On the number of contingency tables and the independence heuristic

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Joint work with Igor Pak

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Outline

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- Sampling $\leftrightarrow$ Counting (self-reduction):

$$\mathbb{P}(X_{11} \geq t) = \frac{\mathrm{T}\begin{pmatrix} \mathbf{a} = (a_1 - t, a_2 \ldots, a_m) \\ \mathbf{b} = (b_1 - t, b_2 \ldots, b_n) \end{pmatrix}}{\mathrm{T}\begin{pmatrix} \mathbf{a} = (a_1, a_2 \ldots, a_m) \\ \mathbf{b} = (b_1, b_2 \ldots, b_n) \end{pmatrix}}$$

Uniform contingency tables in statistics

Data

1	0	3	2	0	7	13
1	2	0	4	3	0	10
7	5	2	1	0	0	15
0	0	3	1	3	9	16
0	3	1	8	0	2	14
5	3	0	3	5	3	19
9	13	9	19	11	21	

$v.s.$

Null model

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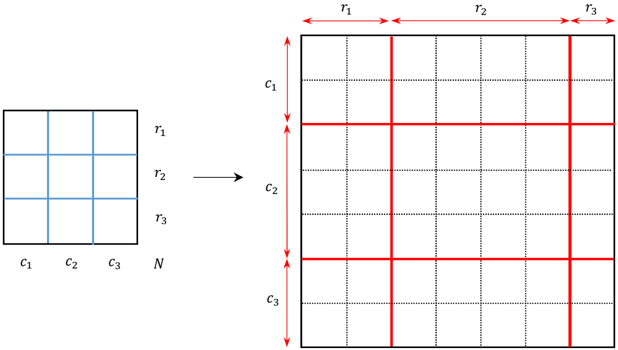
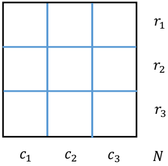
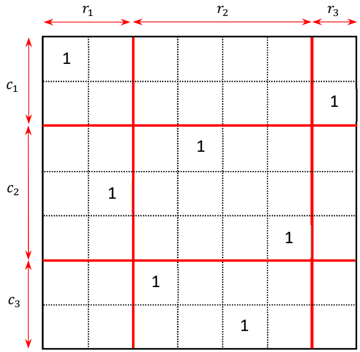
- Contingency tables are fundamental tools in statistics for studying dependence structure between two or more variables
- Uniform contingency table $X = (X_{ij})$ serves as the maximum entropy null model given margins
- It motivates to study the structure of X for given margins

- To sample from $\mathcal{T}(\mathbf{a}, \mathbf{b})$, first consider a 0-1 block matrix of size $N \times N = (a_1 + \cdots + a_m) \times (b_1 + \cdots + b_n)$:

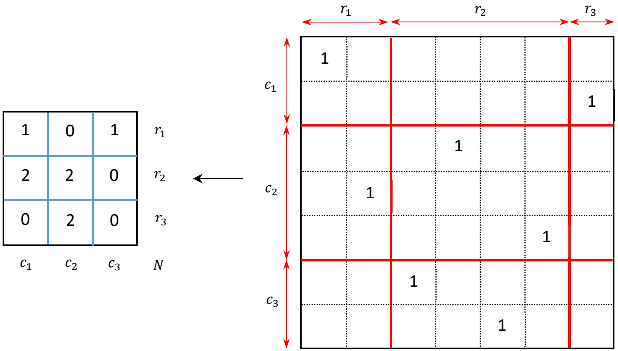


- Fill in the block matrix with a uniform random permutation matrix:





- Collapse each block into each cell in the contingency table



- Resulting contingency table follows hypergeometric distribution: (not uniform)

$$\mathbb{P}(Y = (y_{ij})) \propto \prod_{ij} \frac{1}{y_{ij}!}$$

Counting CTs — Numerical examples (Uniform margins)

- row sums $= s$, column sums $= t$, total sum $= ms = nt (= N)$

Case	m	n	s	t	UB1	UB2	UB3	**Actual**	**New LB**	LB2	LB1
1	3	3	100	100	4.7×10^{17}	1.8×10^{15}	3.4×10^{11}	1.3×10^{7}	3.1×10^{5}	2.4×10^{3}	1.5×10^{-28}
2	3	9	99	33	2.3×10^{40}	1.5×10^{38}	3.7×10^{29}	2.8×10^{21}	7.3×10^{17}	5.6×10^{15}	1.2×10^{-62}
3	3	49	98	6	8.1×10^{121}	1.1×10^{120}	1.1×10^{98}	1.0×10^{68}	9.1×10^{55}	6.4×10^{53}	4.1×10^{-381}
4	10	10	20	20	8.5×10^{82}	1.4×10^{81}	2.2×10^{74}	1.1×10^{59}	5.7×10^{49}	4.8×10^{41}	5.2×10^{-104}
5	18	18	13	13	6.4×10^{164}	1.3×10^{163}	6.0×10^{156}	7.9×10^{127}	1.1×10^{110}	2.7×10^{95}	1.1×10^{-214}
6	30	30	3	3	9.5×10^{130}	3.8×10^{129}	3.8×10^{128}	2.2×10^{92}	2.2×10^{73}	1.6×10^{56}	2.2×10^{-522}
7	100	100	3	3	1.2×10^{589}	2.8×10^{587}	3.4×10^{586}	5.3×10^{459}	4.9×10^{394}	4.1×10^{332}	1.5×10^{-2267}
8	4	4	300	300	9.9×10^{36}	1.3×10^{34}	5.1×10^{25}	2.0×10^{19}	4.1×10^{16}	3.8×10^{12}	2.5×10^{-39}
9	9	9	10^3	10^3	1.1×10^{201}	4.4×10^{197}	1.8×10^{168}	8.0×10^{151}	4.5×10^{142}	7.3×10^{128}	1.8×10^{-32}
10	9	9	10^5	10^5	7.7×10^{362}	3.1×10^{357}	1.4×10^{298}	6.1×10^{279}	3.2×10^{270}	5.2×10^{248}	1.5×10^{44}
11	15	15	10^3	10^3	6.7×10^{508}	2.6×10^{505}	3.8×10^{457}	$\approx 1.7 \times 10^{427}$	1.7×10^{409}	2.3×10^{384}	1.3×10^{80}
12	15	15	10^5	10^5	1.3×10^{958}	5.1×10^{952}	1.1×10^{851}	$\approx 1.7 \times 10^{819}$	3.2×10^{800}	4.5×10^{761}	4.0×10^{383}
13	100	100	10^3	10^3	1.3×10^{14553}	6.0×10^{14549}	8.2×10^{14346}	$\approx 6.3 \times 10^{14072}$	5.3×10^{13869}	4.6×10^{13684}	5.0×10^{10741}
14	100	100	10^5	10^5	1.3×10^{34345}	5.2×10^{34339}	1.1×10^{33751}	$\approx 6.3 \times 10^{33470}$	4.9×10^{33263}	4.4×10^{32979}	6.2×10^{29545}

Figure: Excerpted from [3]

- UB1, LB1 = Barvinok's first upper and lower bounds [1]
- UB2, LB2 = Barvinok's first upper and lower bounds [2]
- UB3 = Shapiro's upper bound [13]
- New LB = Brändén, Leake, Pak [3]

Counting TCs — Numerical examples (Non-uniform margins)

Case	m	n	N	UB1	UB2	UB3	**Actual**	**New LB**	LB2	LB1	Time
1	4	4	592	3.0×10^{30}	6.0×10^{27}	7.1×10^{18}	1.2×10^{15}	9.5×10^{12}	4.6×10^{8}	3.8×10^{-40}	79 sec
2	5	4	1269	1.4×10^{34}	1.2×10^{31}	8.3×10^{20}	3.4×10^{16}	2.0×10^{14}	3.0×10^{7}	1.5×10^{-52}	550 sec
3	4	4	65159458	1.3×10^{112}	?	2.1×10^{65}	4.3×10^{61}	5.8×10^{58}	?	2.3×10^{-49}	N/A
4	50	50	486	7.2×10^{562}	?	1.3×10^{551}	??	5.2×10^{421}	?	6.4×10^{-749}	N/A
5	50	50	302	1.2×10^{350}	?	7.3×10^{338}	??	1.1×10^{239}	?	2.0×10^{-922}	N/A

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- Large gap between rigorous upper and lower bounds on $\mathrm{T}(\mathbf{a}, \mathbf{b})$ for non-uniform margins

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$$\begin{aligned}\log \mathrm{T}(\mathbf{a}, \mathbf{b}) = [(1+C)\log(1+C) - C\log(C)]n^2 - n\log n \\ - n\log 2\pi C(1+C) + \log n + O(1).\end{aligned}$$

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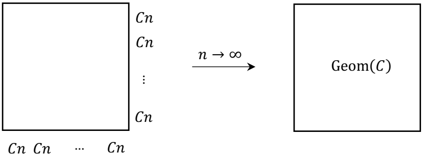
Asymptotically independent entries



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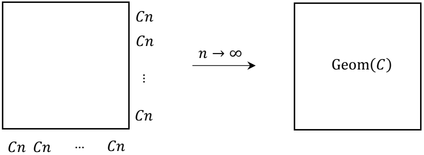

- Empirical distribution of eigenvalues $\Rightarrow$ circular law (Nguyen '14 [12])

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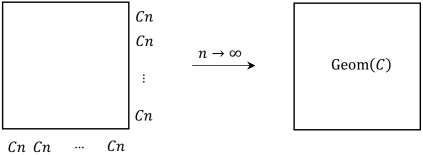

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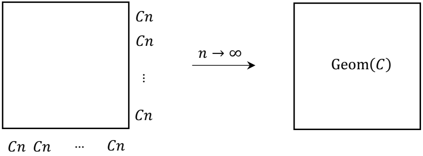

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- Polynomial time approximate algorithm for computing $\mathrm{T}(\mathbf{a}, \mathbf{b})$

Outline

Conjecture (Independent heuristic, Good '50)

$$\mathrm{T}(\mathbf{a},\mathbf{b}) \approx \mathrm{G}(\mathbf{a},\mathbf{b})$$

where

$$\mathrm{G}(\mathbf{a},\mathbf{b}) := \binom{N+mn-1}{mn-1}^{-1} \prod_{i=1}^{m} \binom{a_i+n-1}{n-1} \prod_{j=1}^{n} \binom{b_j+m-1}{m-1}.$$

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- $\mathbb{P}\big(\mathcal{R}_n(\mathbf{r}) \cap \mathcal{C}_m(\mathbf{c})\big) = \dfrac{\mathrm{T}(\mathbf{a}, \mathbf{b})}{|\mathcal{S}_N|}, \quad \mathbb{P}\big(\mathcal{R}_n(\mathbf{r})\big) = \dfrac{|\mathcal{R}_n(\mathbf{r})|}{|\mathcal{S}_N|}, \quad \mathbb{P}\big(\mathcal{C}_n(\mathbf{c})\big) = \dfrac{|\mathcal{C}_n(\mathbf{c})|}{|\mathcal{S}_N|}$

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- $|\mathcal{S}_N| = \dbinom{N+mn-1}{mn-1}, \; |\mathcal{R}_n(\mathbf{a})| = \displaystyle\prod_{i=1}^{m} \binom{a_i+n-1}{n-1}, \; |\mathcal{C}_m(\mathbf{b})| = \prod_{j=1}^{n} \binom{b_j+m-1}{m-1}$

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Reasoning:

- $X \sim \text{Uniform}(\mathcal{S}_N)$, $\mathcal{S}_N := \{\text{CT's with total sum } N = \sum a_i = \sum b_j\}$
- $\mathcal{R}_n(\mathbf{a}) := \{X \text{ has row margins } \mathbf{a}\}$, $\quad \mathcal{C}_m(\mathbf{b}) := \{X \text{ has column margins } \mathbf{b}\}$.
- $\mathbb{P}(\mathcal{R}_n(\mathbf{r}) \cap \mathcal{C}_m(\mathbf{c})) = \dfrac{\mathrm{T}(\mathbf{a},\mathbf{b})}{|\mathcal{S}_N|}$, $\quad \mathbb{P}(\mathcal{R}_n(\mathbf{r})) = \dfrac{|\mathcal{R}_n(\mathbf{r})|}{|\mathcal{S}_N|}$, $\quad \mathbb{P}(\mathcal{C}_n(\mathbf{c})) = \dfrac{|\mathcal{C}_n(\mathbf{c})|}{|\mathcal{S}_N|}$
- $|\mathcal{S}_N| = \dbinom{N+mn-1}{mn-1}$, $|\mathcal{R}_n(\mathbf{a})| = \displaystyle\prod_{i=1}^{m} \binom{a_i+n-1}{n-1}$, $|\mathcal{C}_m(\mathbf{b})| = \displaystyle\prod_{j=1}^{n} \binom{b_j+m-1}{m-1}$
- $$\frac{\mathbb{P}(\mathcal{R}_n(\mathbf{a}) \cap \mathcal{C}_m(\mathbf{b}))}{\mathbb{P}(\mathcal{R}_n(\mathbf{a}))\,\mathbb{P}(\mathcal{C}_m(\mathbf{b}))} = \frac{\mathrm{T}(\mathbf{a},\mathbf{b})}{\mathrm{G}(\mathbf{a},\mathbf{b})}$$

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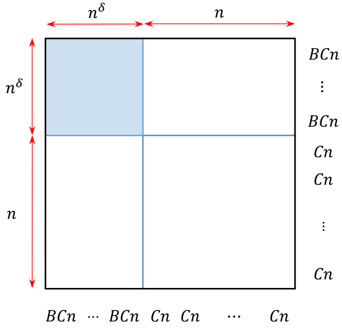
- In 2010, Greenhill and MacKay [4] proved (1) for uniform linear margins $n = m$, $\mathbf{a} = \mathbf{b} = (Cn, Cn, \dots, Cn)$, $C > 0$

Two margins

- Two margins: $\mathbf{a} = \mathbf{b} = (\overbrace{BCn, \dots, BCn}^{n^\delta}, \overbrace{Cn, \dots\dots, Cn}^{(n-n^\delta)}),\ 0 \le \delta \le 1$



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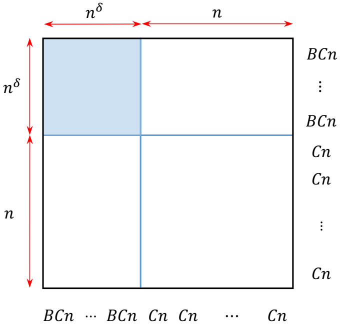

- IH undercounts: For $\delta = 1$, Barvinok [1] shows that

$$\lim_{n\to\infty} \frac{1}{n^2} \log \mathrm{T}(\mathbf{a}, \mathbf{b}) > \lim_{n\to\infty} \frac{1}{n^2} \log \mathrm{G}(\mathbf{a}, \mathbf{b}).$$

In other words, the rows and columns of CTs attract each other

Theorem (L., and Pak '20)

Let $0 < \delta < 1$ *and* $\mathbf{a} = \mathbf{b} = (\overbrace{BCn, \ldots, BCn}^{n^\delta}, \overbrace{Cn, \ldots\ldots\ldots, Cn}^{n - n^\delta}) \in \mathbb{N}^n$.
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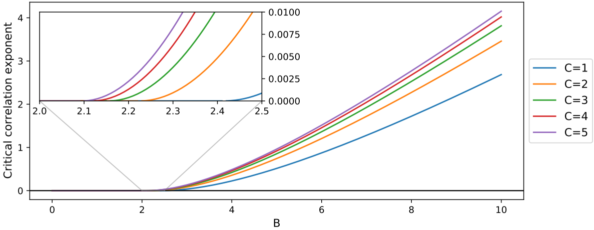

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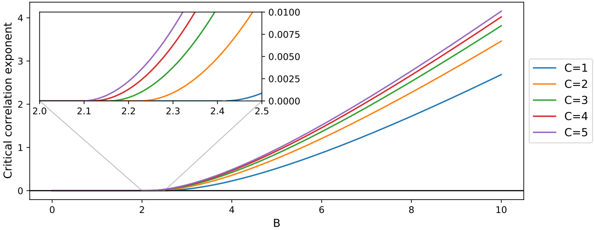

- Asmptotic independence $\xrightarrow{B\nearrow}$ Positive correlation

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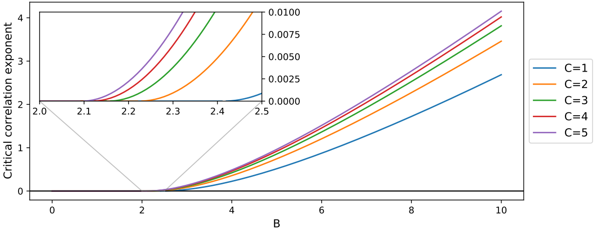
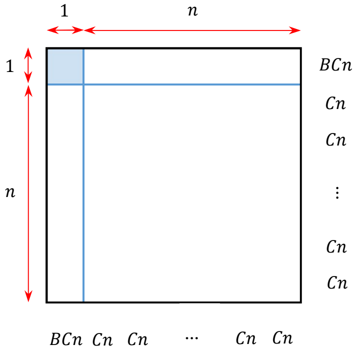


- Asmptotic independence $\xrightarrow{B\nearrow}$ Positive correlation
- Where is this phase transition coming from?

Outline

Barvinok margin



- Let $\mathbf{a} = \mathbf{b} = (\lfloor BCn \rfloor, \lfloor Cn \rfloor, \cdots, \lfloor Cn \rfloor) \in \mathbb{N}^{n+1}$. Let $X = (X_{ij})$ be the uniform contingency table with this margin.

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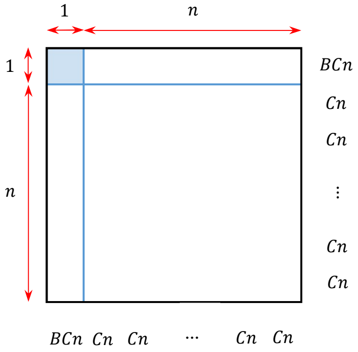

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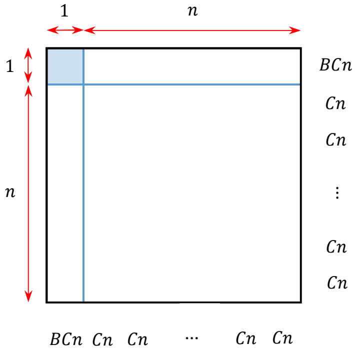
- Do we still have convergence to geometric entries for all $B, C \geq 1$?



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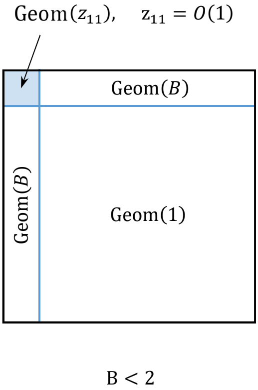
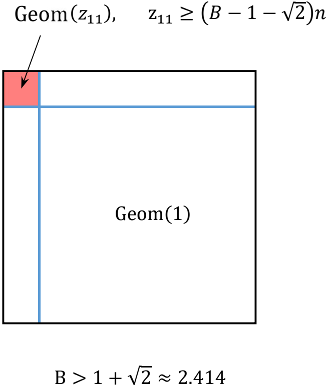
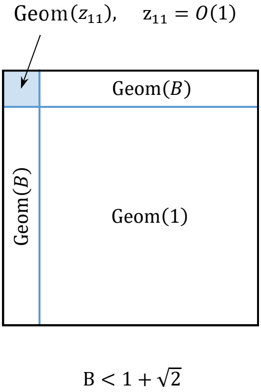
- Do we still have convergence to geometric entries for all $B, C \geq 1$?
- If so, what are the means of the geometric distribution in each block?

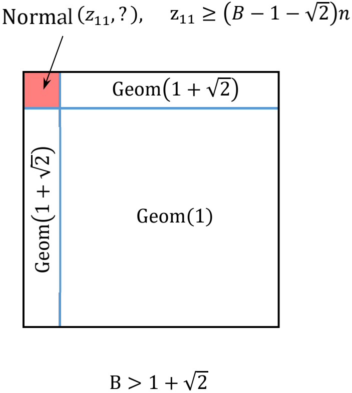
- Based on his **typical table** computation, Barvinok conjectured in 2010 that each entry in X is asymptotically distributed as a geometric variable;
- Furthermore, for $C = 1$, he conjecture that $\mathbb{E}[X_{11}] = O(1)$ for $B < 2$ and $\mathbb{E}[X_{11}] = \Theta(n)$ for $B > 1 + \sqrt{2}$.





- In 2018, Dittmer and Pak tested Barvinok's conjecture using a new MCMC algorithm to sample a uniform contingency table of reasonable size
- They conjectured that $B_c = 1 + \sqrt{2}$ is the critical value and X_{11} actually converges to a normal variable with growing mean

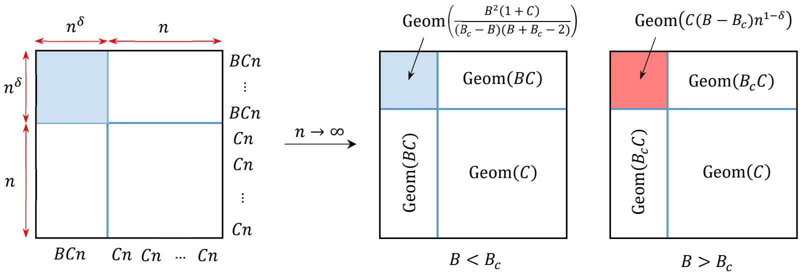




Simulation of corner entry X_{11}

Theorem (Dittmer, L., and Pak '19+)

Let $1/2 < \delta < 1$ *and* $\mathbf{a} = \mathbf{b} = (\overbrace{BCn, \dots, BCn}^{n^\delta}, \overbrace{Cn, \dots\dots, Cn}^{n - n^\delta}) \in \mathbb{N}^n$*. Let* $B_c := 1 + \sqrt{1 + 1/C}$ *and* $X \sim \text{Uniform}(\mathcal{T}(\mathbf{a}, \mathbf{b}))$*. Then* X *marginally converges to the following matrix in total variation distance:*



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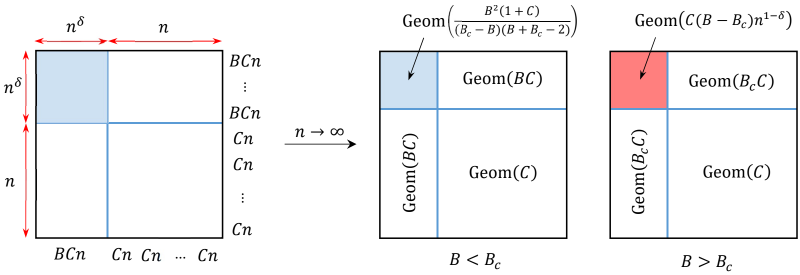

- We also show polynomial rate of convergence in d_{TV}.

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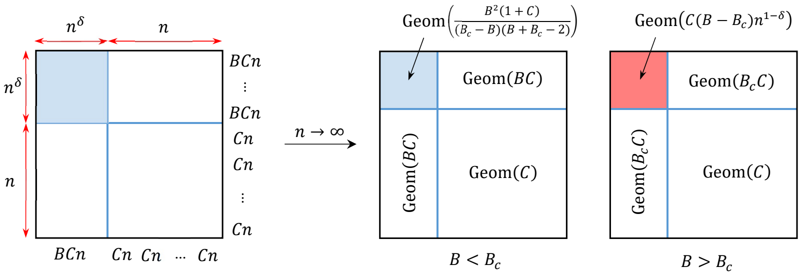

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Outline

Definition

Fix margins $\mathbf{a}, \mathbf{c} \in \mathbb{N}^n$*. Let* $\mathcal{P}(\mathbf{a}, \mathbf{b}) \subseteq \mathbb{R}^{n \times n}_{\geq 0}$ *denote the set of all matrices with non-negative real entries with margins* $\mathbf{r}$ *and* $\mathbf{c}$*. For each* $X = (x_{ij}) \in \mathcal{P}(\mathbf{a}, \mathbf{b})$*, define*

$$g(X) = \sum_{1 \leq i,j \leq n} (x_{ij} + 1) \log(x_{ij} + 1) - x_{ij} \log(x_{ij}).$$

The typical table $Z \in \mathcal{P}(\mathbf{a}, \mathbf{b})$ *for* $\mathcal{T}(\mathbf{a}, \mathbf{b})$ *is defined by*

$$Z = \arg\max_{X \in \mathcal{P}(\mathbf{a}, \mathbf{b})} g(X).$$

Theorem (Barvinok '09, '10)

Fix any margins $\mathbf{a}, \mathbf{b} \in \mathbb{N}^n$*. Let* $Z = (z_{ij})$ *be the typical table for* $\mathcal{T}(\mathbf{a}, \mathbf{b})$*. Let* $N = \sum_{i=1}^{m} a_i = \sum_{j=1}^{m} b_j$ *denote the total sum.*

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(iii) *For the constant* $\gamma > 0$ *in (i), we have*

$$\mathbb{P}(Y \in \mathcal{T}(\mathbf{a}, \mathbf{b})) = e^{-g(Z)}\mathrm{T}(\mathbf{a}, \mathbf{b}) \geq N^{-\gamma n}.$$

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- For **(i)**: Lower bound is hard; Upper bound is immediate from the GF:

$$\prod_{i=1}^{n}\prod_{j=1}^{n} \frac{1}{1 - x_i y_j} = \sum_{\mathbf{a}\in\mathbb{N}^m,\, \mathbf{b}\in\mathbb{N}^n} \mathrm{T}(\mathbf{a}, \mathbf{b}) \prod_{i=1}^{m} x_i^{a_i} \prod_{j=1}^{m} y_j^{b_j}$$

$$\mathrm{T}(\mathbf{a}, \mathbf{b}) \leq \inf \left[\prod_{i=1}^{m} x_i^{a_i} \prod_{j=1}^{m} y_j^{b_j}\right]^{-1} \prod_{j=1}^{n} \frac{1}{1 - x_i y_j}$$

$$= \exp\left(\sup\left[\sum_i a_i \log x_i + \sum_j b_j \log y_j + \sum_{ij} \log(1 - x_i y_j)\right]\right) = \exp(g(Z))$$

Lemma (Dittmer, L., and Pak '19+)

Let $0 < \delta < 1$ *and* $\mathbf{a} = \mathbf{b} = (\overbrace{BCn, \ldots, BCn}^{n^\delta}, \overbrace{Cn, \ldots\ldots, Cn}^{n - n^\delta}) \in \mathbb{N}^n$.
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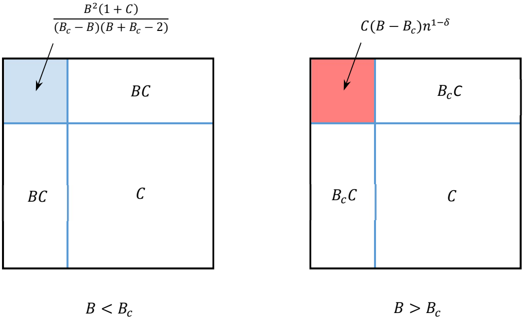

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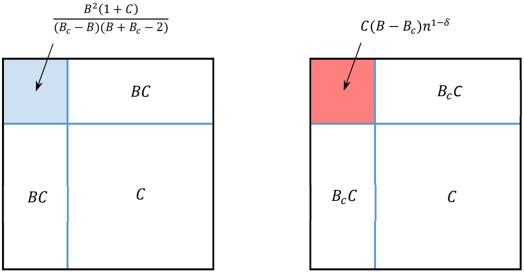
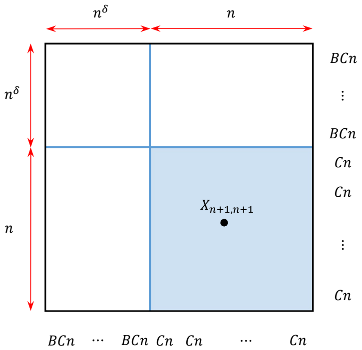
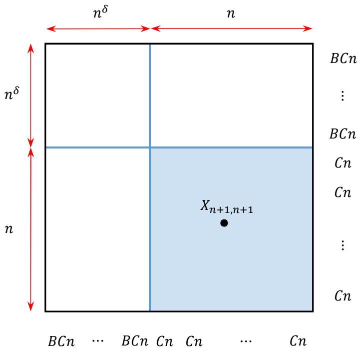


$B < B_c$ $\qquad$ $B > B_c$

- We also show polynomial rate of convergence $\leftarrow$ Crucial in volumn phase transition



- Approximate $\mathbb{P}(X_{n+1,n+1} \in A)$ by the sample mean $S(X)$ of $\mathbf{1}(X_{ij} \in A)$'s within bottom right block



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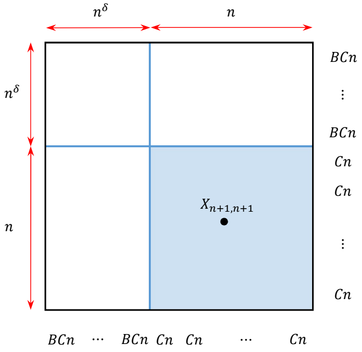
- Approximate X by Y on a rare event and use concentration bounds for Y:

$$
\begin{aligned}
&|\mathbb{P}(X_{ij} \in A) - \mathbb{P}(Y_{ij} \in A)| \\
&\quad = |\mathbb{E}[S(X)] - \mathbb{P}(Y_{ij} \in \mathcal{A})| \\
&\quad \le \mathbb{E}\left[|S(X) - \mathbb{P}(Y_{ij} \in A)|\right] \\
&\quad \le t\mathbb{P}\left(|S(X) - \mathbb{P}(Y_{ij} \in A)| \le t\right) \\
&\qquad\quad + 2\mathbb{P}\left(|S(X) - \mathbb{P}(Y_{ij} \in A)| > t\right) \\
&\quad \le t + 4N^{\gamma^n} \exp\left(-\frac{n^2 t^2}{2}\right).
\end{aligned}
$$



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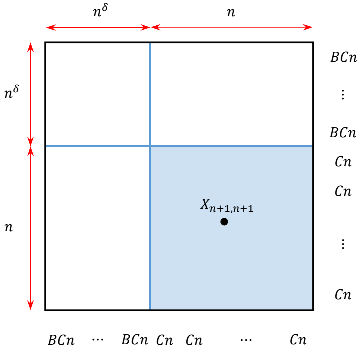
- Approximate X by Y on a rare event and use concentration bounds for Y:

$$\begin{aligned}
&|\mathbb{P}(X_{ij} \in A) - \mathbb{P}(Y_{ij} \in A)| \\
&\quad = |\mathbb{E}[S(X)] - \mathbb{P}(Y_{ij} \in \mathcal{A})| \\
&\quad \le \mathbb{E}\left[|S(X) - \mathbb{P}(Y_{ij} \in A)|\right] \\
&\quad \le t\mathbb{P}\left(|S(X) - \mathbb{P}(Y_{ij} \in A)| \le t\right) \\
&\qquad\quad + 2\mathbb{P}\left(|S(X) - \mathbb{P}(Y_{ij} \in A)| > t\right) \\
&\quad \le t + \exp(cn\log n)\exp\left(-\frac{n^2 t^2}{2}\right).
\end{aligned}$$

Concentration in blocks of volume $\gg n$



- Approximate $\mathbb{P}(X_{n+1,n+1} \in A)$ by the sample mean $S(X)$ of $\mathbf{1}(X_{ij} \in A)$'s within bottom right block
- Approximate X by Y on a rare event and use concentration bounds for Y:

$$\begin{aligned}
&|\mathbb{P}(X_{ij} \in A) - \mathbb{P}(Y_{ij} \in A)| \\
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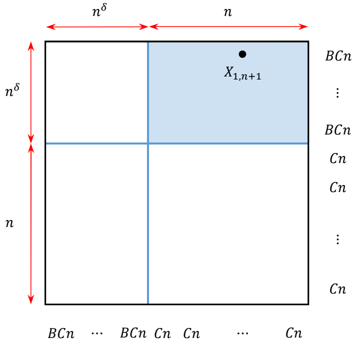
\end{aligned}$$

- This gives $d_{TV}(X, Y) \leq n^{-1/2+\varepsilon}$.



- Approximate $\mathbb{P}(X_{1,n+1} \in A)$ by the sample mean $S(X)$ of $\mathbf{1}(X_{ij} \in A)$'s within top right block
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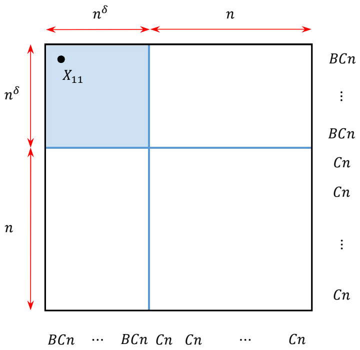
\end{aligned}
$$

- This gives $d_{TV}(X, Y) \le n^{-(\delta/2)+\varepsilon}$ for $\delta > 0$.



- Approximate $\mathbb{P}(X_{11} \in A)$ by the sample mean $S(X)$ of $\mathbf{1}(X_{ij} \in A)$'s within top left block
- Approximate X by Y on a rare event and use concentration bounds for Y:

$$\begin{aligned}
&|\mathbb{P}(X_{ij} \in A) - \mathbb{P}(Y_{ij} \in A)| \\
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&\quad \leq t + \exp(cn \log n) \exp\left(-\frac{n^{2\delta} t^2}{2}\right).
\end{aligned}$$

- This gives $d_{TV}(X, Y) \leq n^{1/2-\delta+\varepsilon}$ for $\delta > 1/2$.

Outline

Theorem (Dittmer, L., and Pak '19+)

Let $X = (X_{ij})_{1 \le i,j \le n}$ *be drawn from* $\mathcal{T}_{n,\delta}(B, C)$ *uniformly at random. Let* $B_c = 1 + \sqrt{1 + 1/C}$*. For* $1/2 < \delta < 1$*, almost surely as* $n \to \infty$*,*

$$\lim_{n\to\infty} \frac{1}{n} \sum_{k=1}^{n} X_{1,k+\lfloor n^{\delta} \rfloor} = \begin{cases} BC & \text{if } B < B_c \\ B_c C & \text{if } B > B_c. \end{cases}$$

Furthermore, for all $B, C \ge 0$ *and* $0 \le \delta < 1$*, almost surely as* $n \to \infty$*,*

$$\lim_{n\to\infty} \frac{1}{n} \sum_{k=1}^{n} X_{n+1,k+\lfloor n^{\delta} \rfloor} = C.$$

Conjecture (CLT)

Fix $0 \leq \delta < 1$. Let $X = (X_{ij})_{1 \leq i,j \leq n}$ be drawn from $\mathcal{T}_{n,\delta}(B, C)$ uniformly at random. Denote $B_c = 1 + \sqrt{1 + 1/C}$ and

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Then as $n \to \infty$,

$$\begin{cases} n^{-1/2}(S_{n,\delta}(B,C) - BCn) \to 0 \ \text{a.s.} & \text{if } B < B_c \\ n^{-1/2}(S_{n,\delta}(B,C) - B_c Cn) \Rightarrow \sqrt{B_c C + (B_c C)^2} Z & \text{if } B > B_c, \end{cases}$$

where $Z \sim N(0,1)$ *and* $\Rightarrow$ *denotes weak convergence.*

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- For $B > B_c$, $S_{n,\delta}(B, C) \to B_cCn \ll BCn =$total row sum so we expect CLT
- However, we don't yet know if $\mathbb{E}[X_{1,n+1}^2] = O(1)$ for $B > B_c$

- From the first row sum, we can write

$$n^{-1/2}\sum_{k=1}^{\lfloor n^{\delta}\rfloor}[X_{1,k} - C(B-B_c)n^{1-\delta}] = n^{-1/2}(S_{n,\delta}(B,C) - B_c Cn).$$

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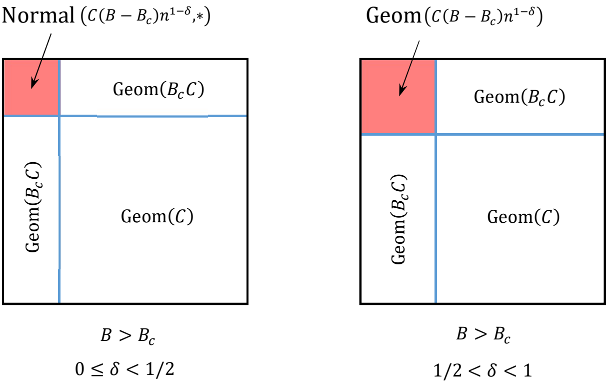
Conjecture

Fix $B, C \geq 1$ and $0<\delta<1/2$. Let $X=(X_{ij})_{1\leq i,j\leq n}$ be drawn from $\mathcal{T}_{n,\delta}(B,C)$ uniformly at random. Denote $B_c = 1+\sqrt{1+1/C}$. Then

$$\frac{X_{11} - C(B-B_c)n^{1-\delta}}{n^{(1-\delta)/2}\sqrt{B_c C + (B_c C)^2}} \Rightarrow N(0,1),$$

where $\Rightarrow$ denotes weak convergence.



- Thin Bezel $\Rightarrow$ Normal corner (Conj), Thick bezel $\Rightarrow$ Geometric corner (Thm)

Thanks a lot!

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