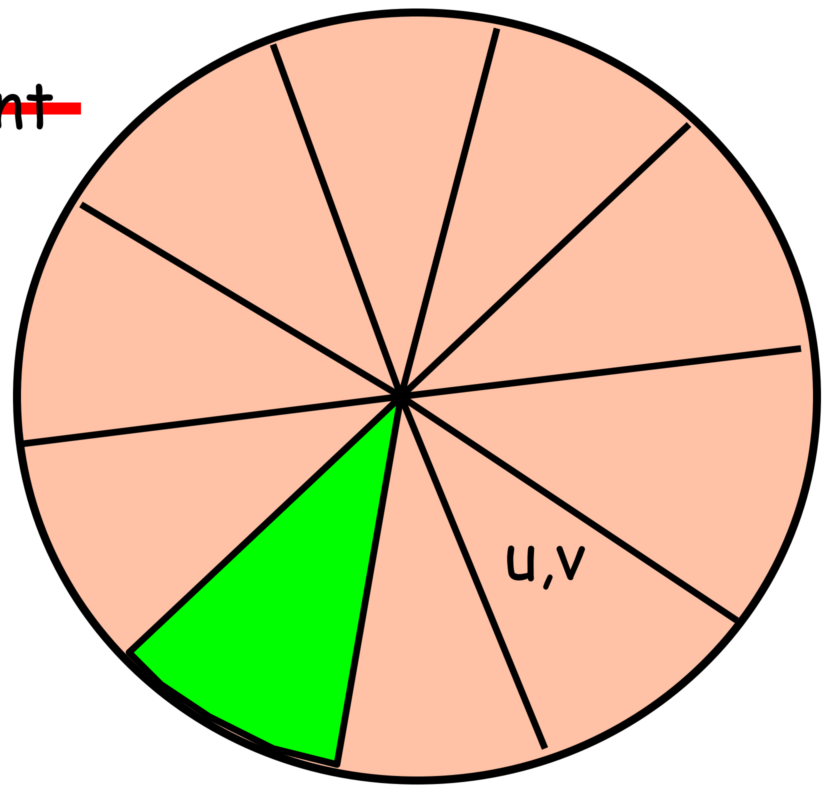

Ideal weights
(for a matching with holes u,v):

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

Simulated Annealing for Permanent

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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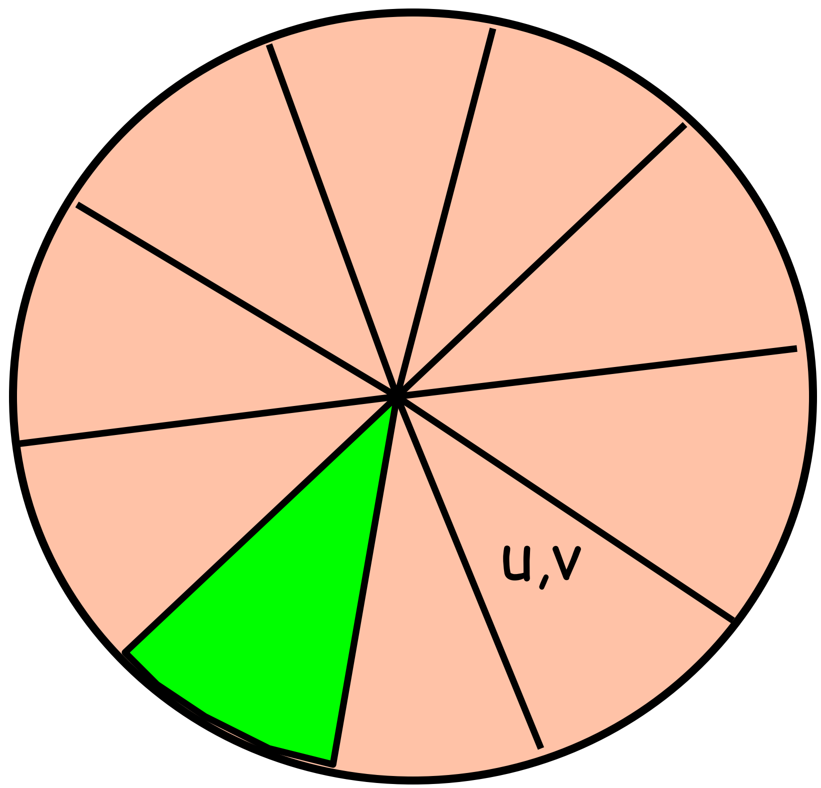

Simulated Annealing for Permanent

Unordered state → Ordered state

(EASY) (DIFFICULT)

G

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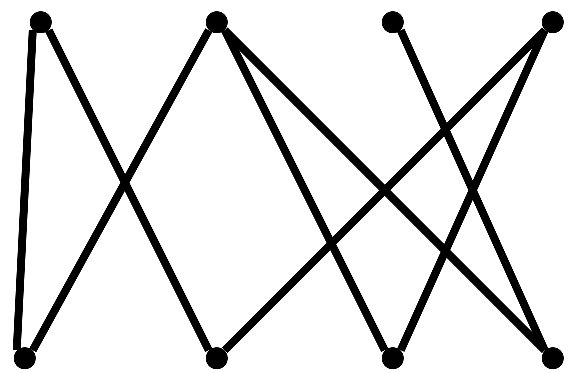

G

Simulated Annealing for Permanent

Unordered state → Ordered state

(EASY) (DIFFICULT)

$K_{n,n}$ → G

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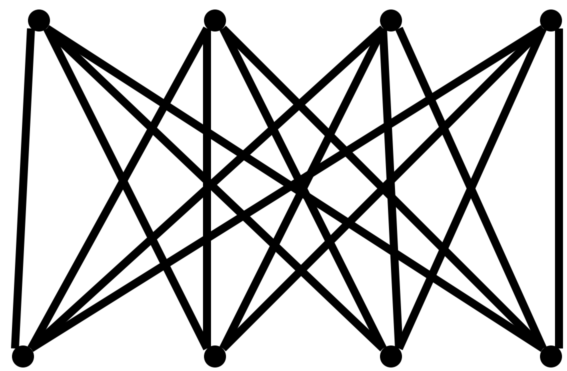

$K_{n,n}$

Simulated Annealing for Permanent

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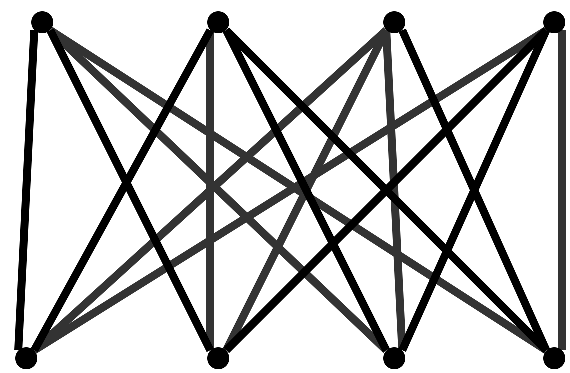

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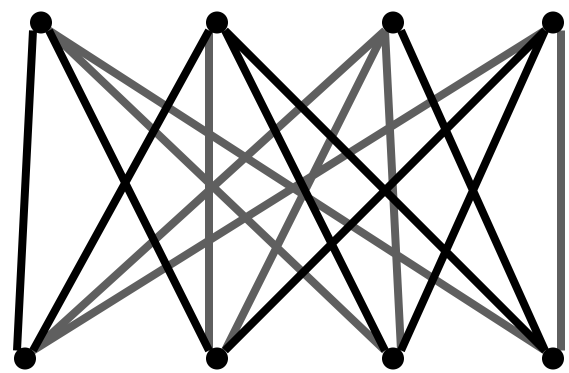

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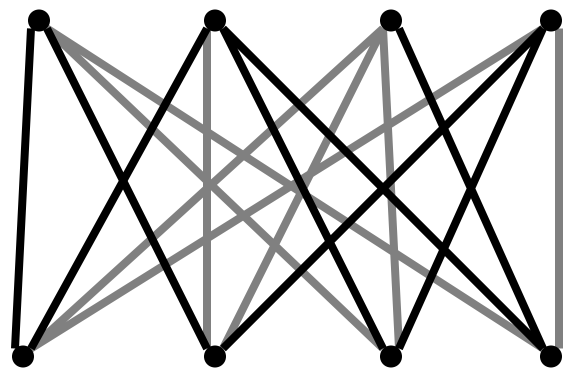

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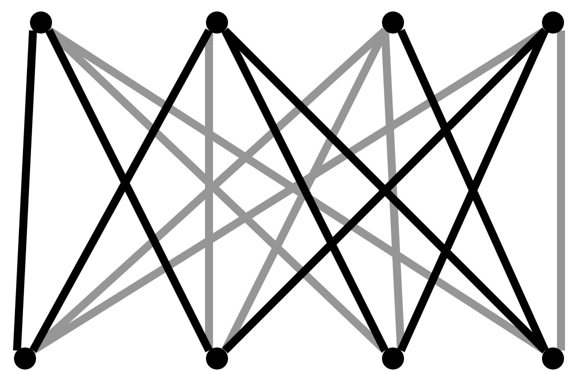

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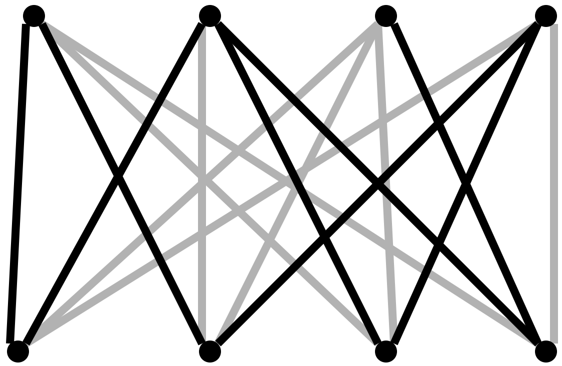


Simulated Annealing for Permanent

Unordered state → Ordered state

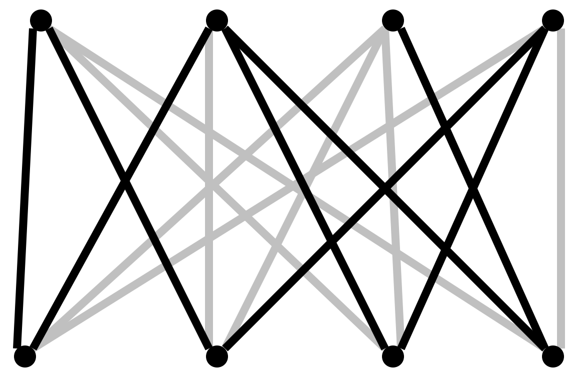
(EASY) (DIFFICULT)

$K_{n,n}$ → G

Solution: **Approximate**

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

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



Simulated Annealing for Permanent

Unordered state → Ordered state

(EASY) (DIFFICULT)

$K_{n,n}$ → G

Solution: **Approximate**

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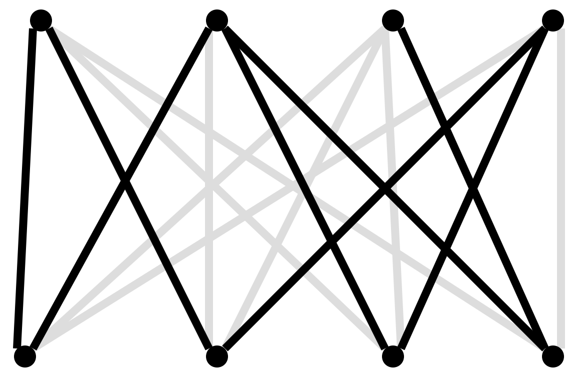


Simulated Annealing for Permanent

Unordered state → Ordered state

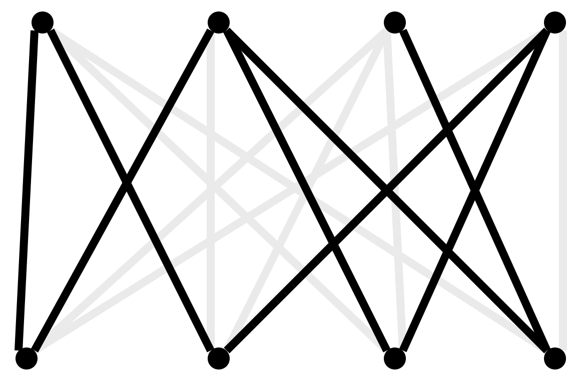
(EASY) (DIFFICULT)

$K_{n,n} \longrightarrow G$

Solution: **Approximate**

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

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



Simulated Annealing for Permanent

Unordered state → Ordered state

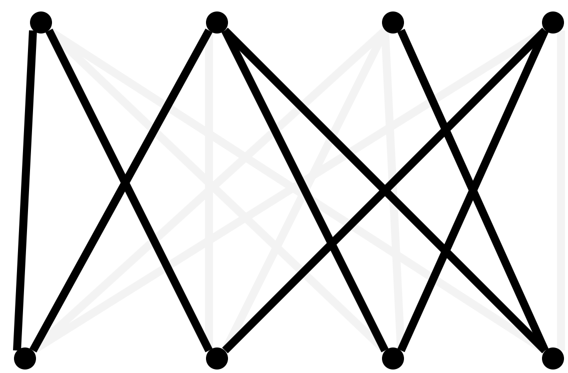
(EASY) (DIFFICULT)

$K_{n,n}$ → G

Solution: **Approximate**

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

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



G

Simulated Annealing for Permanent

Unordered state → Ordered state

(EASY) (DIFFICULT)

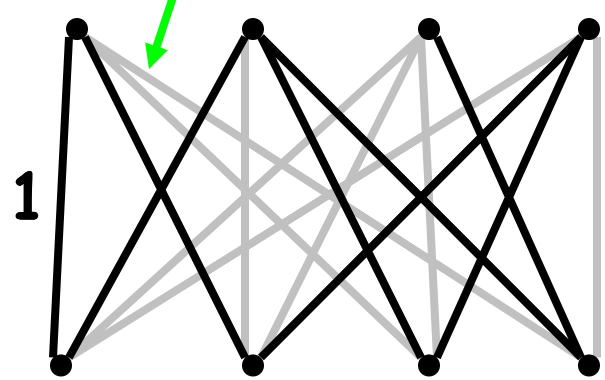
$K_{n,n}$ → G

Solution: **Approximate**

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

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

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



Simulated Annealing for Permanent

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

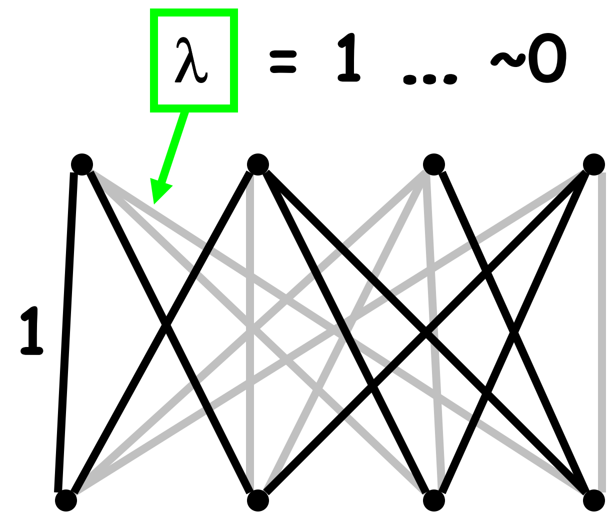
need to be λ-weighted:

$$w(u,v) = \frac{\lambda(\mathcal{P})}{\lambda(\mathcal{N}(u,v))}$$

where

$$\lambda(M) = \lambda^{\#\, \lambda\text{-edges in } M}$$

$$\lambda(S) = \sum_{M \text{ in } S} \lambda(M)$$



Simulated Annealing for Permanent

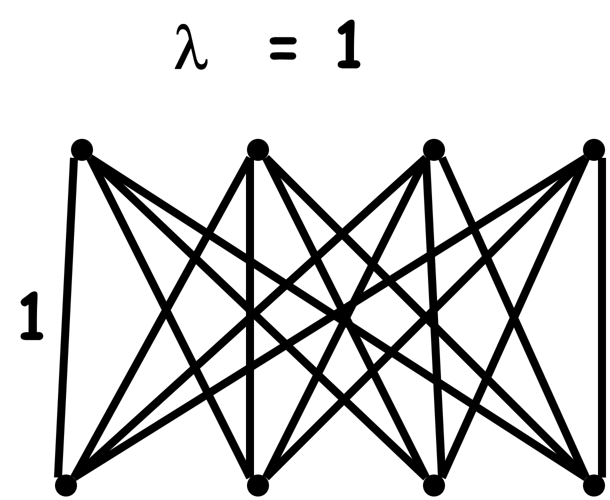
Thm [Jerrum-Sinclair-Vigoda '01]:
Weighted Broder chain mixes if w(u,v) approximated within a constant factor.

$$w(u,v) = \frac{\lambda(\mathcal{P})}{\lambda(\mathcal{N}(u,v))}$$

Algorithm (sketch):

* Initially, $\lambda = 1$.
  Thus $w(u,v) = n!/(n-1)! = n$.

  Later, have approx. of w(u,v).
  Run chain to improve the approx.
  Decrease λ (until ~0).



(Improved approx. of old λ = starting approx. of new λ)

Simulated Annealing for Permanent

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4-apx

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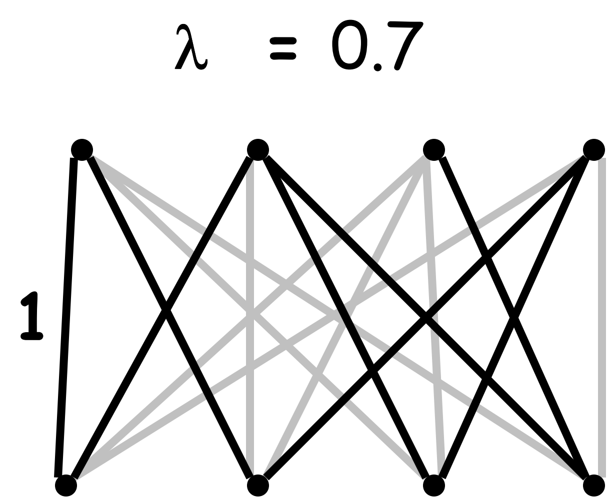

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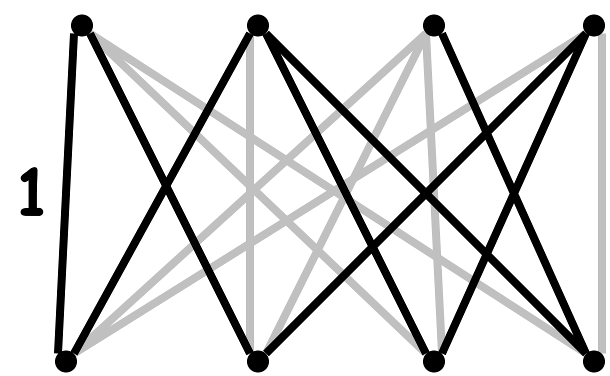
$$w(u,v) = \frac{\lambda(\mathscr{P})}{\lambda(\mathscr{N}(u,v))}$$

~~4~~ 2-apx

Algorithm (sketch):

$\lambda = 0.7$



Initially, $\lambda = 1$.
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Decrease λ (until ~0).

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Simulated Annealing for Permanent

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$$\boxed{w(u,v) = \frac{\lambda(\mathcal{P})}{\lambda(\mathcal{N}(u,v))}}$$

~~4~~-apx
2 = 4-apx for
λ = ~~0.7~~ 0.6

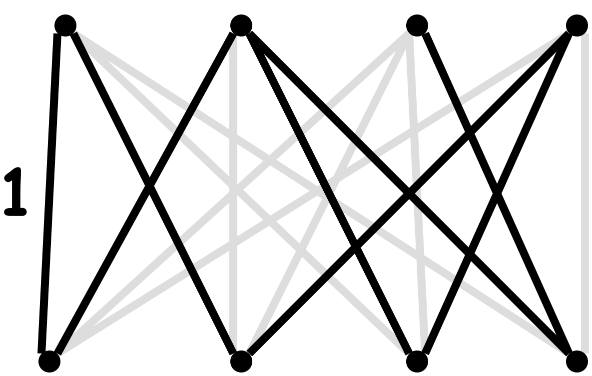
Algorithm (sketch):

Initially, λ = 1.
Thus w(u,v) = n!/(n-1)! = n.

Later, have approx. of w(u,v).
Run chain to improve the approx.
* Decrease λ (until ~0).

(Improved approx. of old λ = starting approx. of new λ)

1



Simulated Annealing for Permanent

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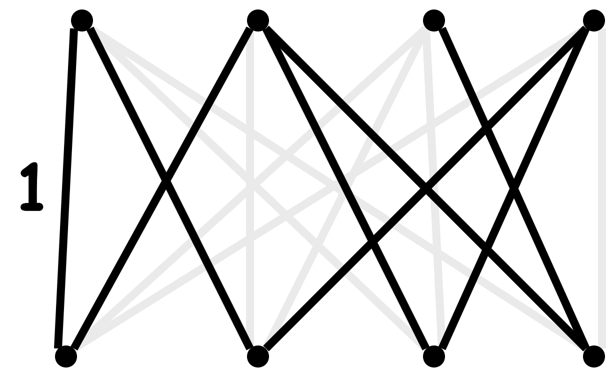

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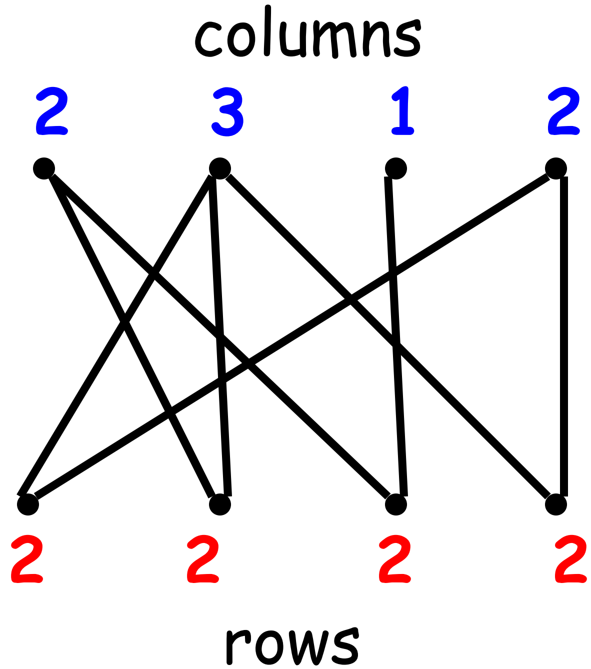
BCT: Bipartite Graphs with Given Degrees



columns

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

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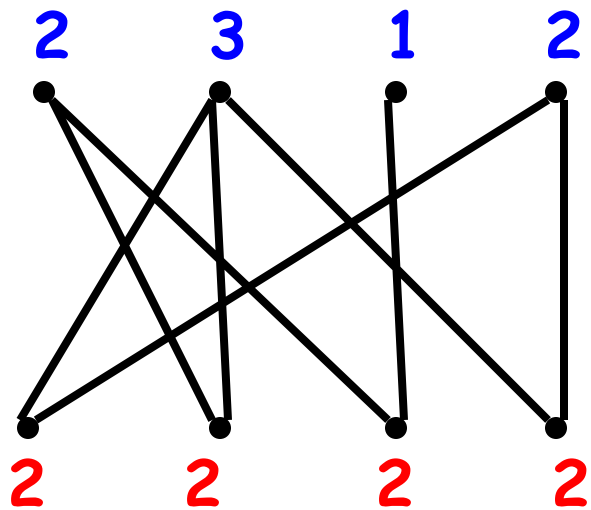

columns

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

"Sliding" Markov Chain on perfect and near tables

Perfect: remove a random edge

Near: slide edges or match

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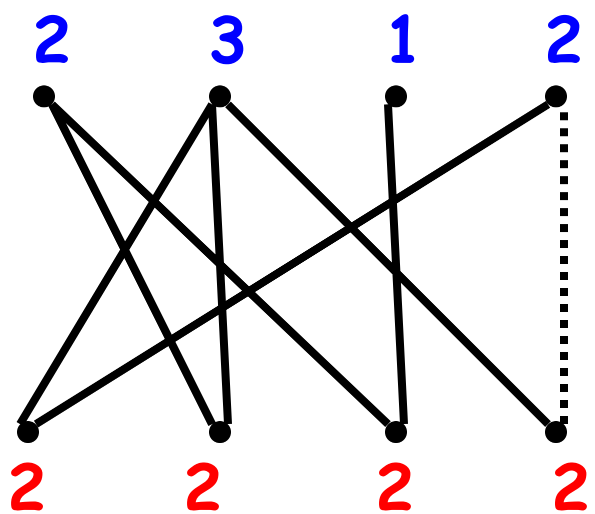

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0	1	0	1	2
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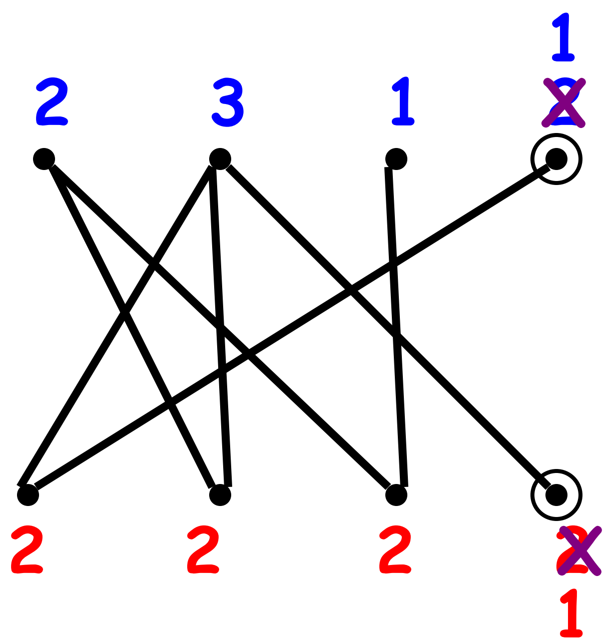

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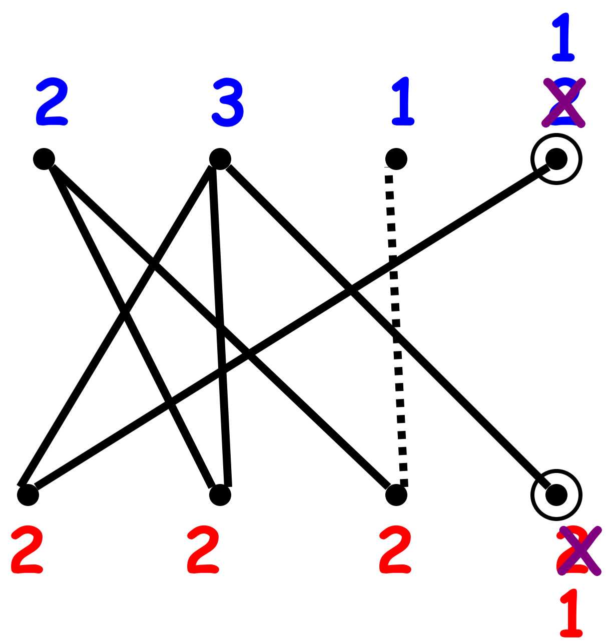

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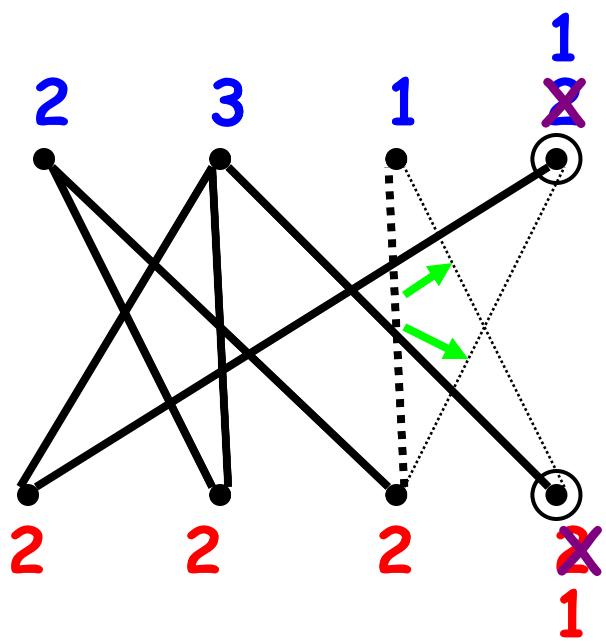

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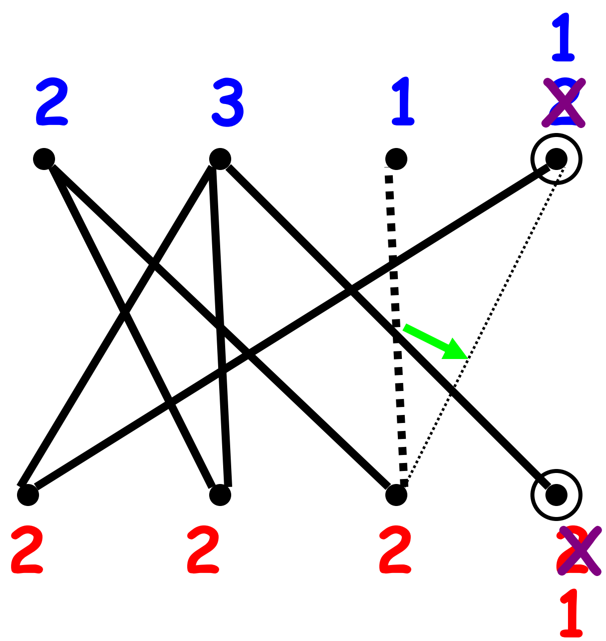

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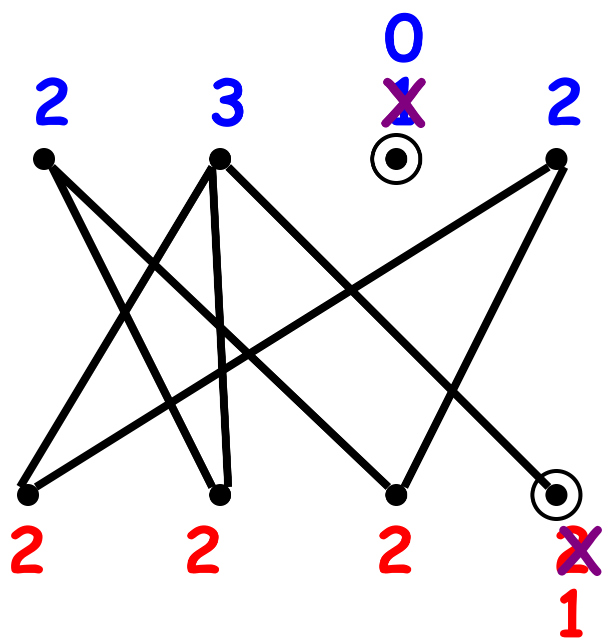

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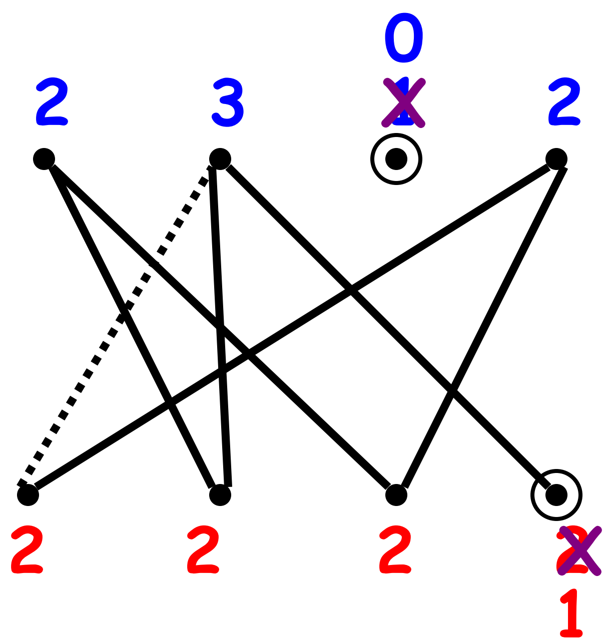

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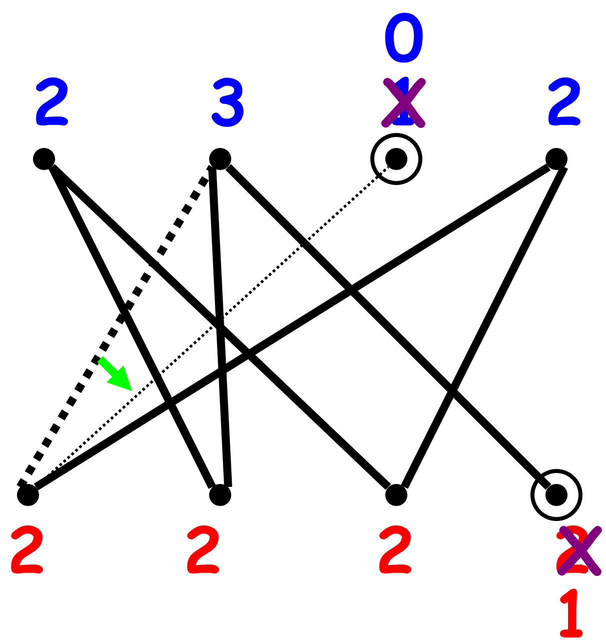

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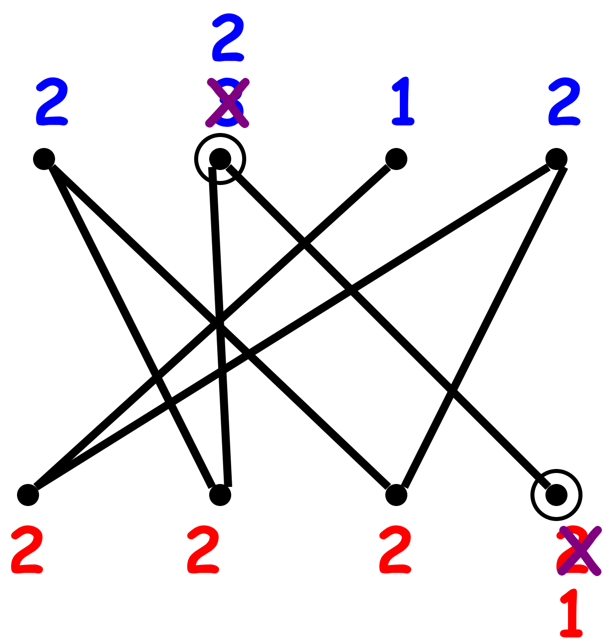

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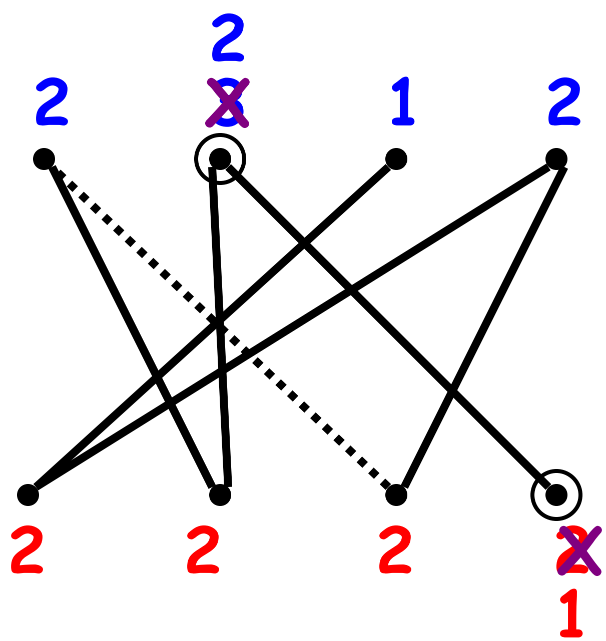

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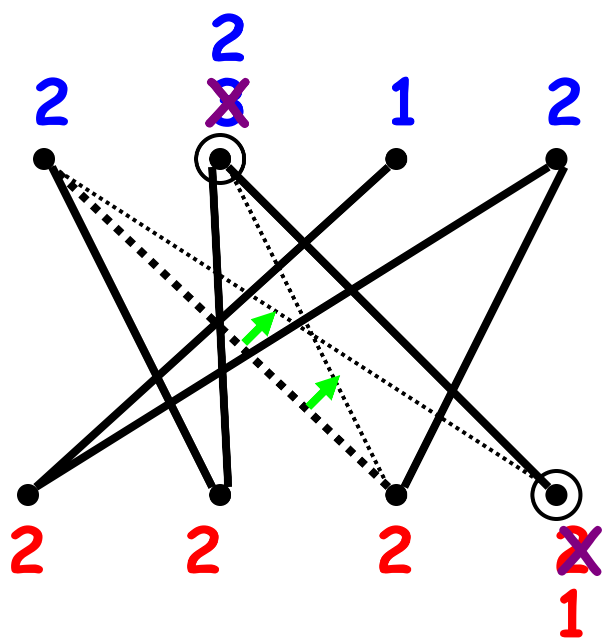

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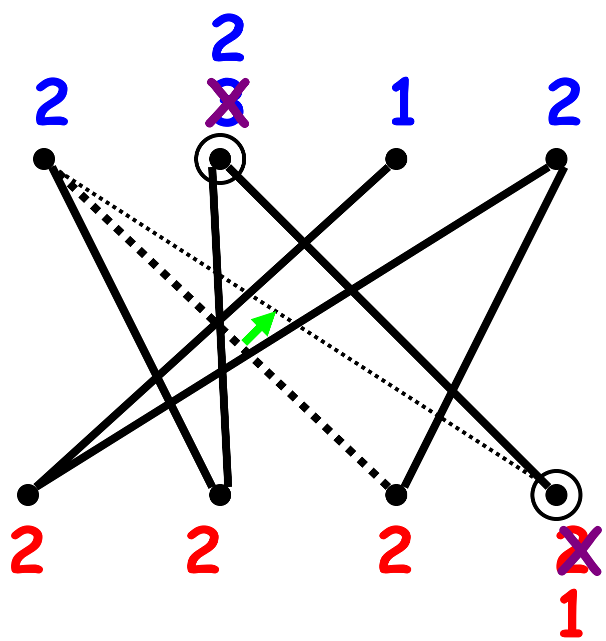

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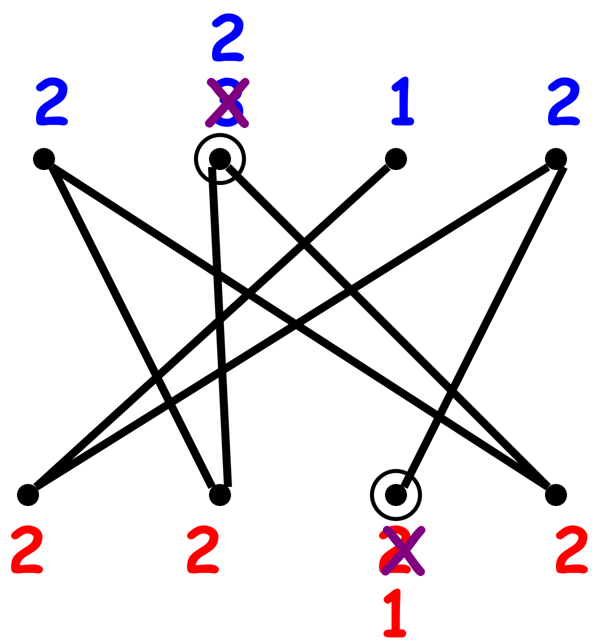

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"Sliding" Markov Chain on perfect and near tables

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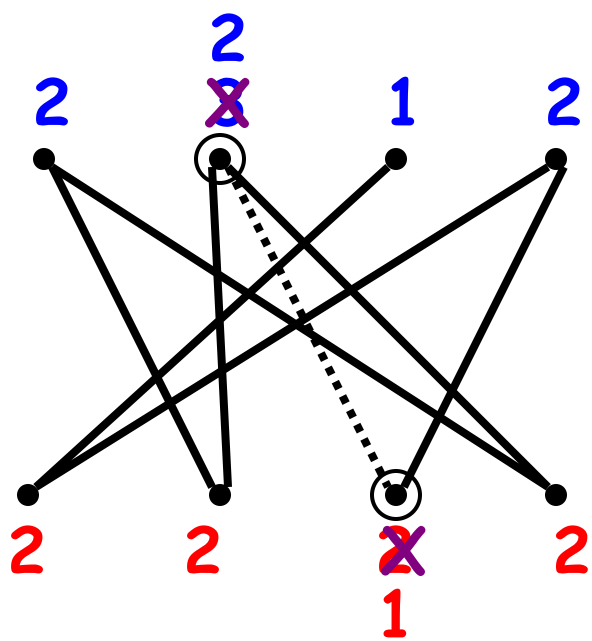

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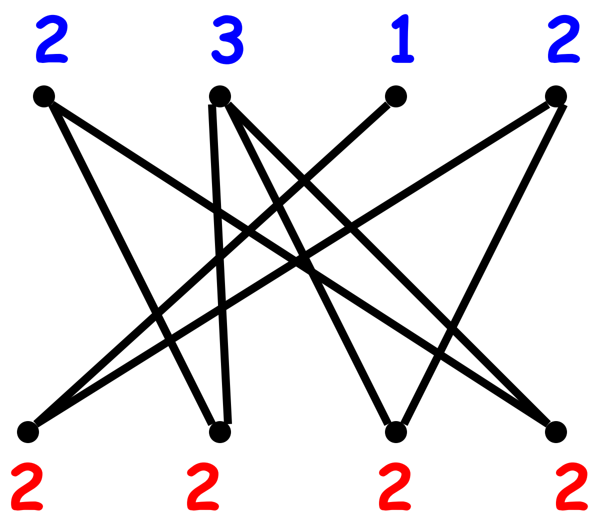

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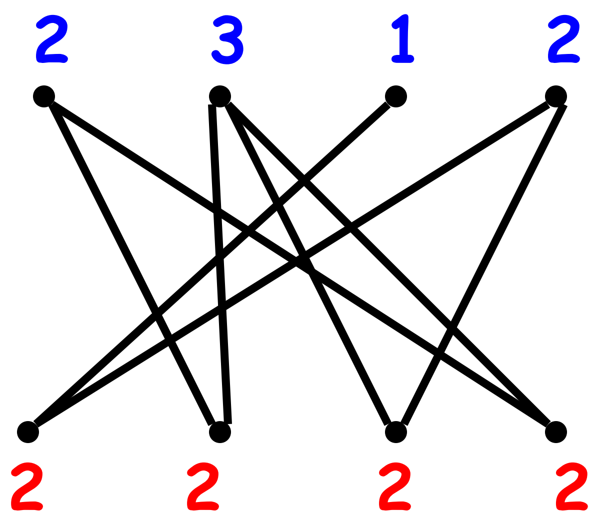
Simulated Annealing for BCT ?

[Bezáková-Bhatnagar-Vigoda '06]



Ideal weights

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

Unordered state → Ordered state

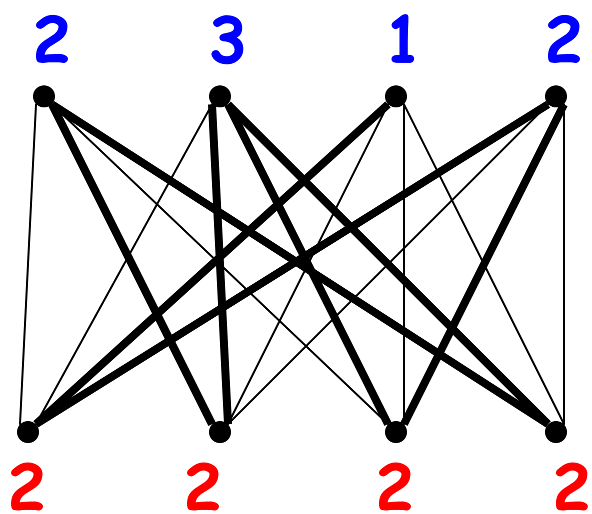
(EASY) (DIFFICULT)

?

2 3 1 2
2 2 2 2

Simulated Annealing for BCT ?

[Bezáková-Bhatnagar-Vigoda '06]



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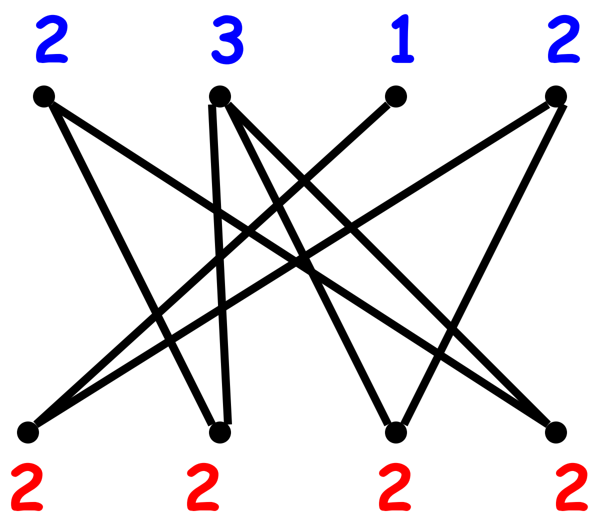
Unordered state → Ordered state

(EASY) (DIFFICULT)

? → 2 3 1 2 / 2 2 2 2 on $K_{n,n}$

Simulated Annealing for BCT ?

[Bezáková-Bhatnagar-Vigoda '06]



Ideal weights

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

Unordered state → Ordered state

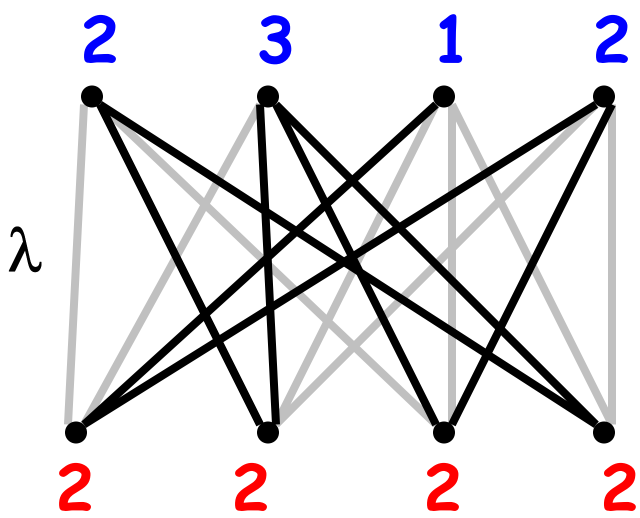
(EASY)

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 ?



Recall that

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where $\lambda(T) = \lambda^{\#\ \lambda\text{-edges in } T}$

$$\lambda(S) = \sum_{T \text{ in } S} \lambda(T)$$

$\lambda = \sim 0$ 1

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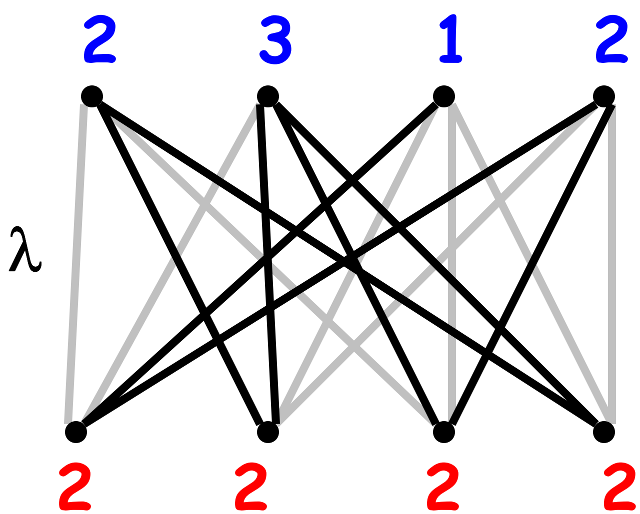
2 2 2 2 on G^*

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

Simulated Annealing for BCT ?



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where $\lambda(T) = \lambda^{\#\ \lambda\text{-edges in } T}$

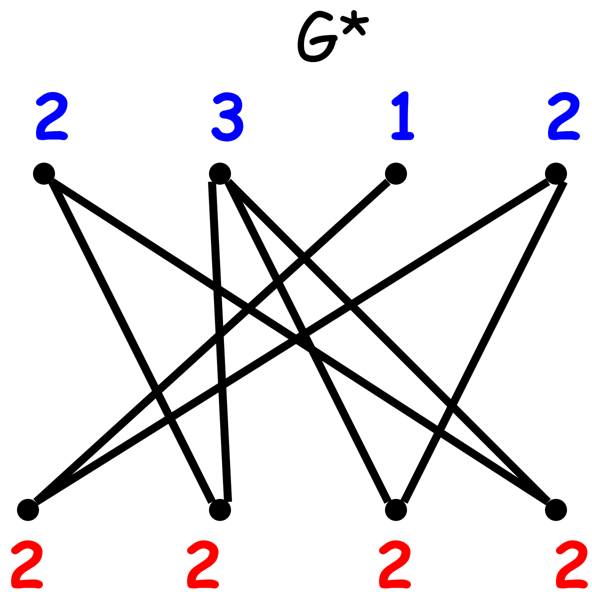
$$\lambda(S) = \sum_{T \text{ in } S} \lambda(T)$$

The catch :

What, if for some u,v, there is no near-table which uses all real edges ? Then,

$$\lambda(\mathscr{N}(u,v)) = 0 \quad \text{for } \lambda = 0.$$

Simulated Annealing for BCT ?



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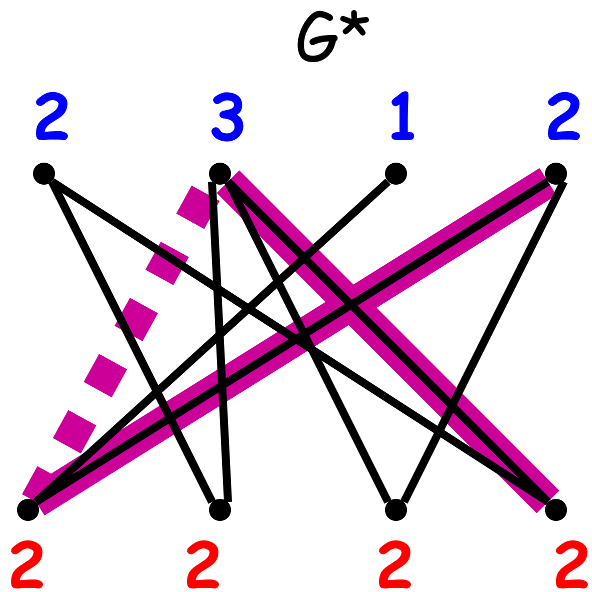
Thm [Bezáková-Bhatnagar-Vigoda '06]:

There exists a graph G^* with given degree sequence s.t. between any two vertices there exists an "alternating" path of length $\leq$ **5**.

Simulated Annealing for BCT ?



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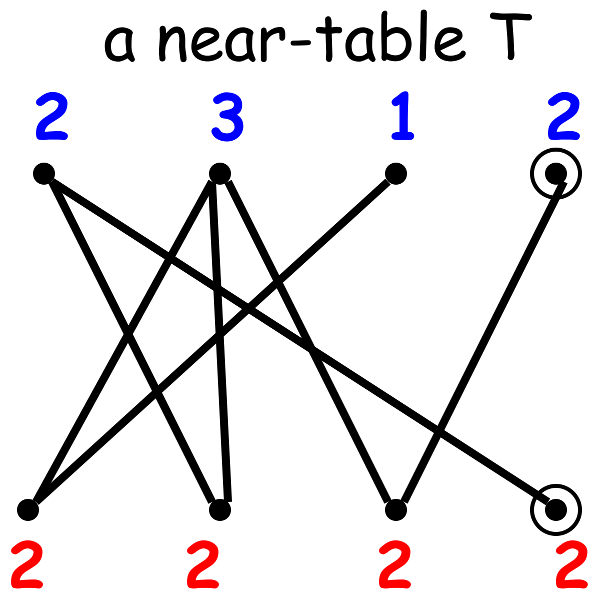

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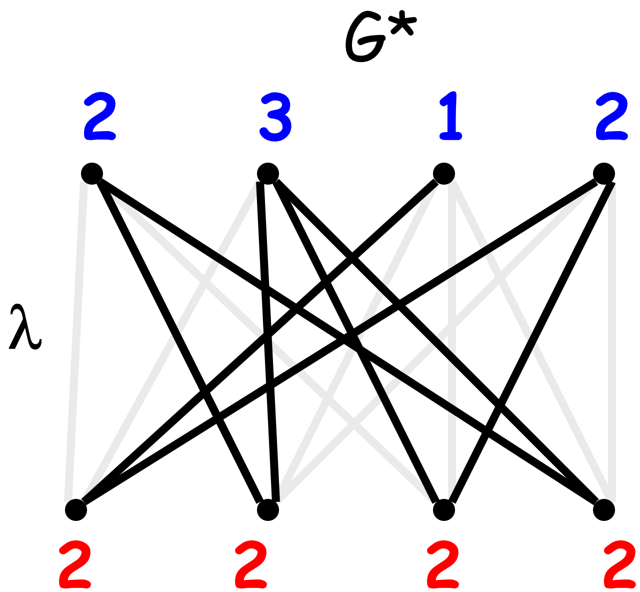
There exists a graph G^* with given degree sequence s.t. between any two vertices there exists an "alternating" path of length $\leq$ **5**.

Corollary: There exists a (u,v)-near-table similar to G^*.

Simulated Annealing for BCT ?



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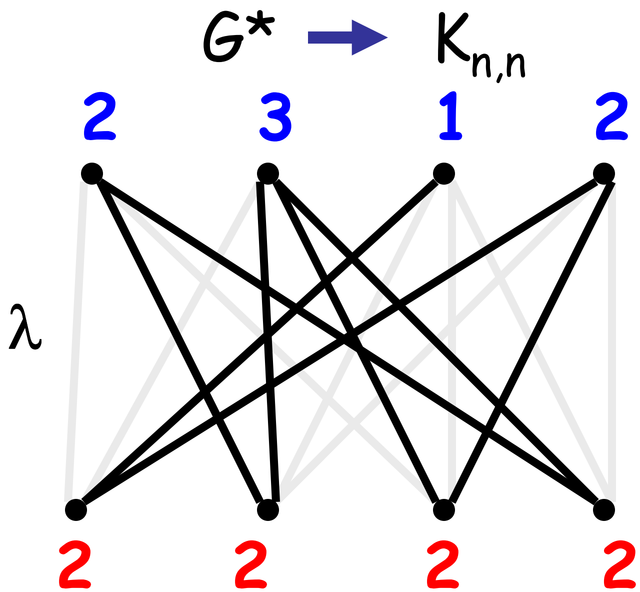

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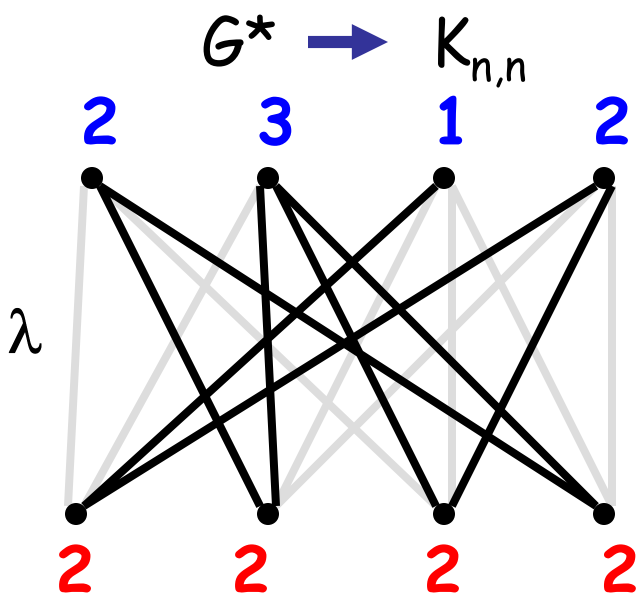

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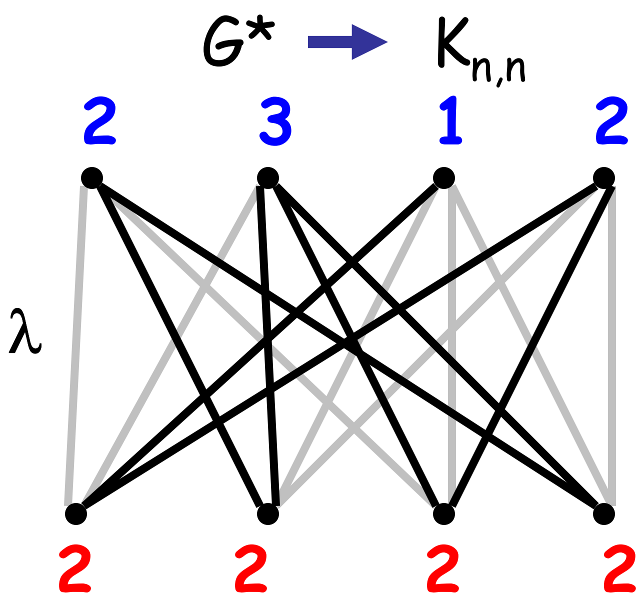

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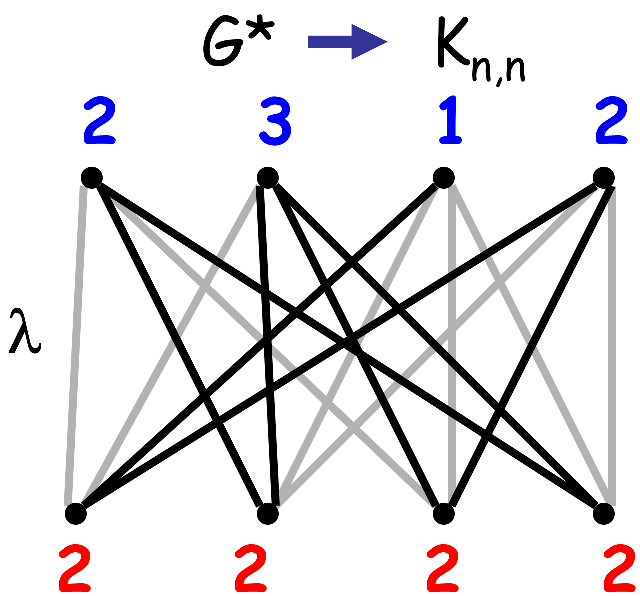

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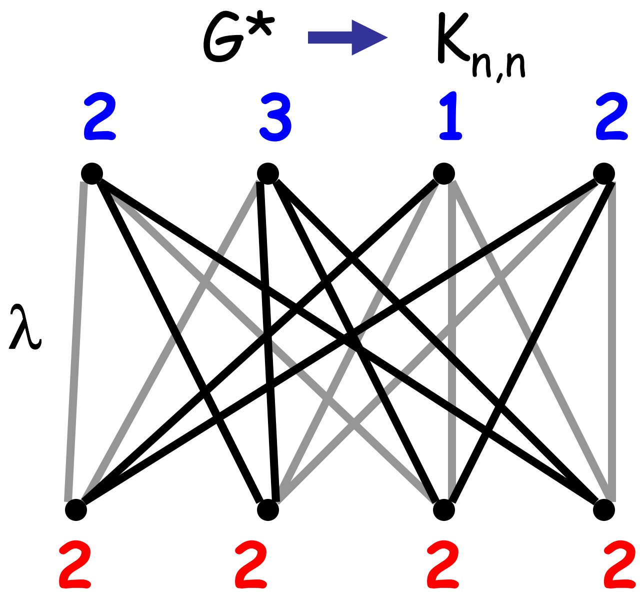

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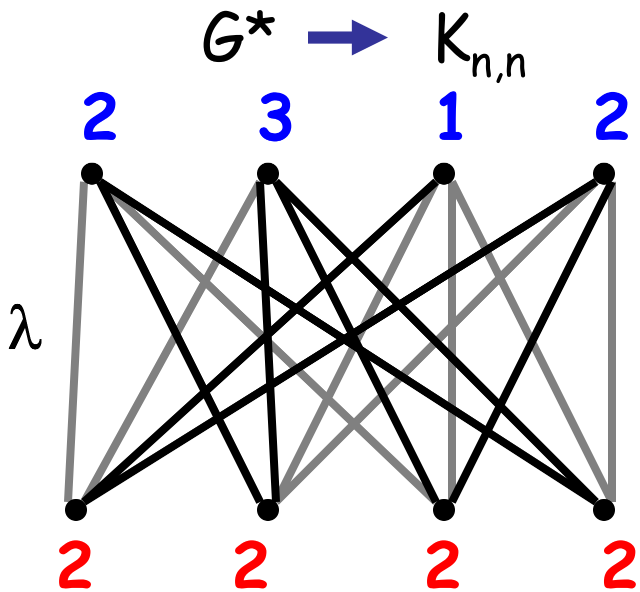

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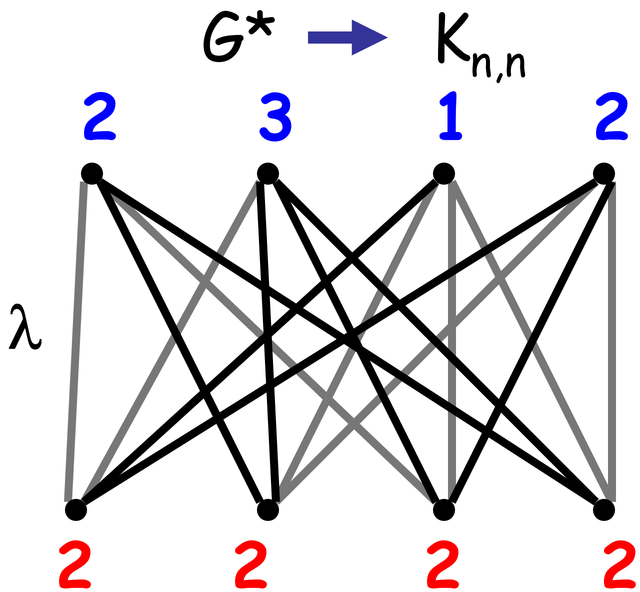

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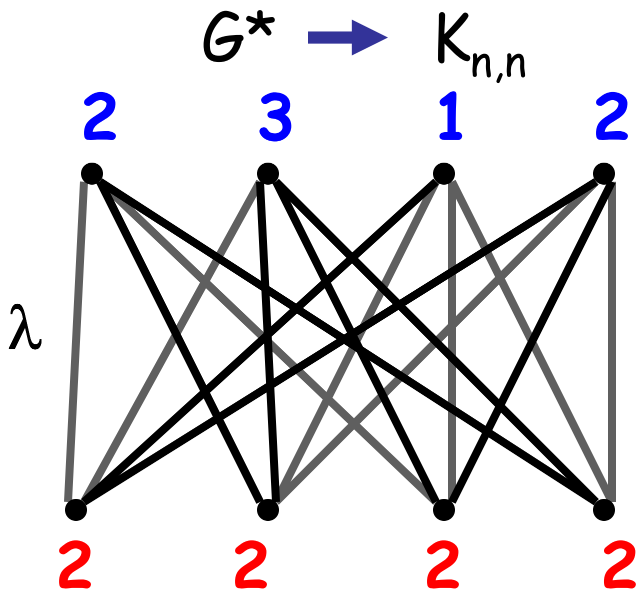

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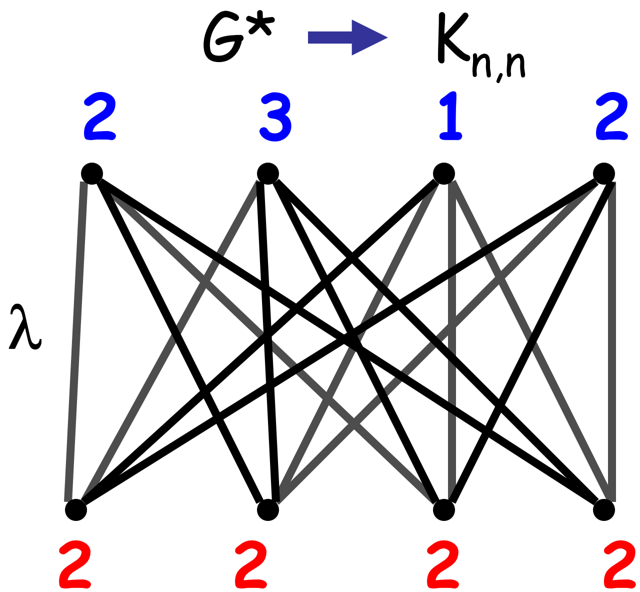

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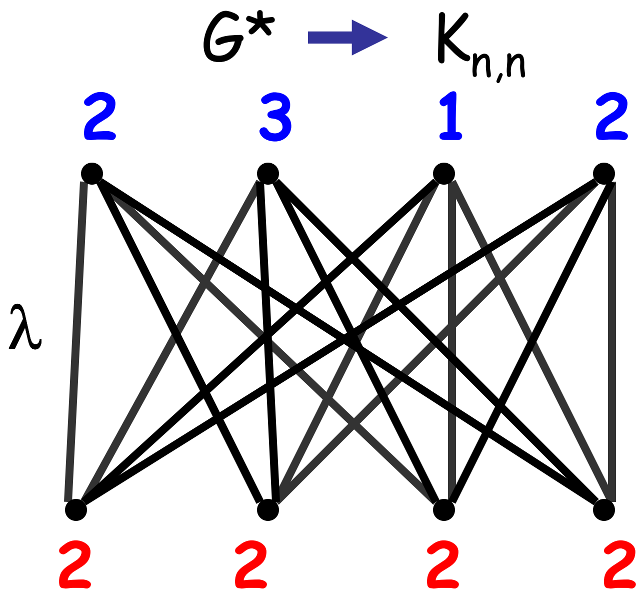

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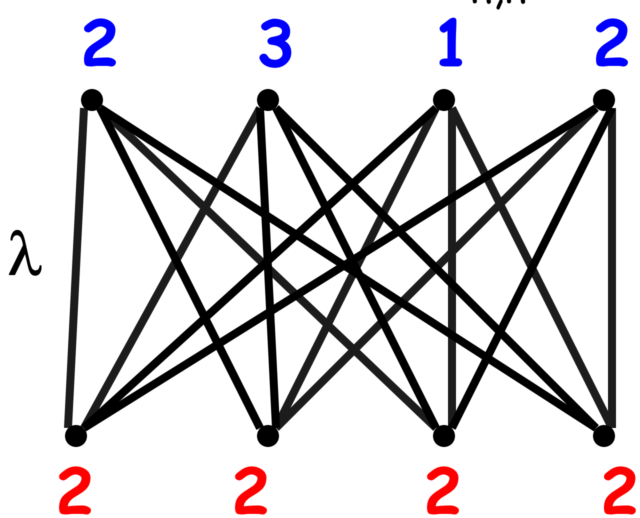

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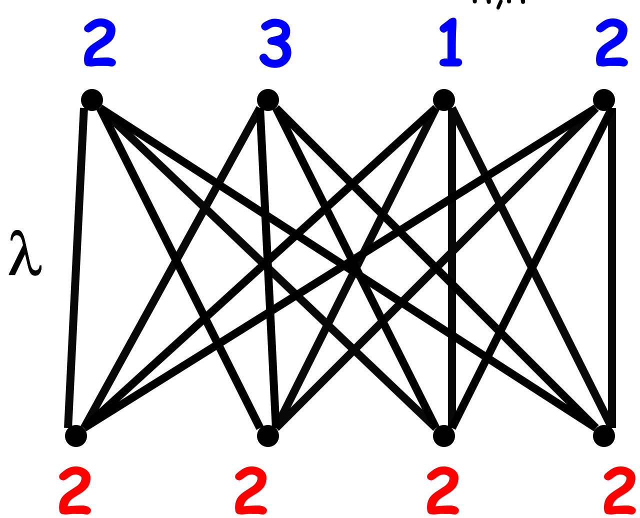

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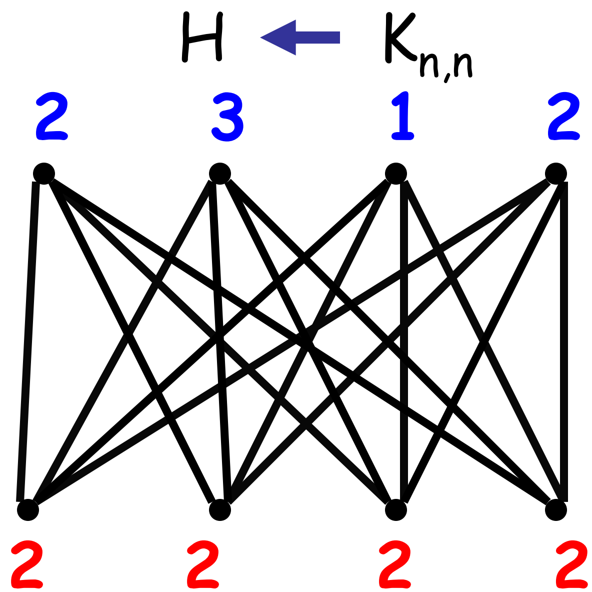

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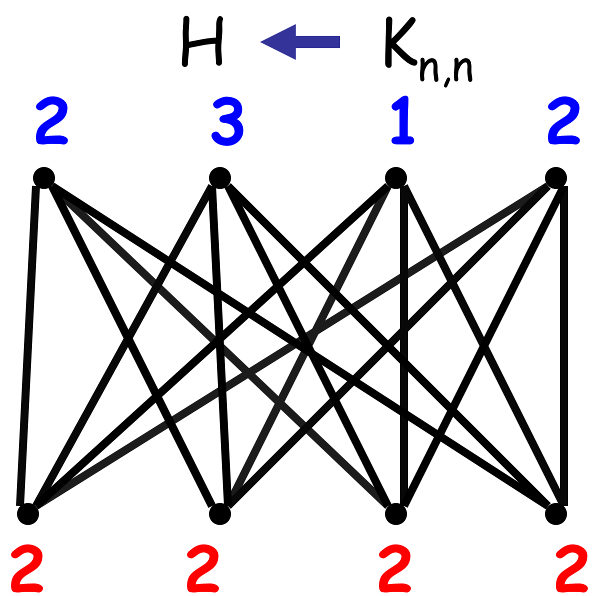

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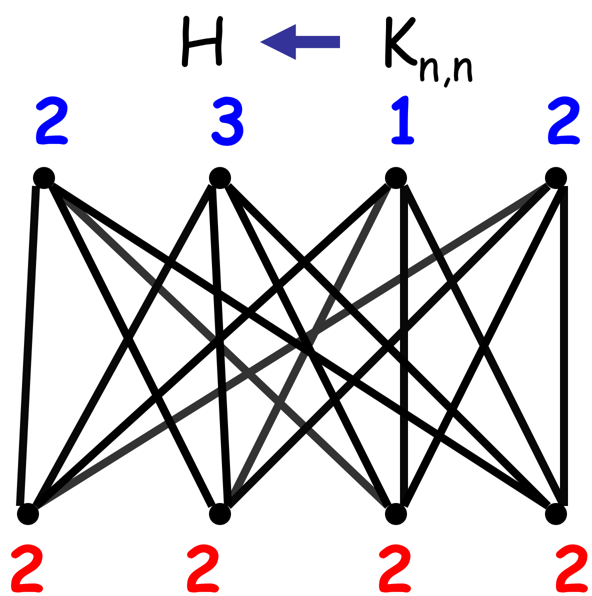

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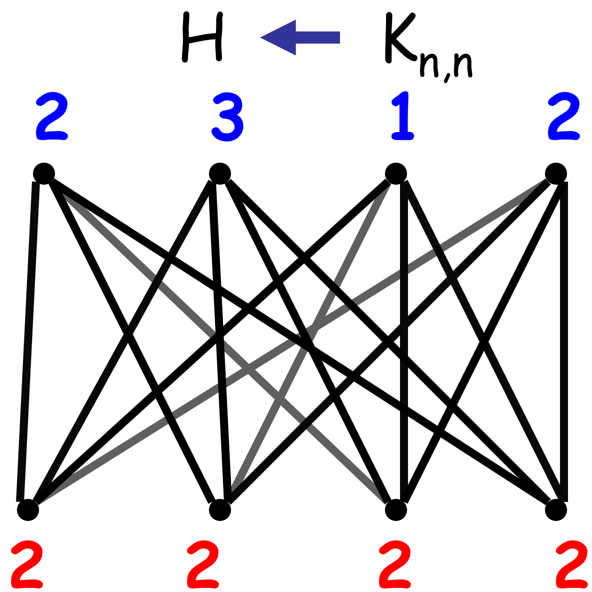

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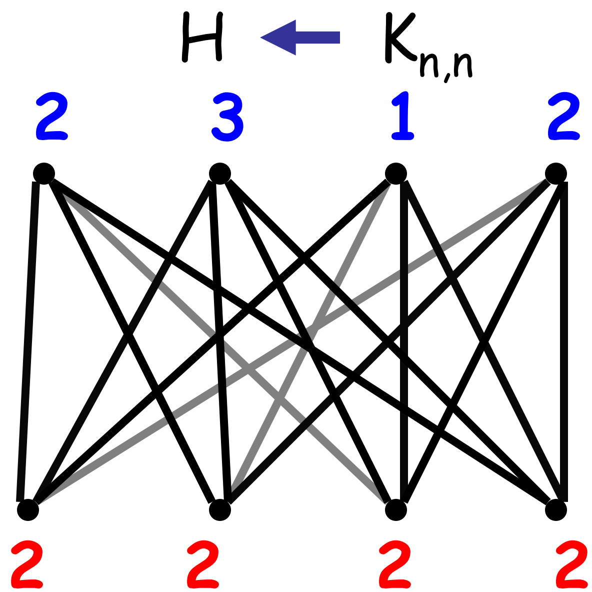

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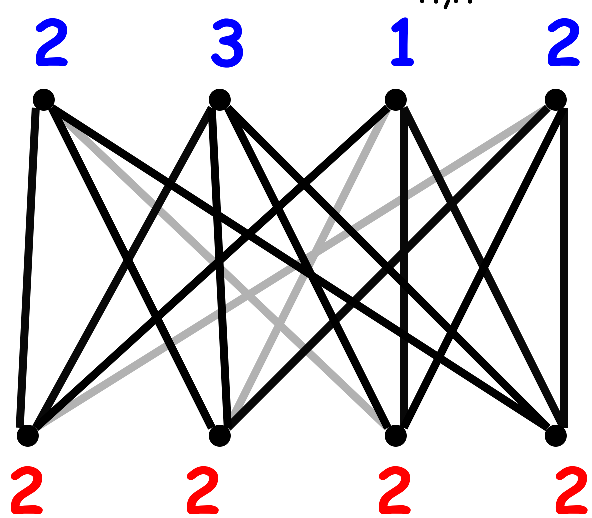

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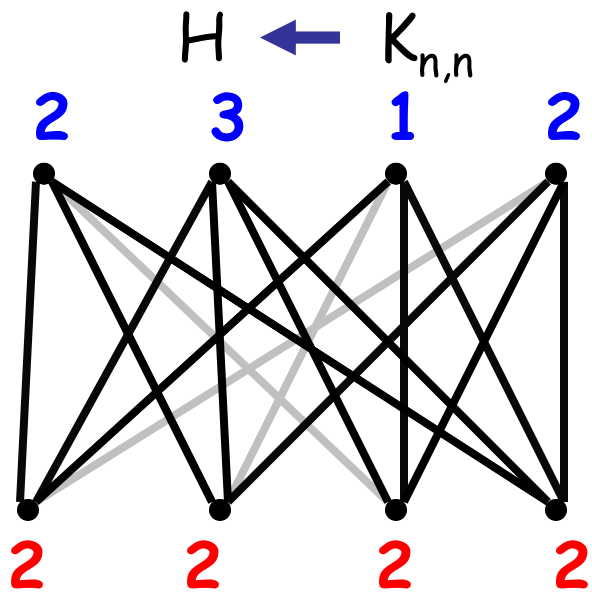

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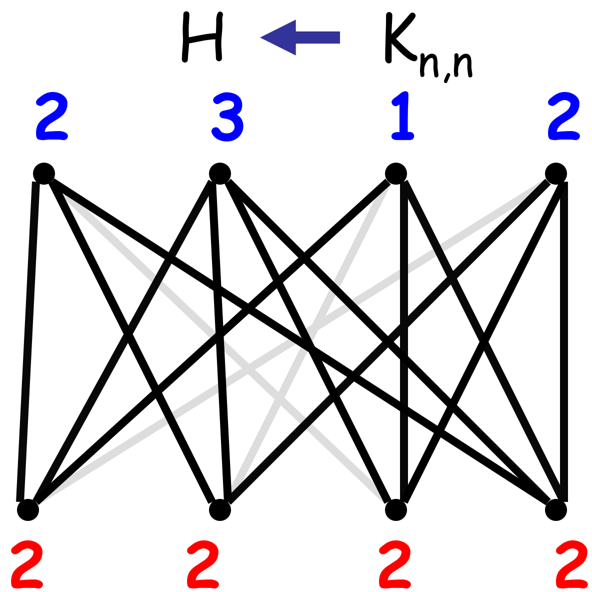

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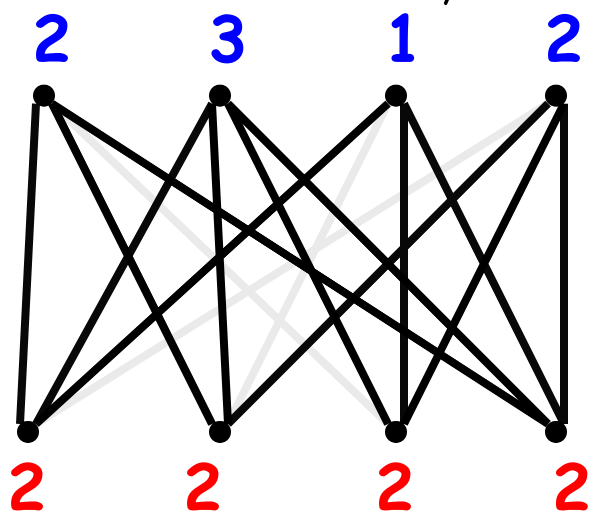

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Different Approaches

Theory (Markov chain Monte Carlo with simulated annealing)

- Jerrum-Sinclair-Vigoda '01: approximate permanent in $O^*(n^{10})$, yields $O^*((mn)^{10})$ algorithm for m x n binary contingency tables
- Bezáková-Bhatnagar-Vigoda '06: $O^*((mn)^3(m+n)^5)$

Practice (sequential importance sampling, Chen-Diaconis-Holmes-Liu '05)

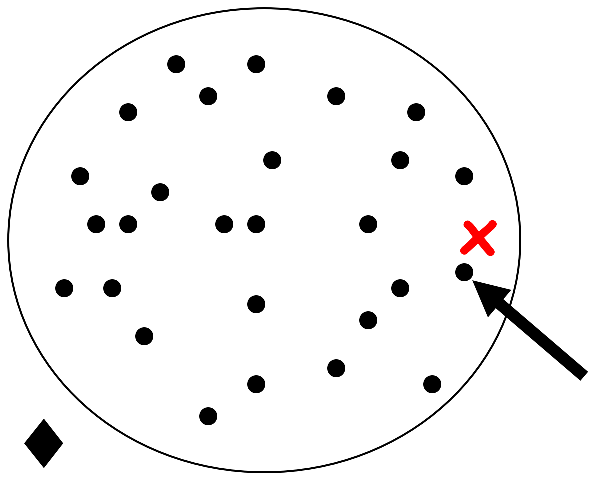
- Bezáková-Sinclair-Štefankovič-Vigoda '06: negative example
- Jose Blanchet '06: SIS works if marginals $O(n^{1/4})$
- Bayati-Kim-Saberi '07: alternative importance sampling method, works if marginals $O(n^{1/4})$

Practice (the switching Markov chain, Diaconis-Gangolli '94)

- Kannan-Tetali-Vempala '97, Cooper-Dyer-Greenhill '05: works for regular marginals

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

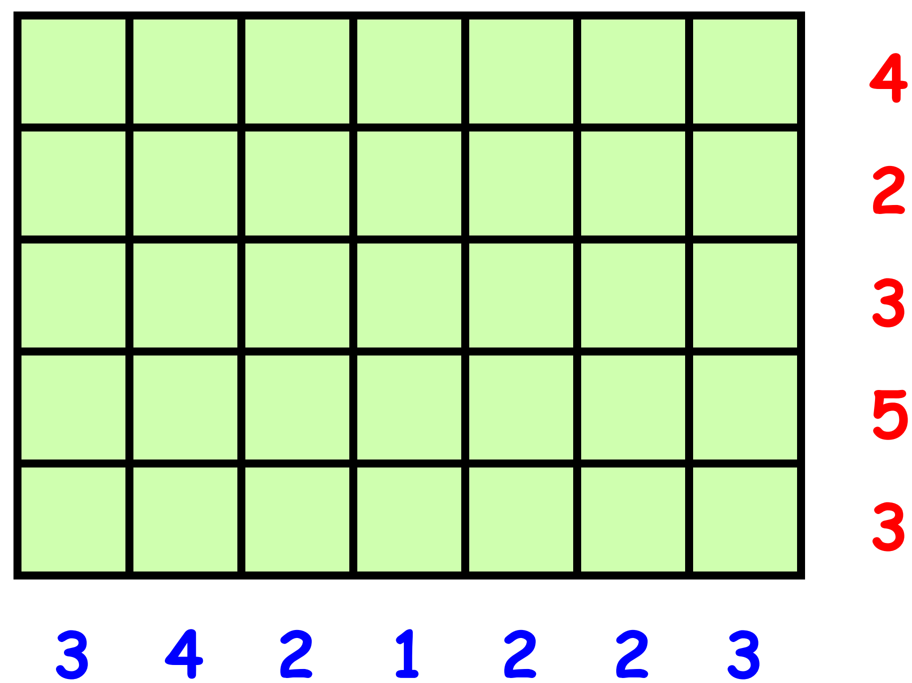
$$E[\eta] = \sum \sigma(x).1/\sigma(x) = \text{size of the set}$$

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



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

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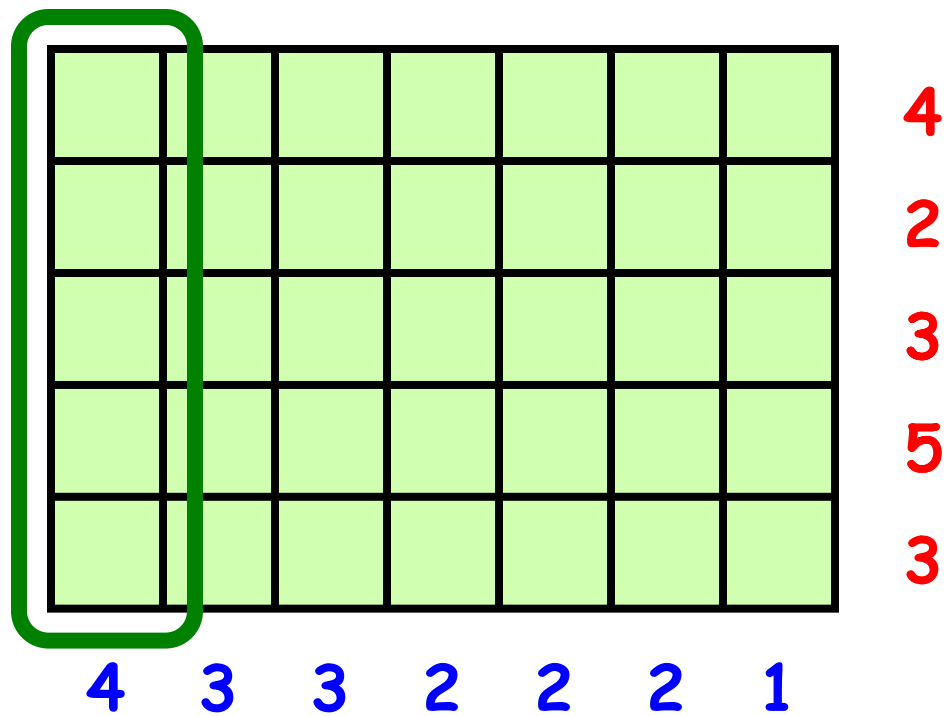

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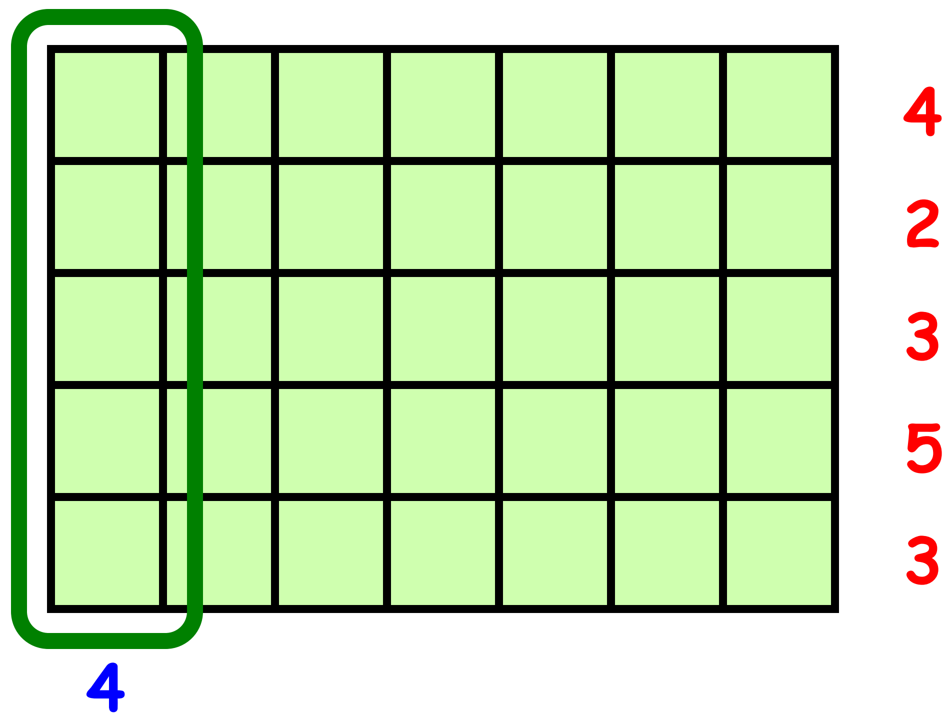

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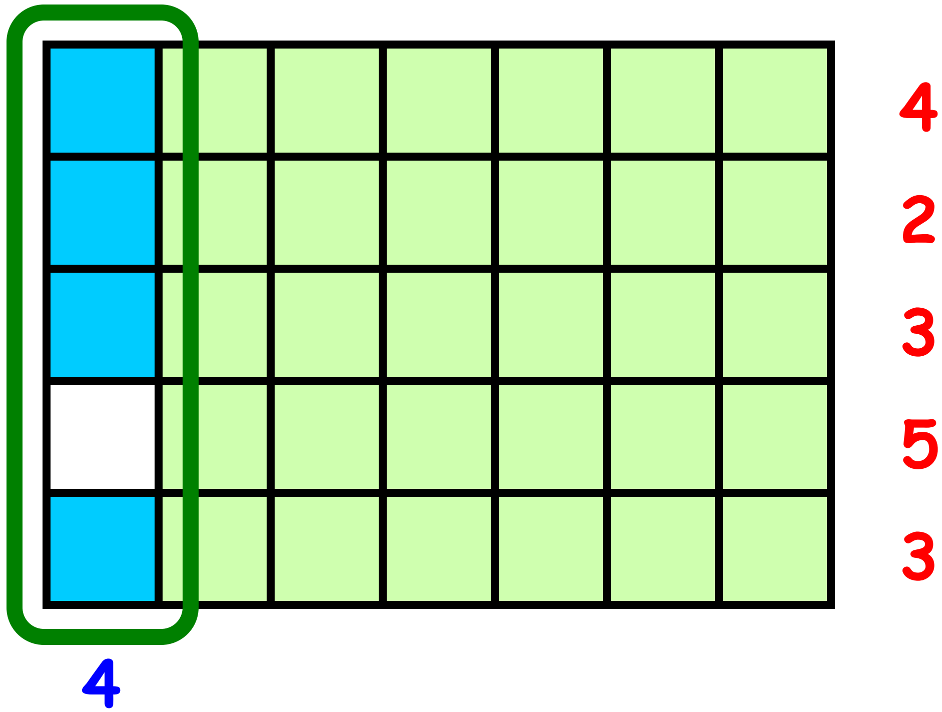

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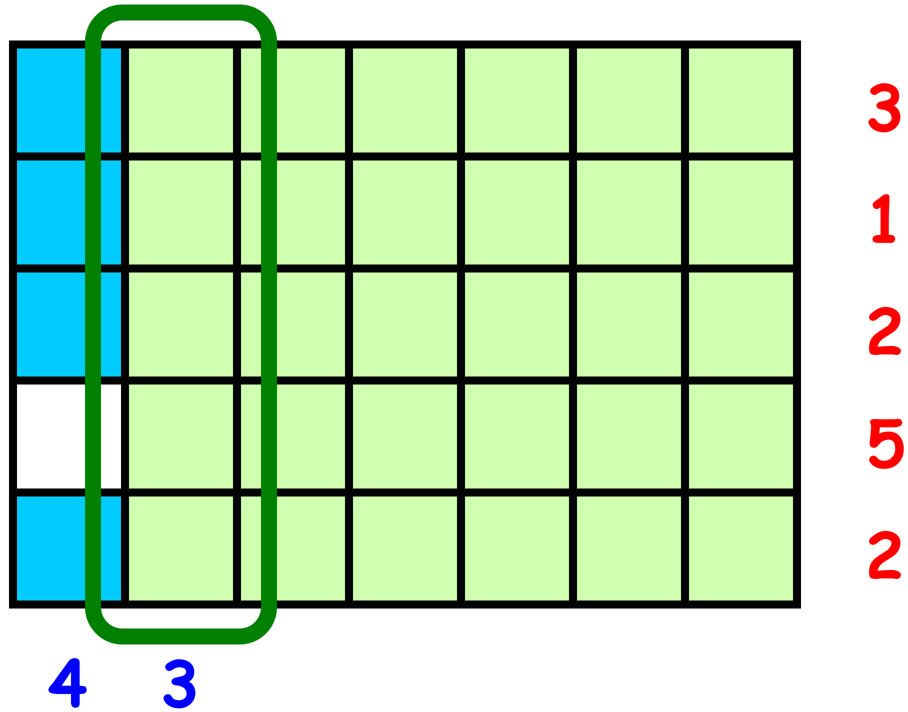

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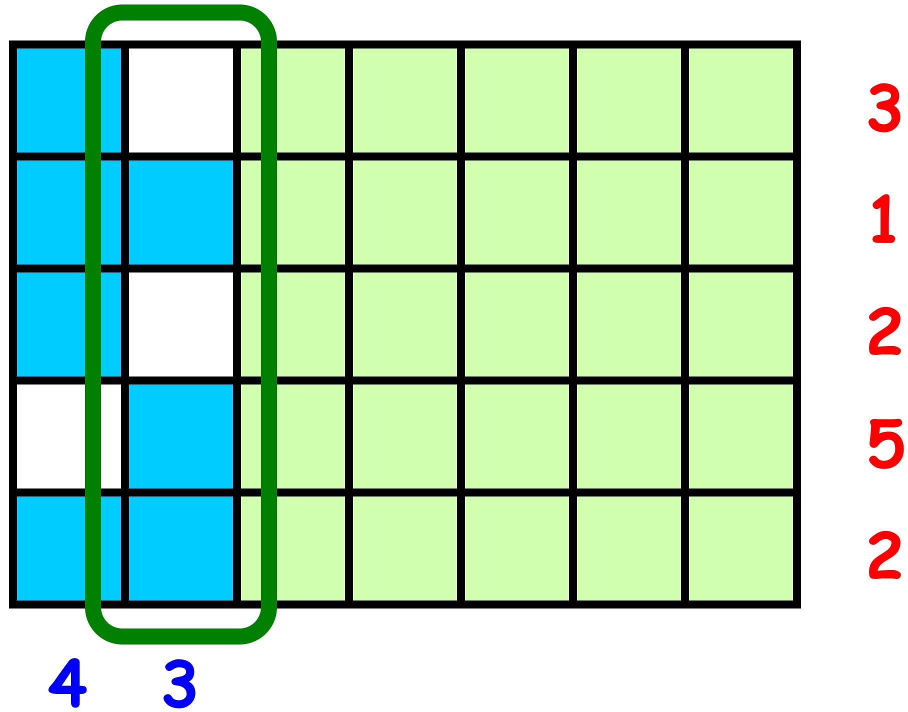

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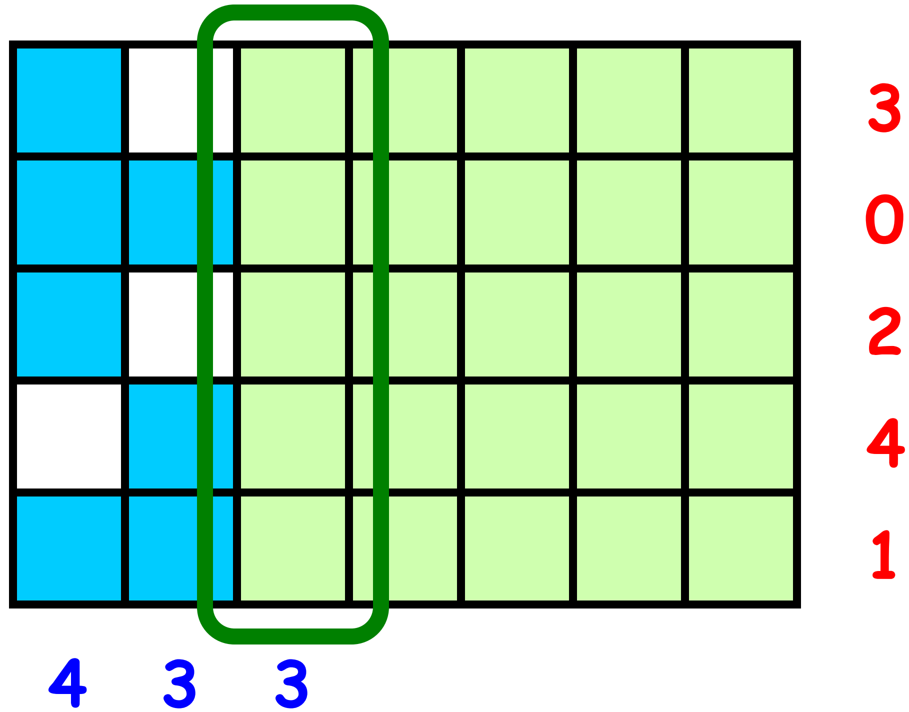

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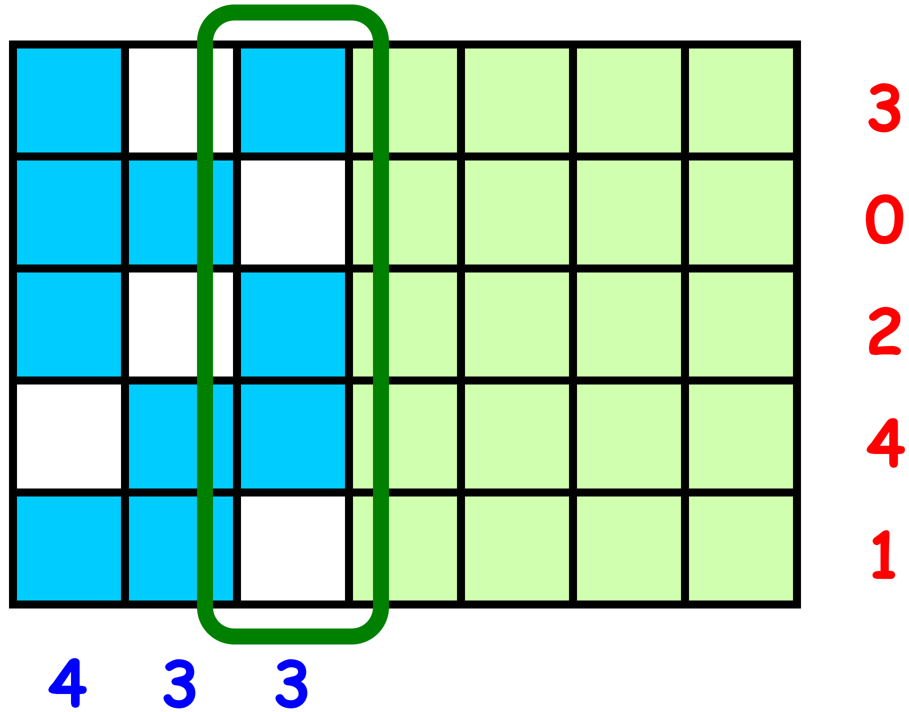

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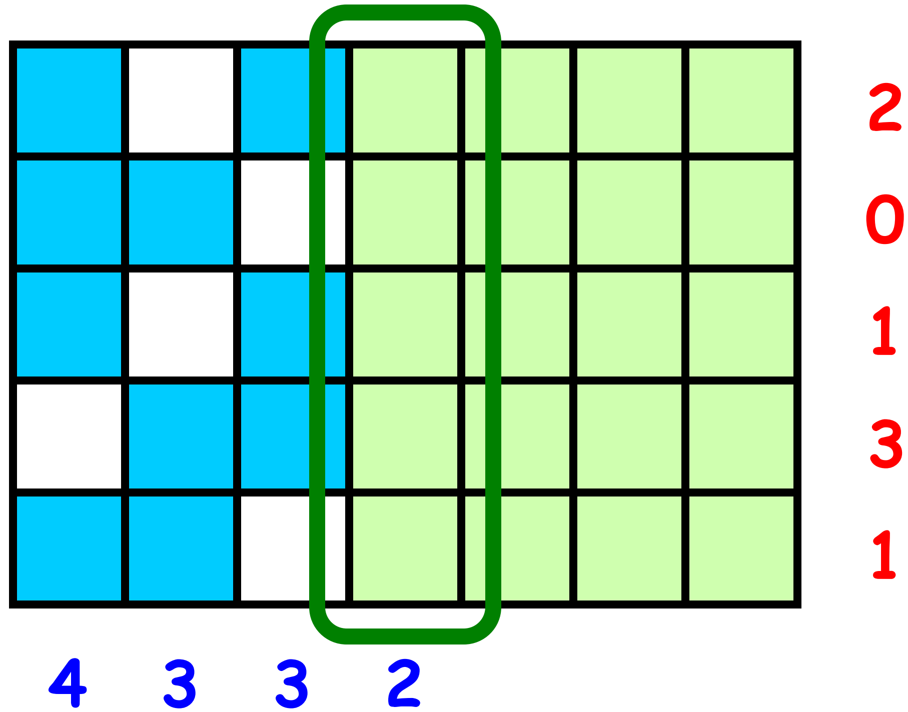

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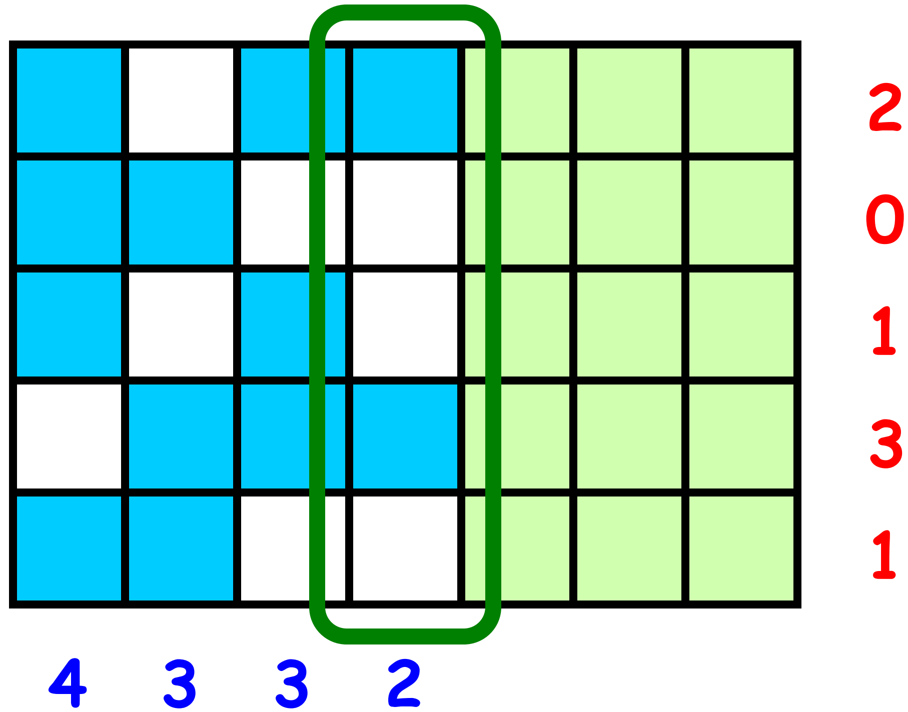

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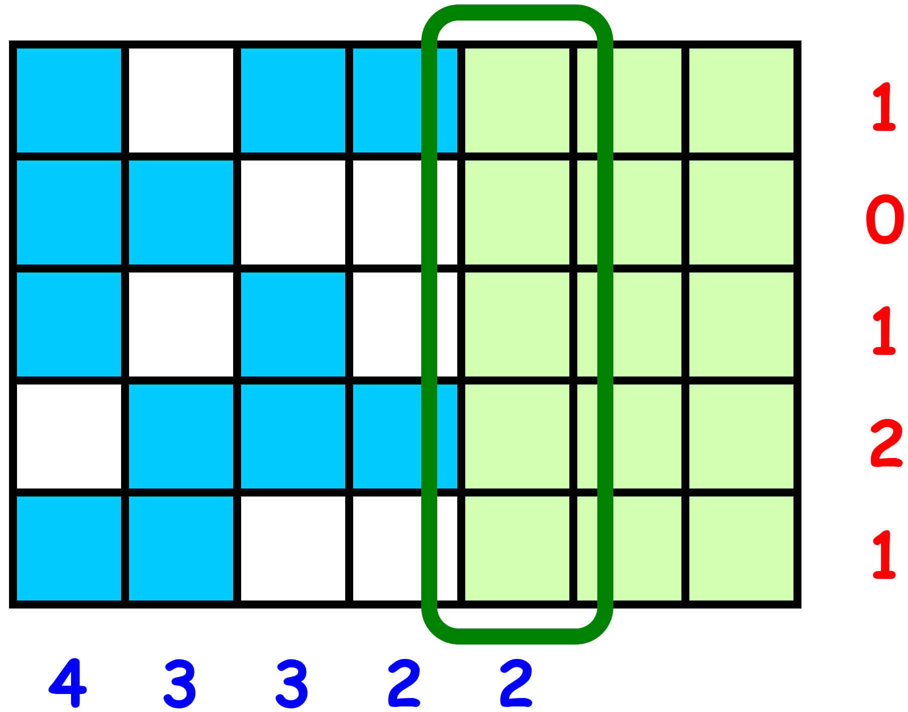

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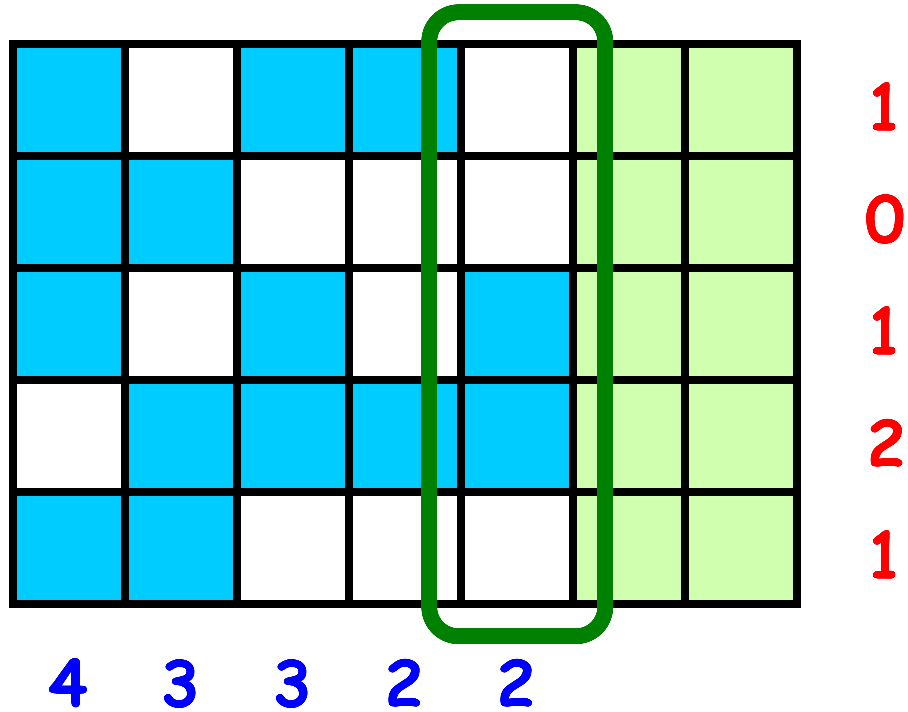

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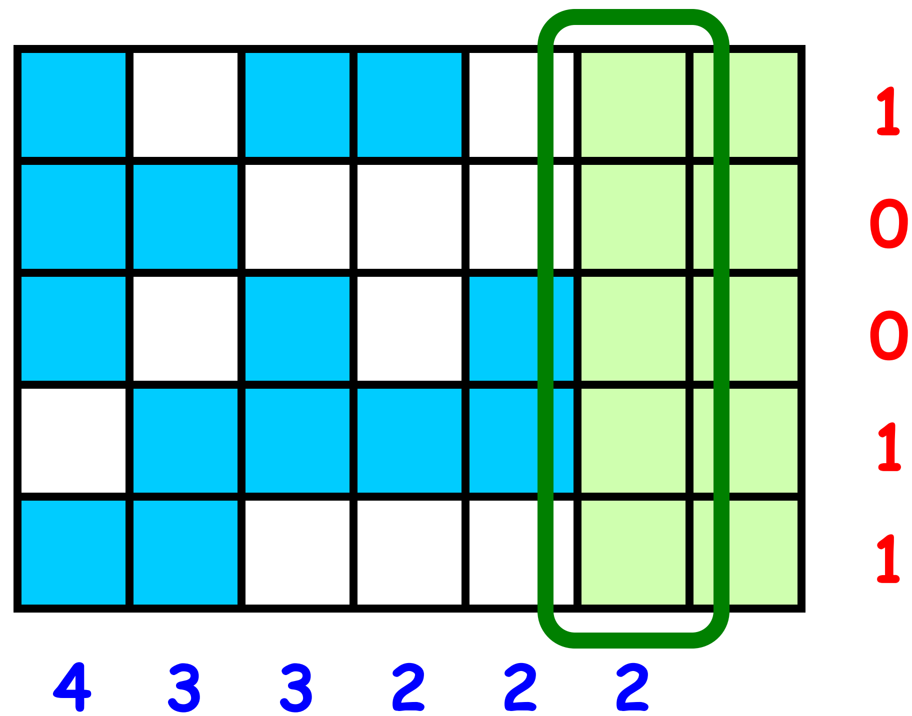

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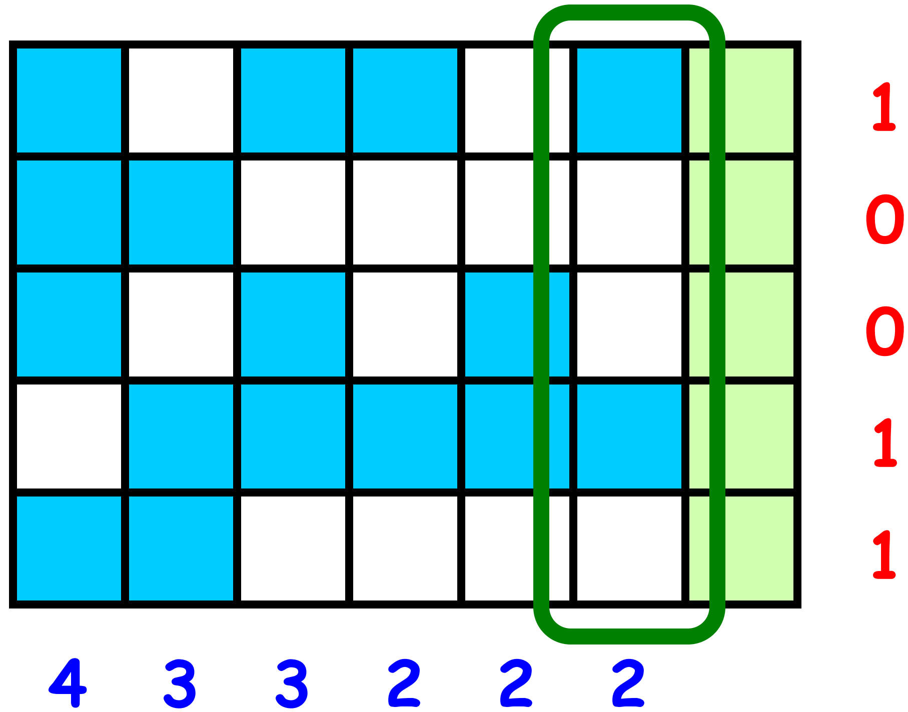

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[Chen-Diaconis-Holmes-Liu '05]

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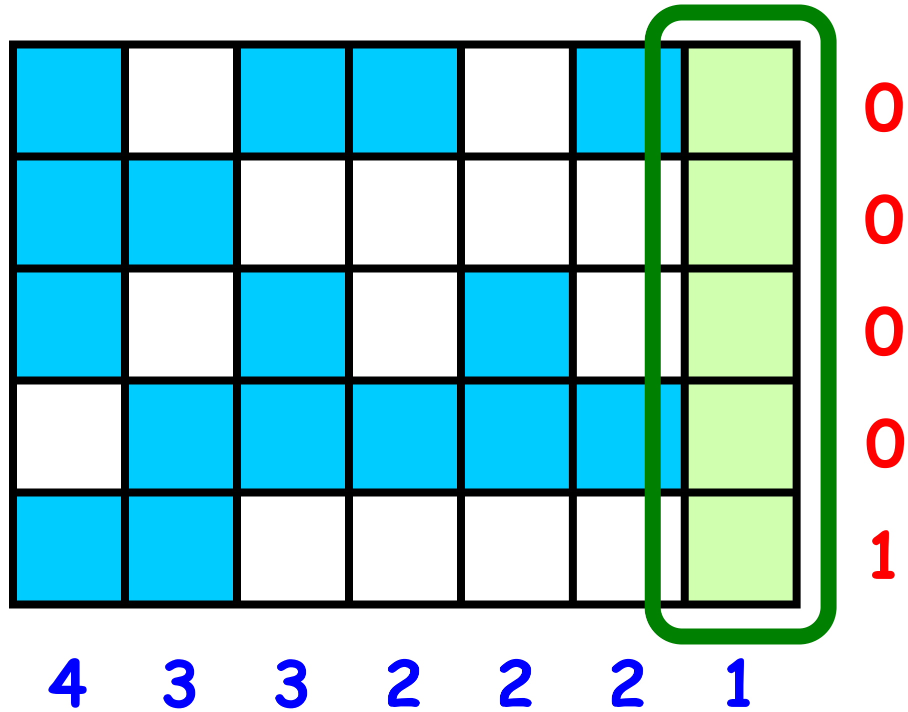

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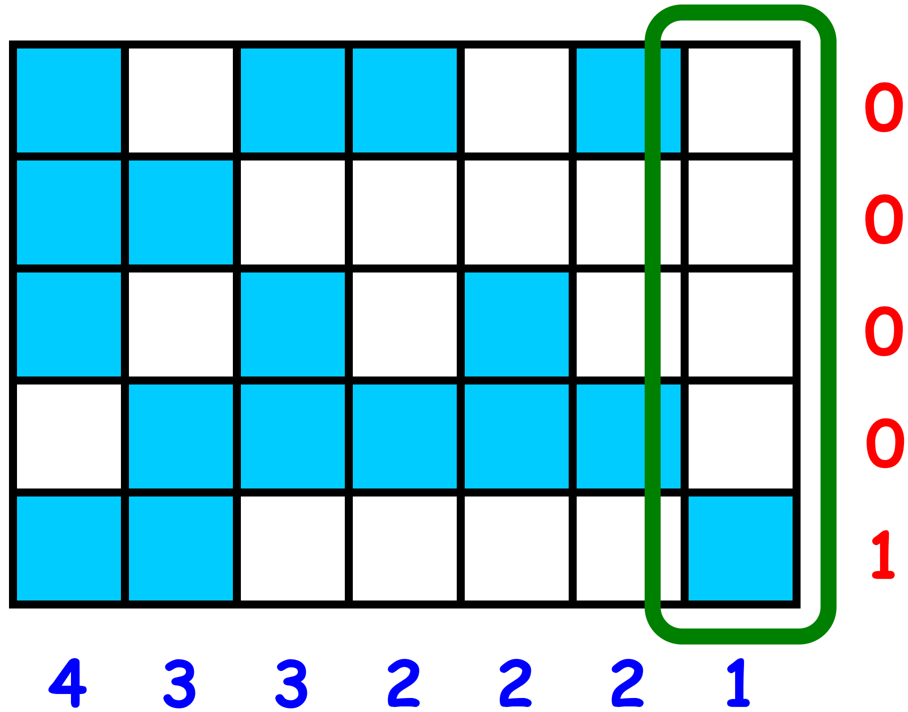

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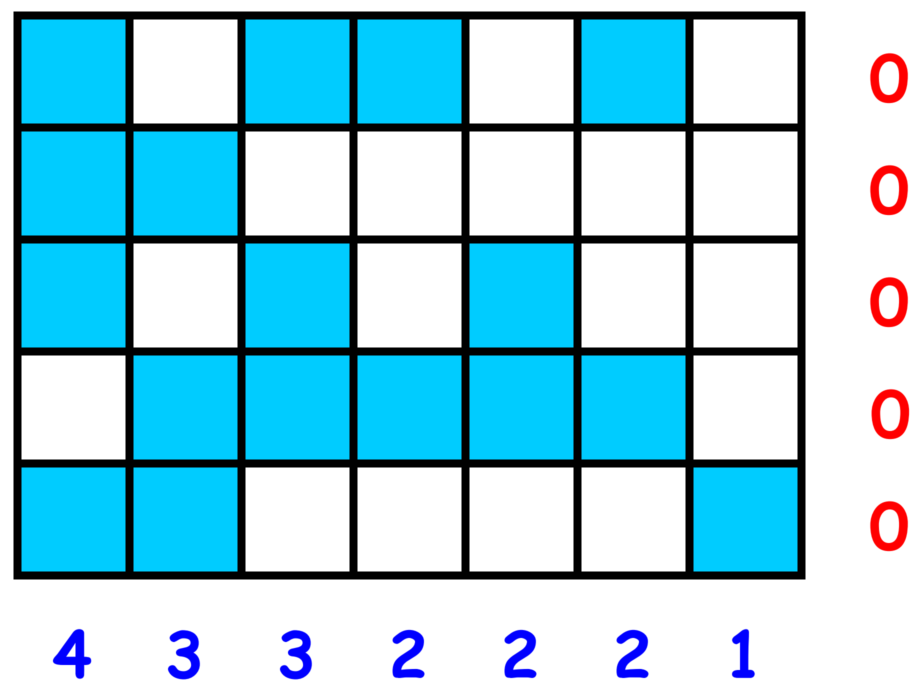

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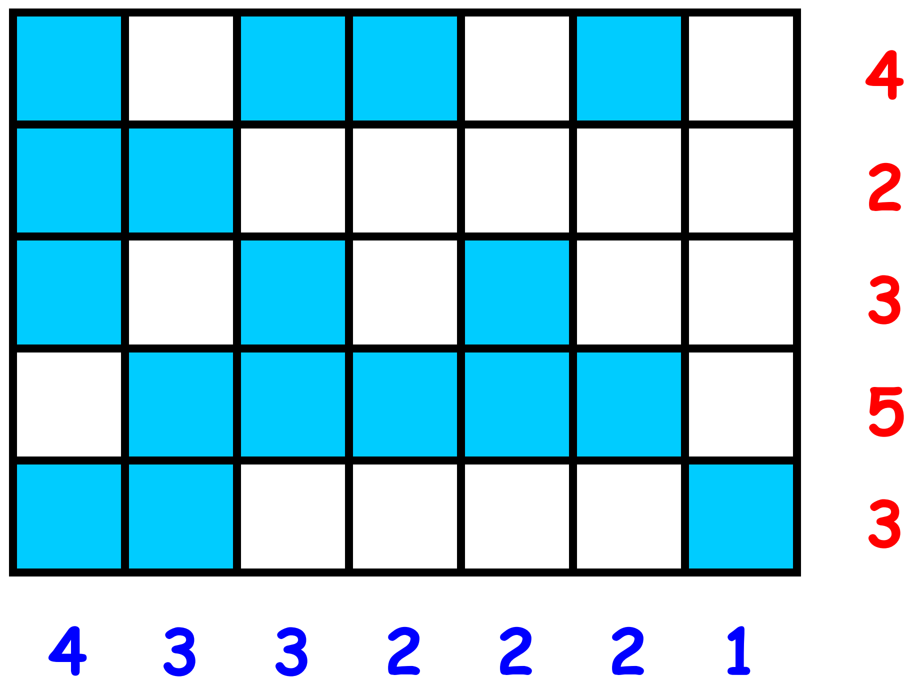
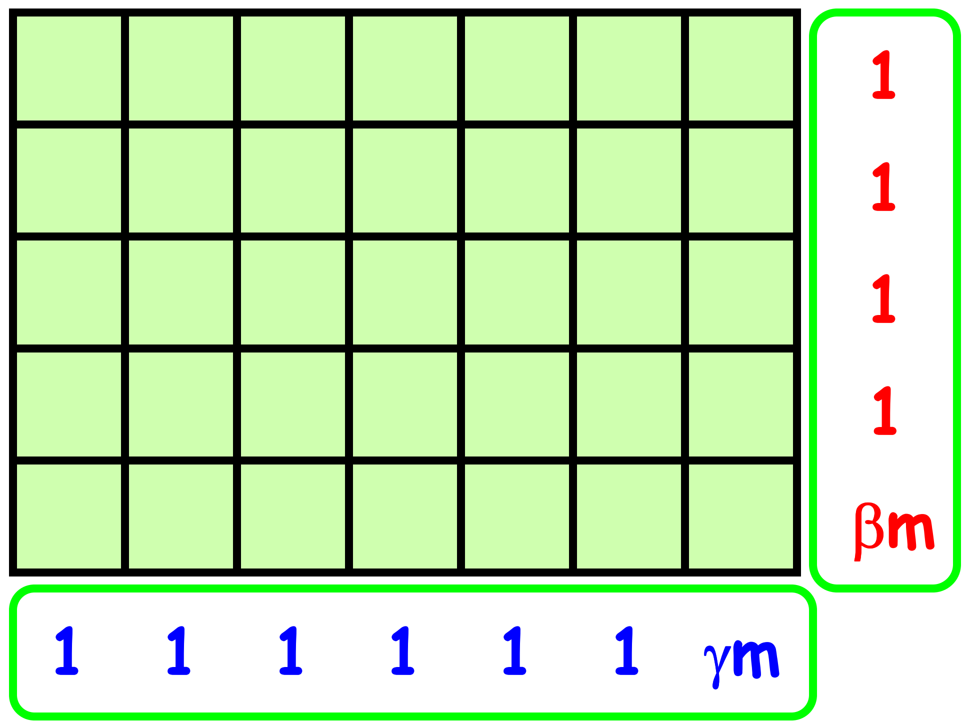


A Counterexample for SIS

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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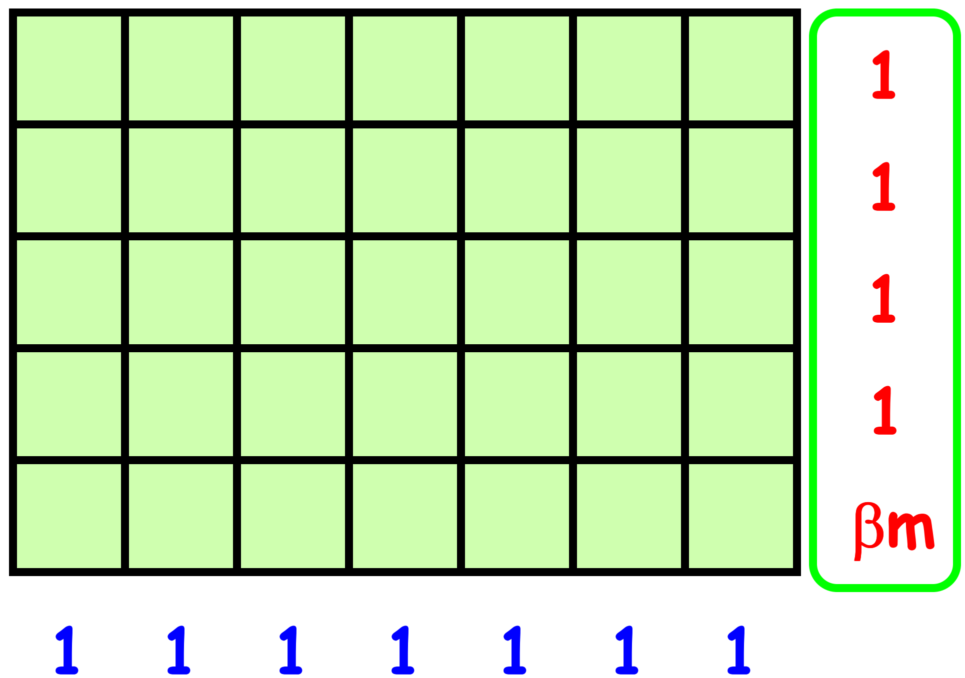
Simpler example



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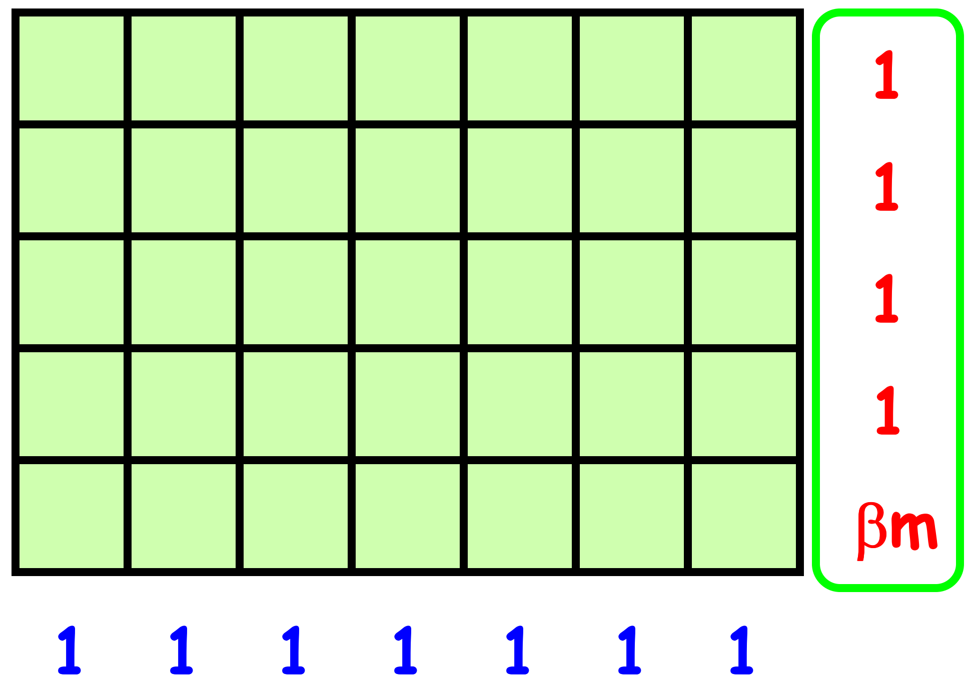

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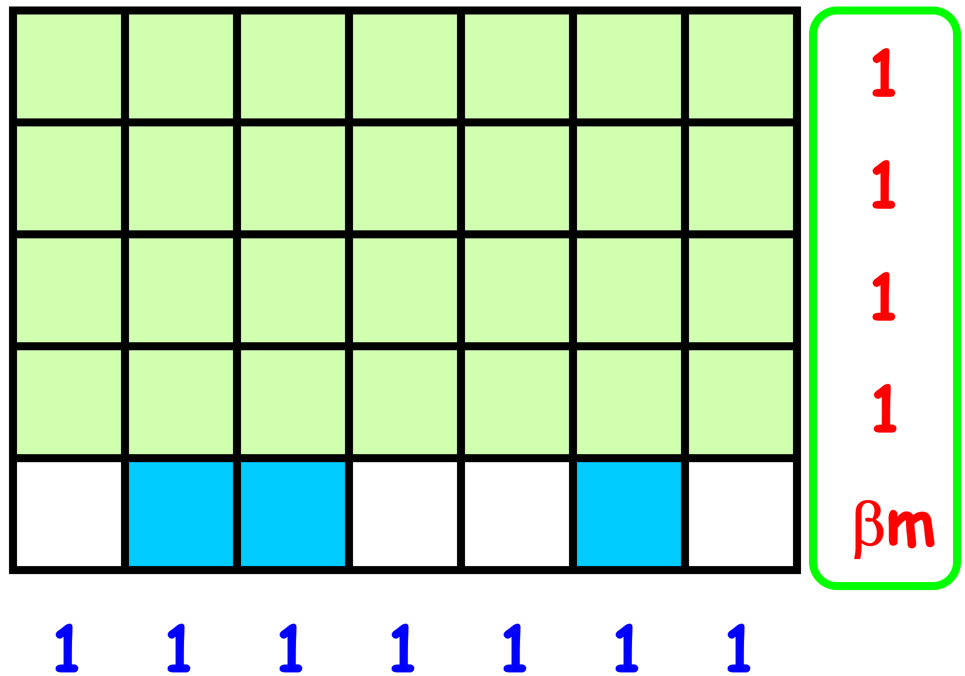

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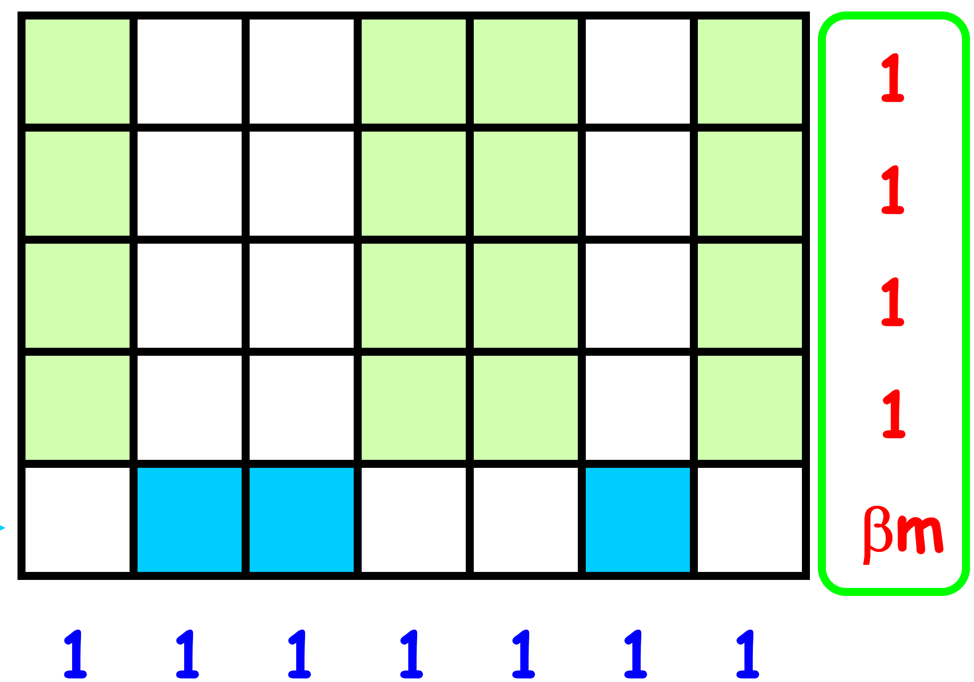

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Expect: $\alpha\beta\mathbf{m}$ ones

SIS: asymptotically fewer

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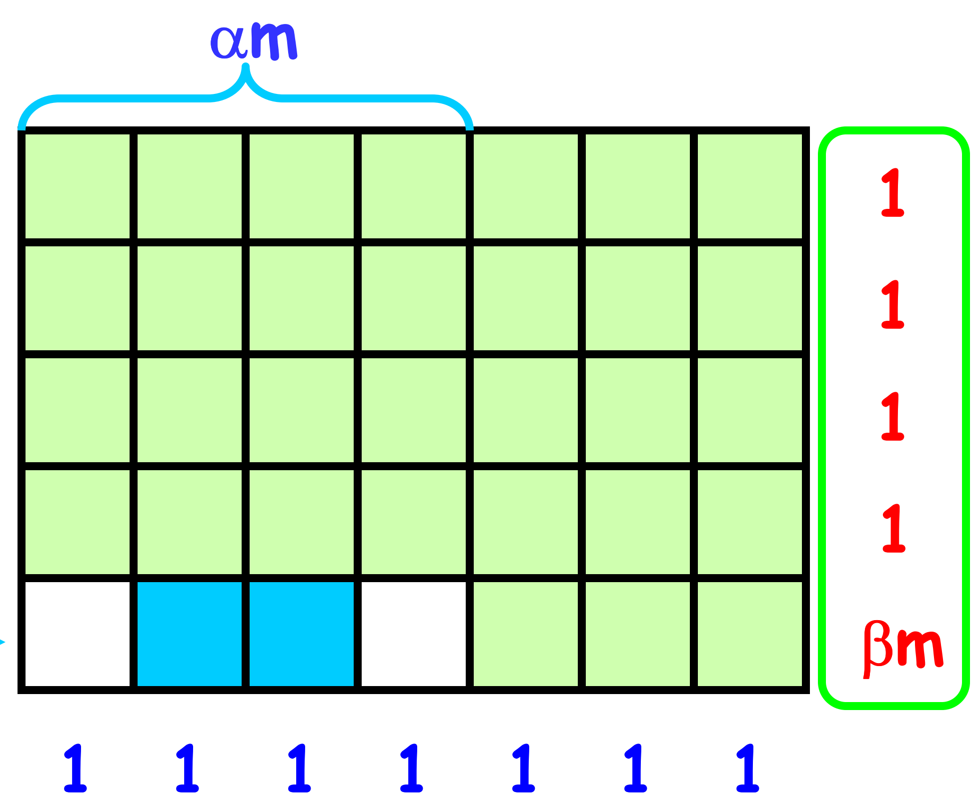

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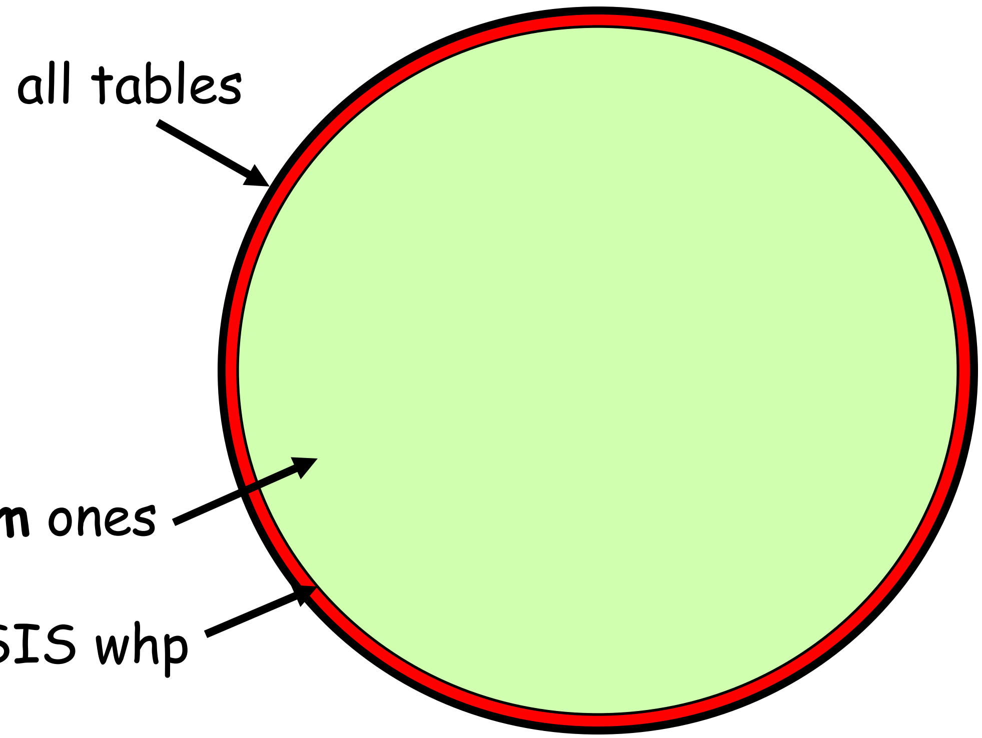

tables with ~$\alpha\beta\mathbf{m}$ ones

tables seen by SIS whp

A Counterexample for SIS

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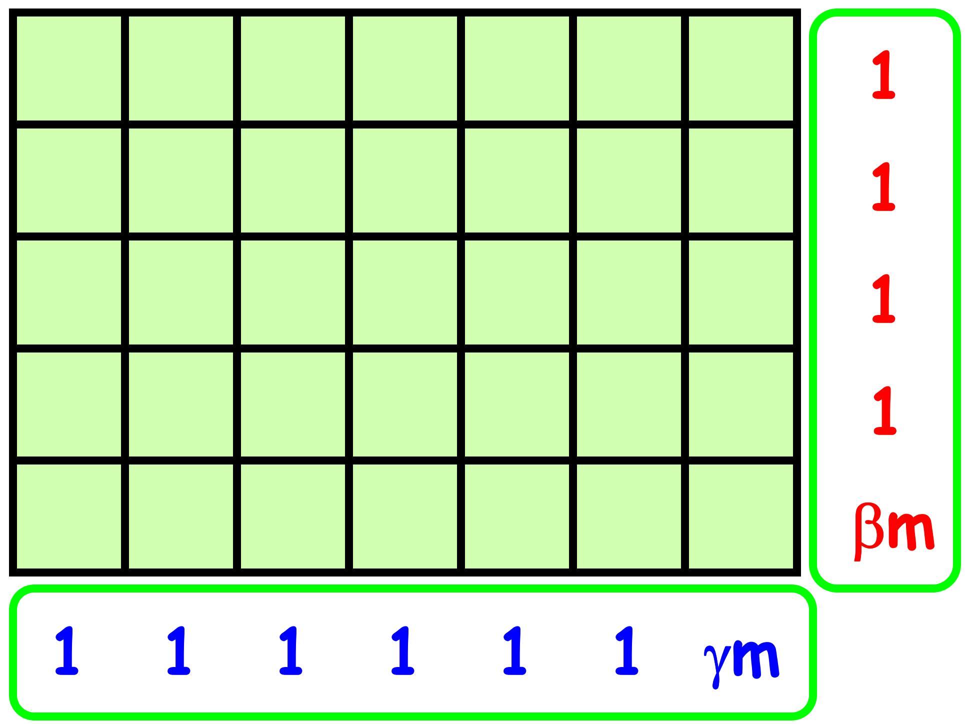
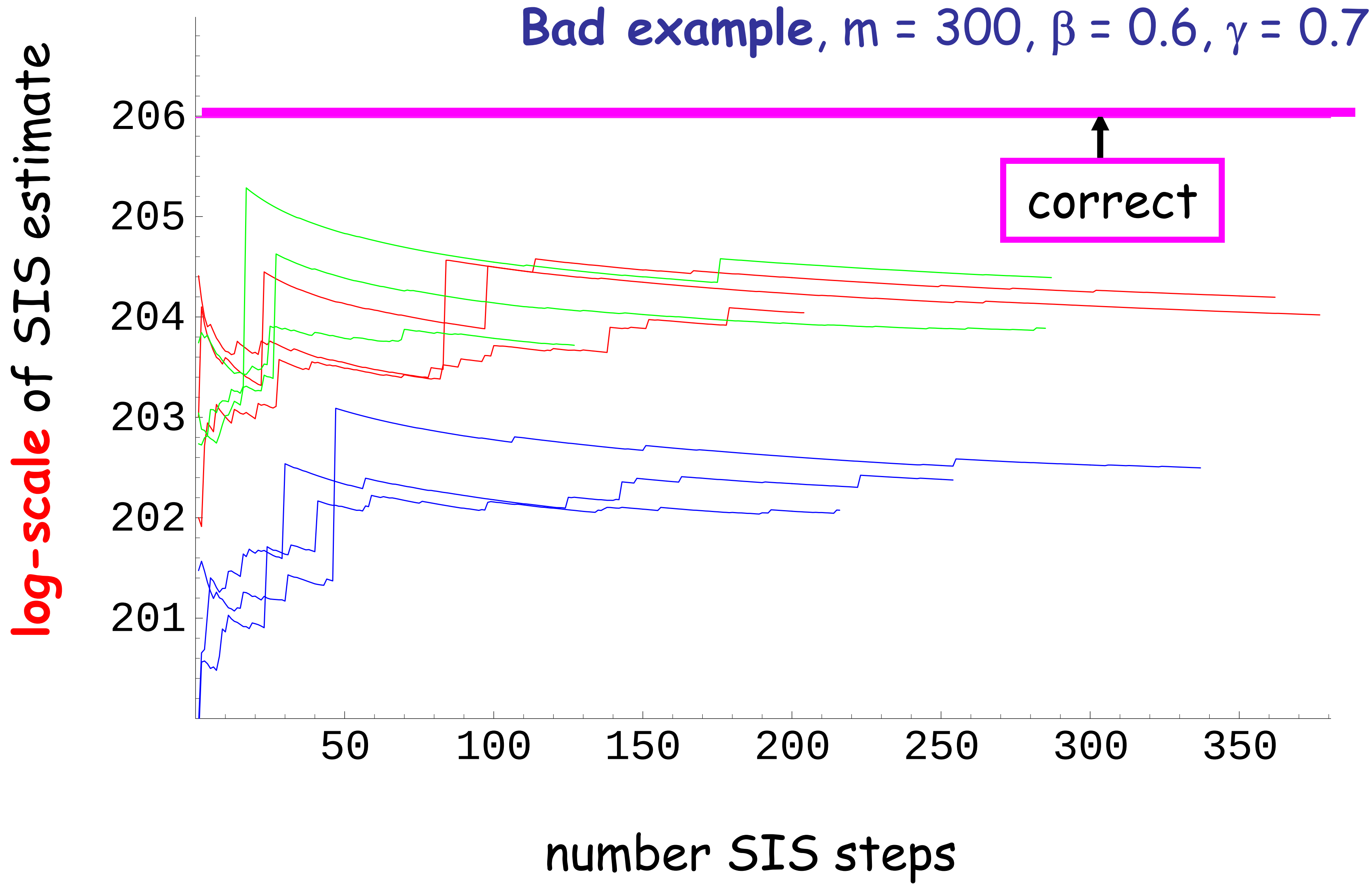
Result holds for any order of rows/columns.

Alternating rows and columns?



SIS - Experimental Results



Open Problems

- Practical algorithm ?
- Detecting convergence of SIS
- SIS for larger marginals ?
- The Switching Markov chain of Diaconis-Gangolli ?

- General contingency tables
- Cell-bounded tables
- Counting non-bipartite graphs with a given degree sequence