Sampling Methods for Random Simple and Bipartite Graphs with Prescribed Degree Sequences

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Overview

Introduction

Problem Definition

- For a sequence of degrees $d_1, ..., d_n$
  - How many graphs are there having a given degree sequence?
  - Ex: $(2, 3, 3, 2, 2, 3, 3, 2)$

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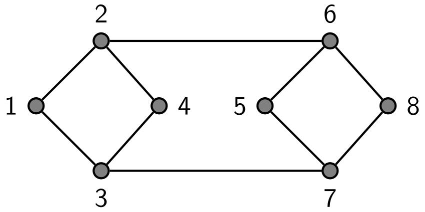

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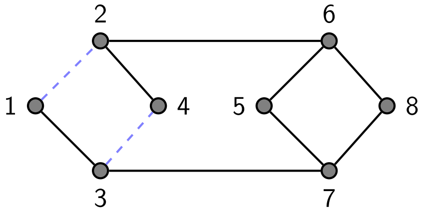

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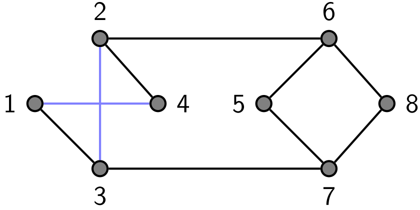

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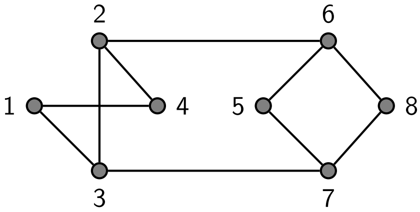

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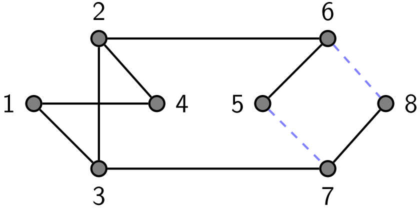

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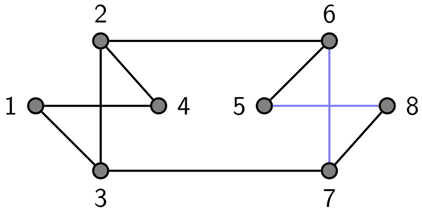

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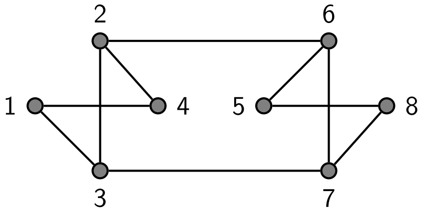

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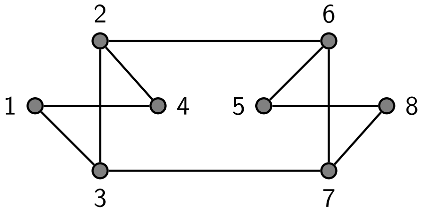

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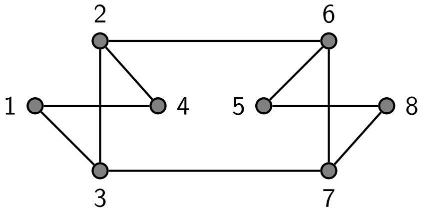


- There are 6057 graphs sharing the same degree sequence.
- How can we draw uniformly distributed samples from the set of graphs satisfying the degree sequence?

Importance Sampling

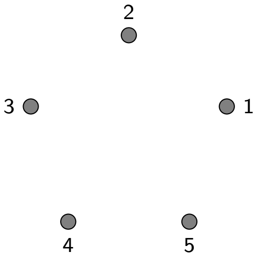
- The expected value of $f(X)$ with respect to the target probability distribution $p(x)$ can be rewritten as

$$\mathbb{E}_p(f(X)) := \int f(x)p(x)dx = \int f(x)\frac{p(x)}{q(x)}q(x)dx = \mathbb{E}_q f(x)w(x)dx$$

- Then, the Monte Carlo estimator of $\mathbb{E}(f(X))$ can be written by

$$\hat{\mu}_{f,N} := \frac{1}{N}\sum_i f(X_i)w(X_i) \quad \textit{where } X_i \sim q(x)$$

$\boldsymbol{d} = (2, 3, 4, 2, 3)$



Input A graphical degree sequence $\boldsymbol{d} = (d_1, ..., d_n)$, and empty edge set $\mathcal{E} = \{\}$

1. If $\boldsymbol{d} = (0, ..., 0)$, return $\mathcal{E}$

2. Choose the least index m where d_m is the smallest non-zero element in $\boldsymbol{d}$

3. Compute the candidate set $\mathcal{C}_m$ where $\mathcal{C}_m = \{i \neq j\colon\ \{i, j\} \notin \mathcal{E}$ and $\ominus_{i,j}\boldsymbol{d}$ is graphical$\}$

4. Choose an index $i \in \mathcal{C}_m$ with probability proportional to d_i

5. Add the edge $\{i, m\}$ to $\mathcal{E}$, and update $\boldsymbol{d}$ to $\ominus_{i,m}\boldsymbol{d}$.

6. Repeat the steps $3 - 5$ until d_m equal to 0

Output edge sequence $E = \{\}$

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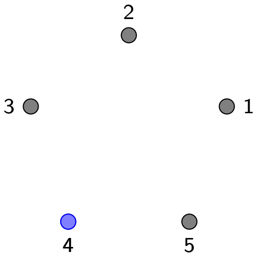

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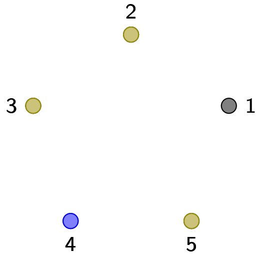

The candidate vertices

$C_4 = \{2, 3, 5\}$

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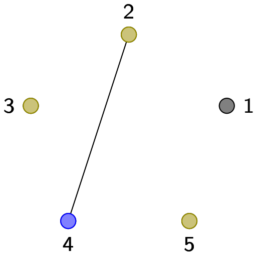

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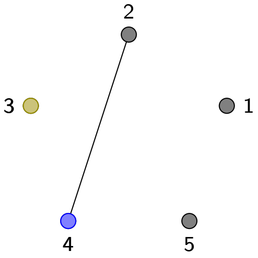

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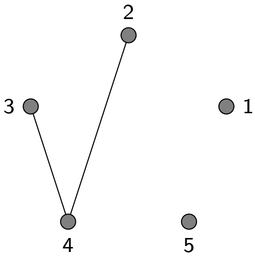

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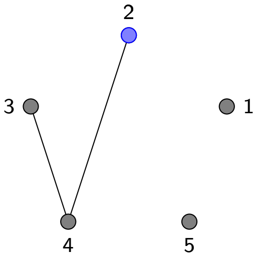

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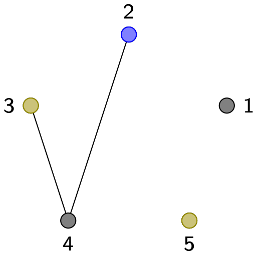

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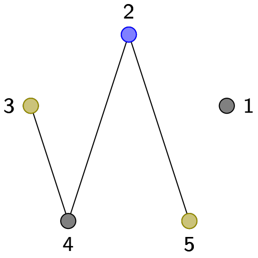

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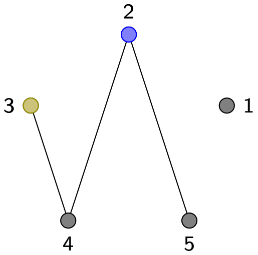

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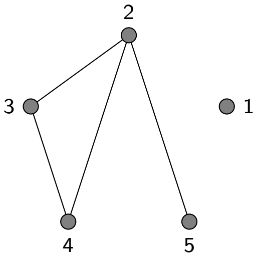

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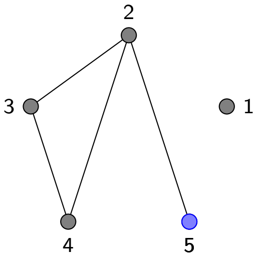

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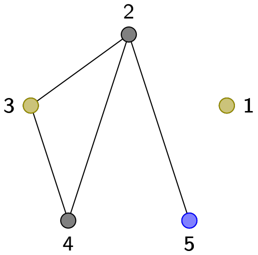

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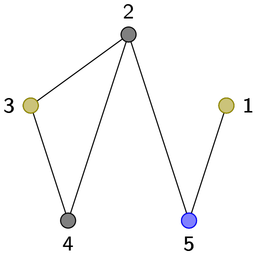

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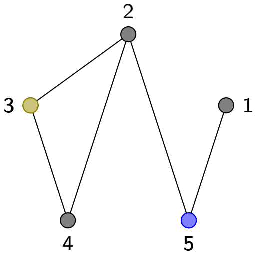

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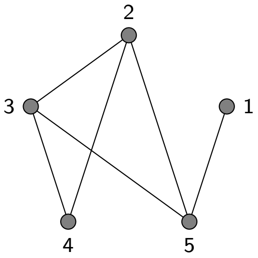

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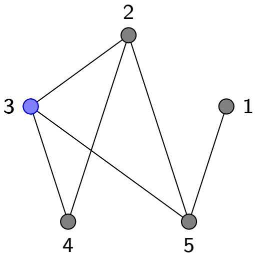

Input A graphical degree sequence $\boldsymbol{d} = (d_1, \ldots, d_n)$, and empty edge set $\mathcal{E} = \{\}$

1. If $\boldsymbol{d} = (0, \ldots, 0)$, return $\mathcal{E}$

2. Choose the least index m where d_m is the smallest non-zero element in $\boldsymbol{d}$

3. Compute the candidate set $\mathcal{C}_m$ where $\mathcal{C}_m = \{i \neq j\colon \ \{i, j\} \notin \mathcal{E} \text{ and } \ominus_{i,j}\boldsymbol{d} \text{ is graphical}\}$

4. Choose an index $i \in \mathcal{C}_m$ with probability proportional to d_i

5. Add the edge $\{i, m\}$ to $\mathcal{E}$, and update $\boldsymbol{d}$ to $\ominus_{i,m}\boldsymbol{d}$.

6. Repeat the steps $3 - 5$ until d_m equal to 0

Output edge sequence $E = \{\{4, 2\}, \{4, 3\}, \{2, 5\}, \{2, 3\}, \{5, 1\}, \{5, 3\}\}$

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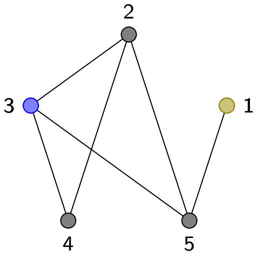

The candidate vertices

$C_3 = \{1\}$

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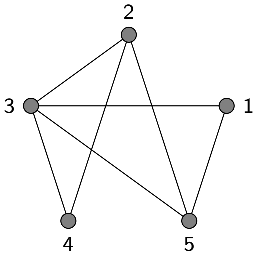

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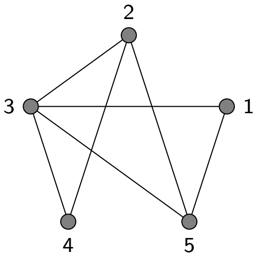

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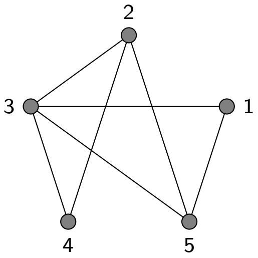

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Output edge sequence $E = \{\{4, 2\}, \{4, 3\}, \{2, 5\}, \{2, 3\}, \{5, 1\}, \{5, 3\}, \{3, 5\}\}$

- In the third step, Erdös-Gallai theorem can be used to check the graphicality of a degree sequence.

Theorem (Erdös-Gallai)

Let $\boldsymbol{d} = (d_1, ..., d_n) \in \mathbb{N}^n$ be a degree sequence with $d_1 \geq d_2 \geq ... \geq d_n$. Then the sequence $\boldsymbol{d} = (d_1, ..., d_n)$ is graphical if and only if $\sum_i^n d_i$ is even and

$$\sum_{i=1}^{k} d_i \leq k(k-1) + \sum_{i=k+1}^{n} min(k, d_i) \text{ for each } k \in \{1, ..., n\} \qquad (1)$$

The algorithm can produce the same graph with different edge sequences. For instance, the edge sequences

$$E = \{\{4,2\},\{4,3\},\{2,5\},\{2,3\},\{5,1\},\{5,3\},\{3,5\}\}$$
$$\widetilde{E} = \{\{4,3\},\{4,2\},\{2,3\},\{2,5\},\{5,3\},\{5,1\},\{3,5\}\}$$

represents the same graph. The probability of generating the edges E and $\widetilde{E}$ is $\sigma(E) = 3/40$ and $\sigma(\widetilde{E}) = 2/40$, respectively.

- Let $\mathcal{E}_{\boldsymbol{d}}$ be the set of all edge sequences produced by the algorithm and $Graph(E)$ be the corresponding graph for E.
- Two edge sequences $E, \widetilde{E}$ are *equivalent* if $Graph(E) = Graph(\widetilde{E})$.
- It defines an equivalence relation on $\mathcal{E}_{\boldsymbol{d}}$, the set of all possible edge sequences produced by the algorithm.
- Let $c(E)$ be the cardinality of the equivalence class of E.

Proposition

[2] Let π be a probability distribution on $\mathcal{G}^{\boldsymbol{d}}$. Then

$$\mathbb{E}_{\sigma}\left(\tilde{f}(E)\frac{\tilde{\pi}(E)}{c(E)\sigma(E)}\right) = \mathbb{E}_{\pi} f(G) \tag{2}$$

where σ is the probability of generating the edge sequence E by the algorithm.

Moreover, an unbiased estimator of $\mathbb{E}f(G)$ is

$$\widehat{f}_{\sigma,N} = \frac{1}{N}\sum_{i=1}^{N} \tilde{f}(E_i)\frac{\tilde{\pi}(E_i)}{c(E_i)\sigma(E_i)} \tag{3}$$

where E_1,...,E_N are the output edge sequences generated by independently running the algorithm N times for the graphical degree sequence $\boldsymbol{d} = (d_1, ..., d_n)$.

- The cardinality of the set $\mathcal{G}^{\boldsymbol{d}}$ can be estimated by choosing π to be uniform distribution, and letting $f(\cdot)$ be $|\mathcal{G}^{\boldsymbol{d}}|$. Then, the equation in the proposition can be written as

$$|\mathcal{G}^{d}| = \mathbb{E}_{\sigma}\left(\frac{1}{c(E)\sigma(E)}\right) \tag{4}$$

Sequential Importance Sampling

- A problem in importance sampling is to choose a good proposal distribution $q(x)$, especially, in high dimensional problems.
- The proposal distribution $q(x)$ can be written by

$$q(x) = q(x_1)q(x_2|x_1) \cdots q(x_n|x_1, ..., x_n)$$

Uniform Sampling Methods

Miller-Harrison Method

- A binary matrix satisfying the row sum $\boldsymbol{p}$ and column sum $\boldsymbol{q}$ can be constructed by sequentially choosing row vectors. Ex: $\boldsymbol{p} = (3, 1, 2)$ and $\boldsymbol{q} = (2, 2, 2)$

$$\begin{array}{c|ccc|} & 2 & 2 & 2 \\ \hline 3 & & & \\ 1 & & & \\ 2 & & & \\ \hline \end{array}$$

- In each step, row and column sums are updated to the vectors $\mathcal{L}\boldsymbol{p}$ and $\boldsymbol{q} - \boldsymbol{u}$.

- Let $N(\boldsymbol{p}, \boldsymbol{q})$ be the number of $(0, 1)$-matrices satisfying the row and column sums $(\boldsymbol{p}, \boldsymbol{q})$.

Miller-Harrison Method

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$$\begin{array}{c|ccc|} & 2 & 2 & 2 \\ \hline 3 & & & \\ 1 & & & \\ 2 & & & \\ \hline \end{array} \qquad \begin{array}{c|ccc|} & 1 & 1 & 1 \\ \hline & 1 & 1 & 1 \\ 1 & & & \\ 2 & & & \\ \hline \end{array}$$

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$$
\begin{array}{c|ccc|}
 & 2 & 2 & 2 \\
\hline
3 & & & \\
1 & & & \\
2 & & & \\
\hline
\end{array}
\qquad
\begin{array}{c|ccc|}
 & 1 & 1 & 1 \\
\hline
 & 1 & 1 & 1 \\
1 & & & \\
2 & & & \\
\hline
\end{array}
\qquad
\begin{array}{c|ccc|}
 & 1 & 0 & 1 \\
\hline
 & 1 & 1 & 1 \\
 & 0 & 1 & 0 \\
2 & & & \\
\hline
\end{array}
$$

- In each step, row and column sums are updated to the vectors $\mathcal{L}\boldsymbol{p}$ and $\boldsymbol{q} - \boldsymbol{u}$.

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- In each step, row and column sums are updated to the vectors $\mathcal{L}\boldsymbol{p}$ and $\boldsymbol{q} - \boldsymbol{u}$.

- Let $N(\boldsymbol{p}, \boldsymbol{q})$ be the number of $(0, 1)$-matrices satisfying the row and column sums $(\boldsymbol{p}, \boldsymbol{q})$.

- The columns of a matrix can be classified into $b := \max_j q_j$ groups.

$$\begin{array}{c|cccccccccc|}
 & 3 & 2 & 1 & 2 & 3 & 3 & 2 & 1 & 1 & 1 \\
\hline
6 & 1 & 0 & 1 & 1 & 0 & 0 & 1 & 0 & 1 & 1 \\
5 & & & & & & & & & & \\
4 & & & & & & & & & & \\
4 & & & & & & & & & & \\
\hline
\end{array}$$

Construction of a binary matrix

- There exist $N(\mathcal{L}\boldsymbol{p}, \boldsymbol{q} - \boldsymbol{u})$ number of matrices having the same first row.

- The columns of a matrix can be classified into $b := \max_j q_j$ groups.

$$
\begin{array}{c|cccccccccc|}
 & 3 & 2 & 1 & 2 & 3 & 3 & 2 & 1 & 1 & 1 \\
\hline
6 & 1 & 0 & 1 & 1 & 0 & 0 & 1 & 0 & 1 & 1 \\
5 & & & & & & & & & & \\
4 & & & & & & & & & & \\
4 & & & & & & & & & & \\
\hline
\end{array}
\quad \longrightarrow \quad
\begin{array}{c|ccc|}
 & 4 & 3 & 3 \\
\hline
6 & 3 & 2 & 1 \\
5 & & & \\
4 & & & \\
4 & & & \\
\hline
\end{array}
$$

Construction of a binary matrix $\qquad\qquad$ $(\boldsymbol{p}, \bar{\boldsymbol{q}})$

- There exist $N(\mathcal{L}\boldsymbol{p}, \boldsymbol{q} - \boldsymbol{u})$ number of matrices having the same first row.

- Let $\overline{\boldsymbol{q}} := (\overline{q}_1, ..., \overline{q}_n)$ where $\{|i : q_j = i, 1 \leq j \leq m|\}$.

  Hence, there exists

$$
\binom{\overline{\boldsymbol{q}}}{\boldsymbol{s}} := \binom{\overline{q_1}}{s_1} \cdots \binom{\overline{q_b}}{s_b} = \binom{4}{3}\binom{3}{2}\binom{3}{1} = 36
$$

number of permutations $\boldsymbol{v}$ of the row $\boldsymbol{u}$ where $N(\mathcal{L}\boldsymbol{p}, \boldsymbol{q} - \boldsymbol{u}) = N(\mathcal{L}\boldsymbol{p}, \boldsymbol{q} - \boldsymbol{v})$

- Alternatively, the possible number of binary matrices can be computed by counting the matrices satisfying the margins $(\boldsymbol{p}, \overline{\boldsymbol{q}})$

Theorem

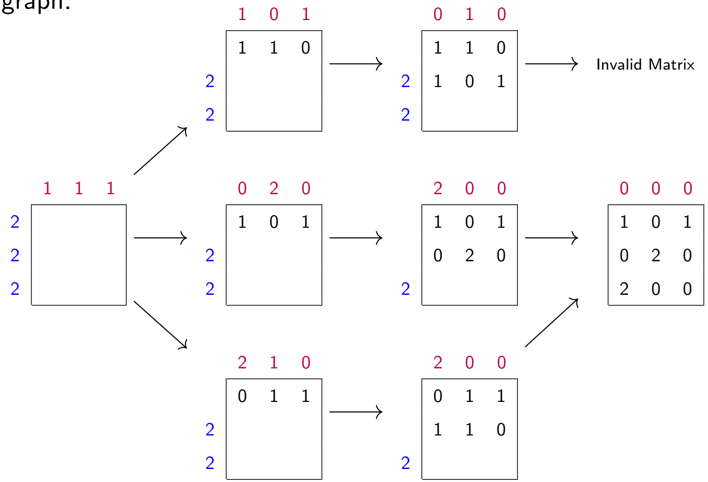
The number of (0-1)-matrices with row and column sums $(\boldsymbol{p}, \boldsymbol{q}) \in \mathbb{N}^n \times \mathbb{N}^m$ *is given by*

$$N(\boldsymbol{p}, \boldsymbol{q}) := \overline{N}(\boldsymbol{p}, \overline{\boldsymbol{q}}) = \sum_{\boldsymbol{s} \in C^{\overline{q}}(p_1)} \binom{\overline{\boldsymbol{q}}}{\boldsymbol{s}} \overline{N}(\mathcal{L}\boldsymbol{p}, \overline{\boldsymbol{q}} \backslash \boldsymbol{s}) \tag{5}$$

where $\overline{\boldsymbol{q}} \backslash \boldsymbol{s} := \boldsymbol{q} - \boldsymbol{s} + \mathcal{L}\boldsymbol{s}$, and

$C^{\overline{q}}(p_1) := \{\boldsymbol{s} \in \mathbb{N}^b : \sum_j s_j = p_1,\ s_j \leq \overline{q}_j \text{ for } 1 \leq j \leq b\}$

- The traversed pair of vectors $(\boldsymbol{u}, \overline{\boldsymbol{v}})$ construct a directed acyclic graph.



- To avoid from invalid matrices, the Gale-Ryser conditions can be used.

Theorem (Gale-Ryser)

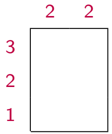
Let $(\boldsymbol{p}, \boldsymbol{q}) \in \mathbb{N}^n \times \mathbb{N}^m$ *be a pair of non-increasing sequences such that* $\sum_{i=1}^{n} p_i = \sum_{j=1}^{m} q_j$.
There exists a (0-1)-matrix $\boldsymbol{A} = (a_{ij})$ *where* $\sum_{j=1}^{m} a_{ij} = \boldsymbol{p}$, $\sum_{i=1}^{n} a_{ij} = \boldsymbol{q}$ *if and only if* $\boldsymbol{p}$ *is dominated by* $\boldsymbol{q}^*$

Definition

It is said that $\boldsymbol{p}$ is dominated by $\boldsymbol{q}$ if $\sum_{i=1}^{k} p_i \leq \sum_{j=1}^{k} q_i$ for all k where $1 \leq k \leq \max\{n, m\}$, $p_i := 0$ for $i > m$, and $q_j := 0$ for $j > n$.

Uniform Sampling Algorithm

- Let $\mathcal{D}(\boldsymbol{p}, \boldsymbol{q})$ be the set of pairs $(\boldsymbol{u}, \overline{\boldsymbol{v}})$ traversed by the algorithm for a given initial input pair $(\boldsymbol{p}, \overline{\boldsymbol{q}})$ where $(\boldsymbol{p}, \boldsymbol{q}) \in \mathbb{N}^n \times \mathbb{N}^m$.



$(\boldsymbol{p}, \bar{\boldsymbol{q}})$

1. Initialize $(\boldsymbol{u}, \boldsymbol{v})$ with $(\boldsymbol{p}, \boldsymbol{q})$

2. If $(\boldsymbol{u}, \boldsymbol{v}) = (\mathbf{0}, \mathbf{0})$, terminate with the set of constructed row vectors.

3. Select a child $(\mathcal{L}\boldsymbol{u}, \overline{\boldsymbol{v}} \setminus \boldsymbol{s}) \in \mathcal{D}(\boldsymbol{p}, \overline{\boldsymbol{q}})$ of $(\boldsymbol{u}, \overline{\boldsymbol{v}})$ with a probability proportional to $\binom{\overline{\boldsymbol{v}}}{\boldsymbol{s}} \overline{N}(\mathcal{L}\boldsymbol{p}, \overline{\boldsymbol{v}} \setminus \boldsymbol{s})$.

4. Uniformly choose a row vector $\boldsymbol{r}$ among the corresponding rows.

5. Set $(\boldsymbol{u}, \boldsymbol{v})$ to $(\mathcal{L}\boldsymbol{u}, \boldsymbol{v} - \boldsymbol{r})$.

6. Return to the step (2)

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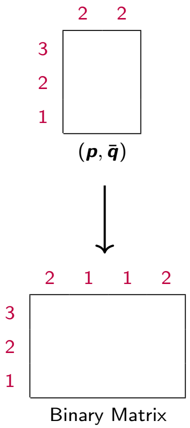

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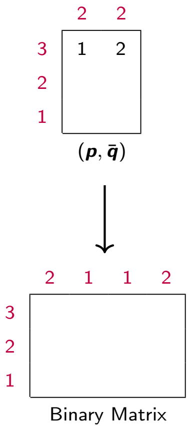

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$$\begin{array}{c|cc|} & 2 & 2 \\ \hline 3 & 1 & 2 \\ 2 & & \\ 1 & & \\ \hline \end{array}$$

$(\boldsymbol{p}, \bar{\boldsymbol{q}})$

$$\downarrow$$

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

Binary Matrix

Uniform Sampling Algorithm

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6. Return to the step (2)

$$\begin{array}{c|cc|}
 & 3 & 0 \\
\hline
 & 1 & 2 \\
2 & & \\
1 & & \\
\hline
\end{array}$$

$(\boldsymbol{p}, \bar{\boldsymbol{q}})$

$$\downarrow$$

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

Binary Matrix

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$$\begin{array}{c|cc|}
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\hline
 & 1 & 2 \\
2 & 2 & 0 \\
1 & & \\
\hline
\end{array}$$

$(\boldsymbol{p}, \bar{\boldsymbol{q}})$

$$\downarrow$$

$$\begin{array}{c|cccc|}
 & 1 & 1 & 0 & 1 \\
\hline
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\hline
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- Let $\mathcal{D}(\boldsymbol{p}, \boldsymbol{q})$ be the set of pairs $(\boldsymbol{u}, \overline{\boldsymbol{v}})$ traversed by the algorithm for a given initial input pair $(\boldsymbol{p}, \overline{\boldsymbol{q}})$ where $(\boldsymbol{p}, \boldsymbol{q}) \in \mathbb{N}^n \times \mathbb{N}^m$.

1. Initialize $(\boldsymbol{u}, \boldsymbol{v})$ with $(\boldsymbol{p}, \boldsymbol{q})$

2. If $(\boldsymbol{u}, \boldsymbol{v}) = (\boldsymbol{0}, \boldsymbol{0})$, terminate with the set of constructed row vectors.

3. Select a child $(\mathcal{L}\boldsymbol{u}, \overline{\boldsymbol{v}} \backslash \boldsymbol{s}) \in \mathcal{D}(\boldsymbol{p}, \overline{\boldsymbol{q}})$ of $(\boldsymbol{u}, \overline{\boldsymbol{v}})$ with a probability proportional to $\binom{\overline{\boldsymbol{v}}}{\boldsymbol{s}} \overline{N}(\mathcal{L}\boldsymbol{p}, \overline{\boldsymbol{v}} \backslash \boldsymbol{s})$.

4. Uniformly choose a row vector $\boldsymbol{r}$ among the corresponding rows.

5. Set $(\boldsymbol{u}, \boldsymbol{v})$ to $(\mathcal{L}\boldsymbol{u}, \boldsymbol{v} - \boldsymbol{r})$.

6. Return to the step (2)

$$\begin{array}{c|cc|} & 3 & 0 \\ \hline & 1 & 2 \\ 2 & 2 & 0 \\ 1 & & \\ \hline \end{array}$$

$(\boldsymbol{p}, \bar{\boldsymbol{q}})$

$$\downarrow$$

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

Binary Matrix

Uniform Sampling Algorithm

- Let $\mathcal{D}(\boldsymbol{p}, \boldsymbol{q})$ be the set of pairs $(\boldsymbol{u}, \overline{\boldsymbol{v}})$ traversed by the algorithm for a given initial input pair $(\boldsymbol{p}, \overline{\boldsymbol{q}})$ where $(\boldsymbol{p}, \boldsymbol{q}) \in \mathbb{N}^n \times \mathbb{N}^m$.

1. Initialize $(\boldsymbol{u}, \boldsymbol{v})$ with $(\boldsymbol{p}, \boldsymbol{q})$

2. If $(\boldsymbol{u}, \boldsymbol{v}) = (\mathbf{0}, \mathbf{0})$, terminate with the set of constructed row vectors.

3. Select a child $(\mathcal{L}\boldsymbol{u}, \overline{\boldsymbol{v}} \backslash \boldsymbol{s}) \in \mathcal{D}(\boldsymbol{p}, \overline{\boldsymbol{q}})$ of $(\boldsymbol{u}, \overline{\boldsymbol{v}})$ with a probability proportional to $\binom{\overline{\boldsymbol{v}}}{\boldsymbol{s}} \overline{N}(\mathcal{L}\boldsymbol{p}, \overline{\boldsymbol{v}} \backslash \boldsymbol{s})$.

4. Uniformly choose a row vector $\boldsymbol{r}$ among the corresponding rows.

5. Set $(\boldsymbol{u}, \boldsymbol{v})$ to $(\mathcal{L}\boldsymbol{u}, \boldsymbol{v} - \boldsymbol{r})$.

6. Return to the step (2)

$$\begin{array}{c|cc|}
 & 1 & 0 \\
\hline
 & 1 & 2 \\
 & 2 & 0 \\
1 & & \\
\hline
\end{array}$$

$(\boldsymbol{p}, \bar{\boldsymbol{q}})$

$$\downarrow$$

$$\begin{array}{c|cccc|}
 & 0 & 0 & 0 & 1 \\
\hline
 & 1 & 0 & 1 & 1 \\
 & 1 & 1 & 0 & 0 \\
1 & & & & \\
\hline
\end{array}$$

Binary Matrix

Uniform Sampling Algorithm

- Let $\mathcal{D}(\boldsymbol{p}, \boldsymbol{q})$ be the set of pairs $(\boldsymbol{u}, \overline{\boldsymbol{v}})$ traversed by the algorithm for a given initial input pair $(\boldsymbol{p}, \overline{\boldsymbol{q}})$ where $(\boldsymbol{p}, \boldsymbol{q}) \in \mathbb{N}^n \times \mathbb{N}^m$.

1. Initialize $(\boldsymbol{u}, \boldsymbol{v})$ with $(\boldsymbol{p}, \boldsymbol{q})$

2. If $(\boldsymbol{u}, \boldsymbol{v}) = (\boldsymbol{0}, \boldsymbol{0})$, terminate with the set of constructed row vectors.

3. Select a child $(\mathcal{L}\boldsymbol{u}, \overline{\boldsymbol{v}} \backslash \boldsymbol{s}) \in \mathcal{D}(\boldsymbol{p}, \overline{\boldsymbol{q}})$ of $(\boldsymbol{u}, \overline{\boldsymbol{v}})$ with a probability proportional to $\binom{\overline{\boldsymbol{v}}}{\boldsymbol{s}} \overline{N}(\mathcal{L}\boldsymbol{p}, \overline{\boldsymbol{v}} \backslash \boldsymbol{s})$.

4. Uniformly choose a row vector $\boldsymbol{r}$ among the corresponding rows.

5. Set $(\boldsymbol{u}, \boldsymbol{v})$ to $(\mathcal{L}\boldsymbol{u}, \boldsymbol{v} - \boldsymbol{r})$.

6. Return to the step (2)

$$\begin{array}{c|cc|} & 1 & 0 \\ \hline & 1 & 2 \\ & 2 & 0 \\ 1 & 1 & 0 \\ \hline \end{array}$$

$(\boldsymbol{p}, \bar{\boldsymbol{q}})$

$$\downarrow$$

$$\begin{array}{c|cccc|} & 0 & 0 & 0 & 1 \\ \hline & 1 & 0 & 1 & 1 \\ & 1 & 1 & 0 & 0 \\ 1 & & & & \\ \hline \end{array}$$

Binary Matrix

Uniform Sampling Algorithm

- Let $\mathcal{D}(\boldsymbol{p}, \boldsymbol{q})$ be the set of pairs $(\boldsymbol{u}, \overline{\boldsymbol{v}})$ traversed by the algorithm for a given initial input pair $(\boldsymbol{p}, \overline{\boldsymbol{q}})$ where $(\boldsymbol{p}, \boldsymbol{q}) \in \mathbb{N}^n \times \mathbb{N}^m$.

1. Initialize $(\boldsymbol{u}, \boldsymbol{v})$ with $(\boldsymbol{p}, \boldsymbol{q})$

2. If $(\boldsymbol{u}, \boldsymbol{v}) = (\mathbf{0}, \mathbf{0})$, terminate with the set of constructed row vectors.

3. Select a child $(\mathcal{L}\boldsymbol{u}, \overline{\boldsymbol{v}} \setminus \boldsymbol{s}) \in \mathcal{D}(\boldsymbol{p}, \overline{\boldsymbol{q}})$ of $(\boldsymbol{u}, \overline{\boldsymbol{v}})$ with a probability proportional to $\binom{\overline{\boldsymbol{v}}}{\boldsymbol{s}} \overline{N}(\mathcal{L}\boldsymbol{p}, \overline{\boldsymbol{v}} \setminus \boldsymbol{s})$.

4. Uniformly choose a row vector $\boldsymbol{r}$ among the corresponding rows.

5. Set $(\boldsymbol{u}, \boldsymbol{v})$ to $(\mathcal{L}\boldsymbol{u}, \boldsymbol{v} - \boldsymbol{r})$.

6. Return to the step (2)

$$\begin{array}{c|cc|} & 1 & 0 \\ \hline & 1 & 2 \\ & 2 & 0 \\ 1 & 1 & 0 \\ \hline \end{array}$$

$(\boldsymbol{p}, \bar{\boldsymbol{q}})$

$$\downarrow$$

$$\begin{array}{c|cccc|} & 0 & 0 & 0 & 1 \\ \hline & 1 & 0 & 1 & 1 \\ & 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 \\ \hline \end{array}$$

Binary Matrix

Uniform Sampling Algorithm

- Let $\mathcal{D}(\boldsymbol{p}, \boldsymbol{q})$ be the set of pairs $(\boldsymbol{u}, \overline{\boldsymbol{v}})$ traversed by the algorithm for a given initial input pair $(\boldsymbol{p}, \overline{\boldsymbol{q}})$ where $(\boldsymbol{p}, \boldsymbol{q}) \in \mathbb{N}^n \times \mathbb{N}^m$.

1. Initialize $(\boldsymbol{u}, \boldsymbol{v})$ with $(\boldsymbol{p}, \boldsymbol{q})$

2. If $(\boldsymbol{u}, \boldsymbol{v}) = (\mathbf{0}, \mathbf{0})$, terminate with the set of constructed row vectors.

3. Select a child $(\mathcal{L}\boldsymbol{u}, \overline{\boldsymbol{v}} \backslash \boldsymbol{s}) \in \mathcal{D}(\boldsymbol{p}, \overline{\boldsymbol{q}})$ of $(\boldsymbol{u}, \overline{\boldsymbol{v}})$ with a probability proportional to $\binom{\overline{\boldsymbol{v}}}{\boldsymbol{s}} \overline{N}(\mathcal{L}\boldsymbol{p}, \overline{\boldsymbol{v}} \backslash \boldsymbol{s})$.

4. Uniformly choose a row vector $\boldsymbol{r}$ among the corresponding rows.

5. **5.** Set $(\boldsymbol{u}, \boldsymbol{v})$ to $(\mathcal{L}\boldsymbol{u}, \boldsymbol{v} - \boldsymbol{r})$.

6. Return to the step (2)

$$\begin{array}{cc} 0 & 0 \\ \hline \begin{array}{|cc|} 1 & 2 \\ 2 & 0 \\ 1 & 0 \\ \hline \end{array} \end{array}$$

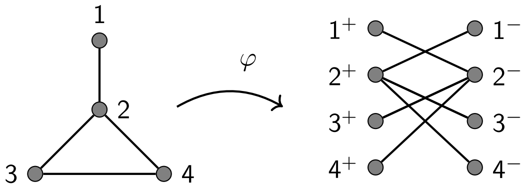
$(\boldsymbol{p}, \bar{\boldsymbol{q}})$

$$\downarrow$$

$$\begin{array}{cccc} 0 & 0 & 0 & 0 \end{array}$$
$$\begin{array}{|cccc|} \hline 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ \hline \end{array}$$

Binary Matrix

- Let $\varphi : \mathcal{G}^{\boldsymbol{d}} \to \mathcal{BP}$ be a function mapping every simple graph to a bipartite graph in the following way.



- Let the image of the set $\mathcal{G}^{\boldsymbol{d}}$ under the function φ be denoted by $\mathcal{SBP}^{(\boldsymbol{d},\boldsymbol{d})}$.
- The map φ is a bijective function from $\mathcal{G}^{\boldsymbol{d}}$ to $\mathcal{SBP}^{(\boldsymbol{d},\boldsymbol{d})}$.
- Hence, the bipartite graphs in the set $\mathcal{SBP}^{(\boldsymbol{d},\boldsymbol{d})}$ can be counted instead of counting the graphs in $\mathcal{G}^{\boldsymbol{d}}$

- Let $\kappa(\boldsymbol{d})$ be the number of simple graphs realizing the degree sequence $\boldsymbol{d}$.
- Similarly, columns of a binary matrix can be classified into $b := \max_j q_j$ groups.

$$
\begin{array}{c|ccccc|}
 & 3 & 3 & 2 & 2 & 2 \\
\hline
3 & 0 & 1 & 0 & 1 & 1 \\
3 & 1 & \mathrm{x} & & & \\
2 & 0 & & \mathrm{x} & & \\
2 & 1 & & & \mathrm{x} & \\
2 & 1 & & & & \mathrm{x} \\
\hline
\end{array}
$$

Binary Matrix

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

Binary Matrix

- There exists $\kappa(\mathcal{L}(\boldsymbol{d} - \boldsymbol{u}))$ number of binary matrices with zero-diagonal entries having the same first column and row vector $\boldsymbol{u} = (0, 1, 0, 1, 1)$

$$
\begin{array}{c|ccccc|}
 & 3 & 3 & 2 & 2 & 2 \\ \hline
3 & 0 & 1 & 0 & 1 & 1 \\
3 & 1 & \times & & & \\
2 & 0 & & \times & & \\
2 & 1 & & & \times & \\
2 & 1 & & & & \times \\ \hline
\end{array}
\quad \longrightarrow \quad
\begin{array}{c|ccc|}
 & 0 & 3 & 1 \\ \hline
3 & 0 & 2 & 1 \\
3 & & & \\
2 & & & \\
2 & & & \\
2 & & & \\ \hline
\end{array}
$$

Binary Matrix $\qquad\qquad$ $(\boldsymbol{p}, \bar{\boldsymbol{r}})$

- There exists $\kappa(\mathcal{L}(\boldsymbol{d} - \boldsymbol{u}))$ number of binary matrices with zero-diagonal entries having the same first column and row vector $\boldsymbol{u} = (0, 1, 0, 1, 1)$
- Since the positions of 1's in the same groups do not affect the number of binary matrices for the remaining part, the number of permutations $\boldsymbol{v}$ of the vector $\boldsymbol{u}$ where $\kappa(\boldsymbol{d} - \boldsymbol{v}) = \kappa(\boldsymbol{d} - \boldsymbol{u})$ is

$$
\binom{\boldsymbol{r}}{\boldsymbol{s}} := \binom{r_1}{s_1} \cdots \binom{r_b}{s_b} = \binom{3}{2}\binom{1}{1} = 3
$$

where $\boldsymbol{r} = (0, d_2, \ldots, d_n)$

- The number of labeled simple graphs realizing the degree sequence can be computed by counting the matrices satisfying the row and column sums $(\boldsymbol{d}, \overline{\boldsymbol{d}})$.

$$
\begin{array}{c|cccc|}
 & 2 & 2 & 2 & 2 \\
\hline
2 & \mathrm{x} & & & \\
2 & & \mathrm{x} & & \\
2 & & & \mathrm{x} & \\
2 & & & & \mathrm{x} \\
\hline
\end{array}
\qquad
\begin{array}{c|cc|}
 & 0 & 3 \\
\hline
2 & & \\
2 & & \\
2 & & \\
2 & & \\
\hline
\end{array}
$$

- In the enumeration of such matrices, update the column sum to $\boldsymbol{r} \backslash \boldsymbol{s} := \boldsymbol{r} - \boldsymbol{s} + \mathcal{L}\boldsymbol{s}$, and the row sum to $\mathcal{L}\xi(\boldsymbol{d}, \boldsymbol{s})$, i.e update the row sum to $\mathcal{L}(\boldsymbol{p} - \boldsymbol{v})$ where $\boldsymbol{v}$ is a corresponding row vector which does not changes the non-increasing order of the row sum.

- The number of labeled simple graphs realizing the degree sequence can be computed by counting the matrices satisfying the row and column sums $(\boldsymbol{d}, \overline{\boldsymbol{d}})$.

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

- In the enumeration of such matrices, update the column sum to $\boldsymbol{r} \backslash \boldsymbol{s} := \boldsymbol{r} - \boldsymbol{s} + \mathcal{L}\boldsymbol{s}$, and the row sum to $\mathcal{L}\xi(\boldsymbol{d}, \boldsymbol{s})$, i.e update the row sum to $\mathcal{L}(\boldsymbol{p} - \boldsymbol{v})$ where $\boldsymbol{v}$ is a corresponding row vector which does not changes the non-increasing order of the row sum.

- The number of labeled simple graphs realizing the degree sequence can be computed by counting the matrices satisfying the row and column sums $(\boldsymbol{d}, \overline{\boldsymbol{d}})$.

$$
\begin{array}{c|cccc|}
 & 2 & 2 & 2 & 2 \\ \hline
 & 0 & 0 & 1 & 1 \\
 & 0 & 0 & 1 & 1 \\
0 & 1 & 1 & x & \\
0 & 1 & 1 & & x \\ \hline
\end{array}
\qquad
\begin{array}{c|cc|}
 & 0 & 3 \\ \hline
2 & & \\
2 & & \\
2 & & \\
2 & & \\ \hline
\end{array}
\qquad
\begin{array}{c|cc|}
 & 2 & 0 \\ \hline
 & 0 & 2 \\
2 & & \\
1 & & \\
1 & & \\ \hline
\end{array}
\qquad
\begin{array}{c|cc|}
 & 0 & 0 \\ \hline
 & 0 & 2 \\
 & 2 & 0 \\
0 & & \\
0 & & \\ \hline
\end{array}
$$

- In the enumeration of such matrices, update the column sum to $\boldsymbol{r} \backslash \boldsymbol{s} := \boldsymbol{r} - \boldsymbol{s} + \mathcal{L}\boldsymbol{s}$, and the row sum to $\mathcal{L}\xi(\boldsymbol{d}, \boldsymbol{s})$, i.e update the row sum to $\mathcal{L}(\boldsymbol{p} - \boldsymbol{v})$ where $\boldsymbol{v}$ is a corresponding row vector which does not changes the non-increasing order of the row sum.

- The number of labeled simple graphs realizing the degree sequence can be computed by counting the matrices satisfying the row and column sums $(\boldsymbol{d}, \overline{\boldsymbol{d}})$.

$$
\begin{array}{cc}
 & \begin{array}{cccc} 2 & 2 & 2 & 2 \end{array} \\
\begin{array}{c} \\ \\ \\ 0 \end{array} & \left|\begin{array}{cccc} 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \end{array}\right|
\end{array}
\quad
\begin{array}{cc}
 & \begin{array}{cc} 0 & 3 \end{array} \\
\begin{array}{c} 2 \\ 2 \\ 2 \\ 2 \end{array} & \left|\begin{array}{cc} & \\ & \\ & \\ & \end{array}\right|
\end{array}
\quad
\begin{array}{cc}
 & \begin{array}{cc} 2 & 0 \end{array} \\
\begin{array}{c} \\ 2 \\ 1 \\ 1 \end{array} & \left|\begin{array}{cc} 0 & 2 \\ & \\ & \\ & \end{array}\right|
\end{array}
\quad
\begin{array}{cc}
 & \begin{array}{cc} 0 & 0 \end{array} \\
\begin{array}{c} \\ \\ 0 \\ 0 \end{array} & \left|\begin{array}{cc} 0 & 2 \\ 2 & 0 \\ & \\ & \end{array}\right|
\end{array}
\quad
\begin{array}{c}
\begin{array}{cc} 0 & 0 \end{array} \\
\left|\begin{array}{cc} 0 & 2 \\ 2 & 0 \\ 0 & 0 \\ 0 & 0 \end{array}\right|
\end{array}
$$

- In the enumeration of such matrices, update the column sum to $\boldsymbol{r} \backslash \boldsymbol{s} := \boldsymbol{r} - \boldsymbol{s} + \mathcal{L}\boldsymbol{s}$, and the row sum to $\mathcal{L}\xi(\boldsymbol{d}, \boldsymbol{s})$, i.e update the row sum to $\mathcal{L}(\boldsymbol{p} - \boldsymbol{v})$ where $\boldsymbol{v}$ is a corresponding row vector which does not changes the non-increasing order of the row sum.

- Similarly, the pair of row and column sums $(\boldsymbol{u}, \overline{\boldsymbol{v}})$ traversed by the algorithm construct a acyclic directed graph.

Theorem

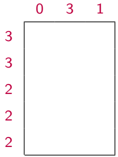
The number of simple graphs $G = (V; E)$ with a given non-increasing degree sequence $\boldsymbol{d} = (d_1, ..., d_n) \in \mathbb{N}^n$, is given by $\kappa(\boldsymbol{d}) := S(\boldsymbol{d}, \overline{\boldsymbol{d}})$, and the function $S(\cdot, \cdot)$ is defined by

$$\kappa(\boldsymbol{d}) := S(\boldsymbol{d}, \overline{\boldsymbol{d}}) = \sum_{\boldsymbol{s} \in C^{\overline{r}}(d_1)} \binom{\overline{\boldsymbol{r}}}{\boldsymbol{s}} S(\mathcal{L}\xi(\boldsymbol{d}, \boldsymbol{s}), \overline{\boldsymbol{r}} \backslash \boldsymbol{s})$$

where the sequence $\boldsymbol{r} := (0, \mathcal{L}\boldsymbol{d}) = (0, d_2, ..., d_n)$.

Uniform Sampling Algorithm

- Let $\mathcal{C}(\boldsymbol{d}, \bar{\boldsymbol{d}})$ be the set of all pairs $(\boldsymbol{u}, \bar{\boldsymbol{v}})$ traversed by the algorithm where $(\boldsymbol{d}, \bar{\boldsymbol{d}})$ is the starting node.



$(\boldsymbol{d}, \bar{\boldsymbol{d}})$

1 Initialize $(\boldsymbol{u}, \overline{\boldsymbol{v}})$ with $(\boldsymbol{d}, \overline{\boldsymbol{d}})$

2 If $(\boldsymbol{u}, \overline{\boldsymbol{v}}) = (\mathbf{0}, \mathbf{0})$, terminate with the set of constructed rows.

3 Select a child $(\mathcal{L}\xi(\boldsymbol{d}, \boldsymbol{s}), \overline{\boldsymbol{r}} \backslash \boldsymbol{s}) \in \mathcal{C}(\boldsymbol{d}, \overline{\boldsymbol{d}})$ of $(\boldsymbol{u}, \overline{\boldsymbol{v}})$ with a probability proportional to $\binom{\overline{\boldsymbol{r}}}{\boldsymbol{s}} S(\mathcal{L}\xi(\boldsymbol{d}, \boldsymbol{s}), \overline{\boldsymbol{r}} \backslash \boldsymbol{s})$.

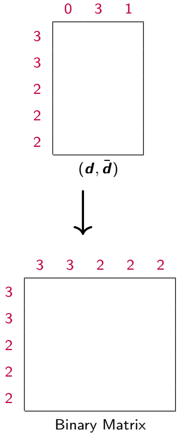
4 Uniformly choose a row vector $\boldsymbol{\pi}$ among the corresponding rows.

5 Set $(\boldsymbol{u}, \overline{\boldsymbol{v}})$ to $(\mathcal{L}\xi(\boldsymbol{d}, \boldsymbol{s}), \overline{\boldsymbol{r}} \backslash \boldsymbol{s})$.

6 Return to the step (2).

Uniform Sampling Algorithm

- Let $\mathcal{C}(\boldsymbol{d}, \bar{\boldsymbol{d}})$ be the set of all pairs $(\boldsymbol{u}, \bar{\boldsymbol{v}})$ traversed by the algorithm where $(\boldsymbol{d}, \bar{\boldsymbol{d}})$ is the starting node.



1 Initialize $(\boldsymbol{u}, \overline{\boldsymbol{v}})$ with $(\boldsymbol{d}, \overline{\boldsymbol{d}})$

2 If $(\boldsymbol{u}, \overline{\boldsymbol{v}}) = (\mathbf{0}, \mathbf{0})$, terminate with the set of constructed rows.

3 Select a child $(\mathcal{L}\xi(\boldsymbol{d}, \boldsymbol{s}), \overline{\boldsymbol{r}} \backslash \boldsymbol{s}) \in \mathcal{C}(\boldsymbol{d}, \overline{\boldsymbol{d}})$ of $(\boldsymbol{u}, \overline{\boldsymbol{v}})$ with a probability proportional to $\binom{\overline{\boldsymbol{r}}}{\boldsymbol{s}} S(\mathcal{L}\xi(\boldsymbol{d}, \boldsymbol{s}), \overline{\boldsymbol{r}} \backslash \boldsymbol{s})$.

4 Uniformly choose a row vector $\boldsymbol{\pi}$ among the corresponding rows.

5 Set $(\boldsymbol{u}, \overline{\boldsymbol{v}})$ to $(\mathcal{L}\xi(\boldsymbol{d}, \boldsymbol{s}), \overline{\boldsymbol{r}} \backslash \boldsymbol{s})$.

6 Return to the step (2).

Uniform Sampling Algorithm

- Let $\mathcal{C}(\boldsymbol{d}, \bar{\boldsymbol{d}})$ be the set of all pairs $(\boldsymbol{u}, \bar{\boldsymbol{v}})$ traversed by the algorithm where $(\boldsymbol{d}, \bar{\boldsymbol{d}})$ is the starting node.

$$\begin{array}{c|ccc|}
 & 0 & 3 & 1 \\
\hline
3 & 0 & 2 & 1 \\
3 & & & \\
2 & & & \\
2 & & & \\
2 & & & \\
\hline
\end{array}$$

$(\boldsymbol{d}, \bar{\boldsymbol{d}})$

$$\downarrow$$

$$\begin{array}{c|ccccc|}
 & 3 & 3 & 2 & 2 & 2 \\
\hline
3 & & & & & \\
3 & & & & & \\
2 & & & & & \\
2 & & & & & \\
2 & & & & & \\
\hline
\end{array}$$

Binary Matrix

1 Initialize $(\boldsymbol{u}, \overline{\boldsymbol{v}})$ with $(\boldsymbol{d}, \overline{\boldsymbol{d}})$

2 If $(\boldsymbol{u}, \overline{\boldsymbol{v}}) = (\mathbf{0}, \mathbf{0})$, terminate with the set of constructed rows.

3 Select a child $(\mathcal{L}\xi(\boldsymbol{d}, \boldsymbol{s}), \overline{\boldsymbol{r}} \backslash \boldsymbol{s}) \in \mathcal{C}(\boldsymbol{d}, \overline{\boldsymbol{d}})$ of $(\boldsymbol{u}, \overline{\boldsymbol{v}})$ with a probability proportional to $\binom{\overline{\boldsymbol{r}}}{\boldsymbol{s}} S(\mathcal{L}\xi(\boldsymbol{d}, \boldsymbol{s}), \overline{\boldsymbol{r}} \backslash \boldsymbol{s})$.

4 Uniformly choose a row vector $\boldsymbol{\pi}$ among the corresponding rows.

5 Set $(\boldsymbol{u}, \overline{\boldsymbol{v}})$ to $(\mathcal{L}\xi(\boldsymbol{d}, \boldsymbol{s}), \overline{\boldsymbol{r}} \backslash \boldsymbol{s})$.

6 Return to the step (2).

Uniform Sampling Algorithm

- Let $\mathcal{C}(\boldsymbol{d}, \bar{\boldsymbol{d}})$ be the set of all pairs $(\boldsymbol{u}, \bar{\boldsymbol{v}})$ traversed by the algorithm where $(\boldsymbol{d}, \bar{\boldsymbol{d}})$ is the starting node.

$$
\begin{array}{c|ccc|}
 & 0 & 3 & 1 \\
\hline
3 & 0 & 2 & 1 \\
3 & & & \\
2 & & & \\
2 & & & \\
2 & & & \\
\hline
\end{array}
$$

$(\boldsymbol{d}, \bar{\boldsymbol{d}})$

$$\downarrow$$

$$
\begin{array}{c|ccccc|}
 & 3 & 3 & 2 & 2 & 2 \\
\hline
3 & 0 & 1 & 0 & 1 & 1 \\
3 & 1 & & & & \\
2 & 0 & & & & \\
2 & 1 & & & & \\
2 & 1 & & & & \\
\hline
\end{array}
$$

Binary Matrix

1 Initialize $(\boldsymbol{u}, \overline{\boldsymbol{v}})$ with $(\boldsymbol{d}, \overline{\boldsymbol{d}})$

2 If $(\boldsymbol{u}, \overline{\boldsymbol{v}}) = (\mathbf{0}, \mathbf{0})$, terminate with the set of constructed rows.

3 Select a child $(\mathcal{L}\xi(\boldsymbol{d}, \boldsymbol{s}), \overline{\boldsymbol{r}} \backslash \boldsymbol{s}) \in \mathcal{C}(\boldsymbol{d}, \overline{\boldsymbol{d}})$ of $(\boldsymbol{u}, \overline{\boldsymbol{v}})$ with a probability proportional to $\binom{\overline{\boldsymbol{r}}}{\boldsymbol{s}} S(\mathcal{L}\xi(\boldsymbol{d}, \boldsymbol{s}), \overline{\boldsymbol{r}} \backslash \boldsymbol{s})$.

4 Uniformly choose a row vector $\boldsymbol{\pi}$ among the corresponding rows.

5 Set $(\boldsymbol{u}, \overline{\boldsymbol{v}})$ to $(\mathcal{L}\xi(\boldsymbol{d}, \boldsymbol{s}), \overline{\boldsymbol{r}} \backslash \boldsymbol{s})$.

6 Return to the step (2).

Uniform Sampling Algorithm

- Let $\mathcal{C}(\boldsymbol{d}, \bar{\boldsymbol{d}})$ be the set of all pairs $(\boldsymbol{u}, \bar{\boldsymbol{v}})$ traversed by the algorithm where $(\boldsymbol{d}, \bar{\boldsymbol{d}})$ is the starting node.

$$
\begin{array}{c|ccc|}
 & 2 & 1 & 0 \\
\hline
 & 0 & 2 & 1 \\
2 & & & \\
2 & & & \\
1 & & & \\
1 & & & \\
\hline
\end{array}
$$

$(\boldsymbol{d}, \bar{\boldsymbol{d}})$

$$\downarrow$$

$$
\begin{array}{c|ccccc|}
 & & 2 & 2 & 1 & 1 \\
\hline
 & 0 & 1 & 0 & 1 & 1 \\
2 & 1 & & & & \\
2 & 0 & & & & \\
1 & 1 & & & & \\
1 & 1 & & & & \\
\hline
\end{array}
$$

Binary Matrix

1 Initialize $(\boldsymbol{u}, \overline{\boldsymbol{v}})$ with $(\boldsymbol{d}, \overline{\boldsymbol{d}})$

2 If $(\boldsymbol{u}, \overline{\boldsymbol{v}}) = (\mathbf{0}, \mathbf{0})$, terminate with the set of constructed rows.

3 Select a child $(\mathcal{L}\xi(\boldsymbol{d}, \boldsymbol{s}), \overline{\boldsymbol{r}} \backslash \boldsymbol{s}) \in \mathcal{C}(\boldsymbol{d}, \overline{\boldsymbol{d}})$ of $(\boldsymbol{u}, \overline{\boldsymbol{v}})$ with a probability proportional to $\binom{\overline{\boldsymbol{r}}}{\boldsymbol{s}} S(\mathcal{L}\xi(\boldsymbol{d}, \boldsymbol{s}), \overline{\boldsymbol{r}} \backslash \boldsymbol{s})$.

4 Uniformly choose a row vector $\boldsymbol{\pi}$ among the corresponding rows.

5 Set $(\boldsymbol{u}, \overline{\boldsymbol{v}})$ to $(\mathcal{L}\xi(\boldsymbol{d}, \boldsymbol{s}), \overline{\boldsymbol{r}} \backslash \boldsymbol{s})$.

6 Return to the step (2).

Uniform Sampling Algorithm

- Let $\mathcal{C}(\boldsymbol{d}, \bar{\boldsymbol{d}})$ be the set of all pairs $(\boldsymbol{u}, \bar{\boldsymbol{v}})$ traversed by the algorithm where $(\boldsymbol{d}, \bar{\boldsymbol{d}})$ is the starting node.

$$
\begin{array}{c|ccc|}
 & 2 & 1 & 0 \\
\hline
 & 0 & 2 & 1 \\
2 & 1 & 1 & 0 \\
2 & & & \\
1 & & & \\
1 & & & \\
\hline
\end{array}
$$

$(\boldsymbol{d}, \bar{\boldsymbol{d}})$

$$\downarrow$$

$$
\begin{array}{c|ccccc|}
 & & 2 & 2 & 1 & 1 \\
\hline
 & 0 & 1 & 0 & 1 & 1 \\
2 & 1 & & & & \\
2 & 0 & & & & \\
1 & 1 & & & & \\
1 & 1 & & & & \\
\hline
\end{array}
$$

Binary Matrix

1 Initialize $(\boldsymbol{u}, \overline{\boldsymbol{v}})$ with $(\boldsymbol{d}, \overline{\boldsymbol{d}})$

2 If $(\boldsymbol{u}, \overline{\boldsymbol{v}}) = (\boldsymbol{0}, \boldsymbol{0})$, terminate with the set of constructed rows.

3 Select a child $(\mathcal{L}\xi(\boldsymbol{d}, \boldsymbol{s}), \overline{\boldsymbol{r}} \backslash \boldsymbol{s}) \in \mathcal{C}(\boldsymbol{d}, \overline{\boldsymbol{d}})$ of $(\boldsymbol{u}, \overline{\boldsymbol{v}})$ with a probability proportional to $\binom{\overline{\boldsymbol{r}}}{\boldsymbol{s}} S(\mathcal{L}\xi(\boldsymbol{d}, \boldsymbol{s}), \overline{\boldsymbol{r}} \backslash \boldsymbol{s})$.

4 Uniformly choose a row vector $\boldsymbol{\pi}$ among the corresponding rows.

5 Set $(\boldsymbol{u}, \overline{\boldsymbol{v}})$ to $(\mathcal{L}\xi(\boldsymbol{d}, \boldsymbol{s}), \overline{\boldsymbol{r}} \backslash \boldsymbol{s})$.

6 Return to the step (2).

Uniform Sampling Algorithm

- Let $\mathcal{C}(\boldsymbol{d}, \bar{\boldsymbol{d}})$ be the set of all pairs $(\boldsymbol{u}, \bar{\boldsymbol{v}})$ traversed by the algorithm where $(\boldsymbol{d}, \bar{\boldsymbol{d}})$ is the starting node.

$$
\begin{array}{c|ccc|}
 & 2 & 1 & 0 \\
\hline
 & 0 & 2 & 1 \\
2 & 1 & 1 & 0 \\
2 & & & \\
1 & & & \\
1 & & & \\
\hline
\end{array}
$$

$(\boldsymbol{d}, \bar{\boldsymbol{d}})$

$$\downarrow$$

$$
\begin{array}{c|ccccc|}
 & & 2 & 2 & 1 & 1 \\
\hline
 & 0 & 1 & 0 & 1 & 1 \\
2 & 1 & 0 & 1 & 0 & 1 \\
2 & 0 & 1 & & & \\
1 & 1 & 0 & & & \\
1 & 1 & 1 & & & \\
\hline
\end{array}
$$

Binary Matrix

1 Initialize $(\boldsymbol{u}, \overline{\boldsymbol{v}})$ with $(\boldsymbol{d}, \overline{\boldsymbol{d}})$

2 If $(\boldsymbol{u}, \overline{\boldsymbol{v}}) = (\mathbf{0}, \mathbf{0})$, terminate with the set of constructed rows.

3 Select a child $(\mathcal{L}\xi(\boldsymbol{d}, \boldsymbol{s}), \overline{\boldsymbol{r}} \backslash \boldsymbol{s}) \in \mathcal{C}(\boldsymbol{d}, \overline{\boldsymbol{d}})$ of $(\boldsymbol{u}, \overline{\boldsymbol{v}})$ with a probability proportional to $\binom{\overline{\boldsymbol{r}}}{\boldsymbol{s}} S(\mathcal{L}\xi(\boldsymbol{d}, \boldsymbol{s}), \overline{\boldsymbol{r}} \backslash \boldsymbol{s})$.

4 Uniformly choose a row vector $\boldsymbol{\pi}$ among the corresponding rows.

5 Set $(\boldsymbol{u}, \overline{\boldsymbol{v}})$ to $(\mathcal{L}\xi(\boldsymbol{d}, \boldsymbol{s}), \overline{\boldsymbol{r}} \backslash \boldsymbol{s})$.

6 Return to the step (2).

Uniform Sampling Algorithm

- Let $\mathcal{C}(\boldsymbol{d}, \bar{\boldsymbol{d}})$ be the set of all pairs $(\boldsymbol{u}, \bar{\boldsymbol{v}})$ traversed by the algorithm where $(\boldsymbol{d}, \bar{\boldsymbol{d}})$ is the starting node.

$$
\begin{array}{c|ccc|}
 & 1 & 0 & 0 \\
\hline
 & 0 & 2 & 1 \\
 & 1 & 1 & 0 \\
1 & & & \\
1 & & & \\
0 & & & \\
\hline
\end{array}
$$

$(\boldsymbol{d}, \bar{\boldsymbol{d}})$

$$\downarrow$$

$$
\begin{array}{c|ccccc|}
 & & & 1 & 1 & 0 \\
\hline
 & 0 & 1 & 0 & 1 & 1 \\
 & 1 & 0 & 1 & 0 & 1 \\
1 & 0 & 1 & & & \\
1 & 1 & 0 & & & \\
0 & 1 & 1 & & & \\
\hline
\end{array}
$$

Binary Matrix

1 Initialize $(\boldsymbol{u}, \overline{\boldsymbol{v}})$ with $(\boldsymbol{d}, \overline{\boldsymbol{d}})$

2 If $(\boldsymbol{u}, \overline{\boldsymbol{v}}) = (\mathbf{0}, \mathbf{0})$, terminate with the set of constructed rows.

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5 Set $(\boldsymbol{u}, \overline{\boldsymbol{v}})$ to $(\mathcal{L}\xi(\boldsymbol{d}, \boldsymbol{s}), \overline{\boldsymbol{r}} \backslash \boldsymbol{s})$.

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Uniform Sampling Algorithm

- Let $\mathcal{C}(\boldsymbol{d}, \bar{\boldsymbol{d}})$ be the set of all pairs $(\boldsymbol{u}, \bar{\boldsymbol{v}})$ traversed by the algorithm where $(\boldsymbol{d}, \bar{\boldsymbol{d}})$ is the starting node.

$$
\begin{array}{c|ccc|}
 & 1 & 0 & 0 \\
\hline
 & 0 & 2 & 1 \\
 & 1 & 1 & 0 \\
1 & 1 & 0 & 0 \\
1 & & & \\
0 & & & \\
\hline
\end{array}
$$

$(\boldsymbol{d}, \bar{\boldsymbol{d}})$

$$\downarrow$$

$$
\begin{array}{c|ccccc|}
 & & & 1 & 1 & 0 \\
\hline
 & 0 & 1 & 0 & 1 & 1 \\
 & 1 & 0 & 1 & 0 & 1 \\
1 & 0 & 1 & & & \\
1 & 1 & 0 & & & \\
0 & 1 & 1 & & & \\
\hline
\end{array}
$$

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1 Initialize $(\boldsymbol{u}, \overline{\boldsymbol{v}})$ with $(\boldsymbol{d}, \overline{\boldsymbol{d}})$

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3 **3** Select a child $(\mathcal{L}\xi(\boldsymbol{d}, \boldsymbol{s}), \overline{\boldsymbol{r}} \backslash \boldsymbol{s}) \in \mathcal{C}(\boldsymbol{d}, \overline{\boldsymbol{d}})$ of $(\boldsymbol{u}, \overline{\boldsymbol{v}})$ with a probability proportional to $\binom{\overline{\boldsymbol{r}}}{\boldsymbol{s}} S(\mathcal{L}\xi(\boldsymbol{d}, \boldsymbol{s}), \overline{\boldsymbol{r}} \backslash \boldsymbol{s})$.

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$$
\begin{array}{c|ccc|}
 & 1 & 0 & 0 \\
\hline
 & 0 & 2 & 1 \\
 & 1 & 1 & 0 \\
1 & 1 & 0 & 0 \\
1 & & & \\
0 & & & \\
\hline
\end{array}
$$

$(\boldsymbol{d}, \bar{\boldsymbol{d}})$

$$\downarrow$$

$$
\begin{array}{c|ccccc|}
 & & & 1 & 1 & 0 \\
\hline
 & 0 & 1 & 0 & 1 & 1 \\
 & 1 & 0 & 1 & 0 & 1 \\
1 & 0 & 1 & 0 & 1 & 0 \\
1 & 1 & 0 & 1 & & \\
0 & 1 & 1 & 0 & & \\
\hline
\end{array}
$$

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$$\begin{array}{c|ccc|}
 & 0 & 0 & 0 \\ \hline
 & 0 & 2 & 1 \\
 & 1 & 1 & 0 \\
 & 1 & 0 & 0 \\
0 & & & \\
0 & & & \\ \hline
\end{array}$$

$(\boldsymbol{d}, \bar{\boldsymbol{d}})$

$$\downarrow$$

$$\begin{array}{c|ccccc|}
 & & & & 0 & 0 \\ \hline
 & 0 & 1 & 0 & 1 & 1 \\
 & 1 & 0 & 1 & 0 & 1 \\
 & 0 & 1 & 0 & 1 & 0 \\
0 & 1 & 0 & 1 & & \\
0 & 1 & 1 & 0 & & \\ \hline
\end{array}$$

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$$
\begin{array}{c|ccc|}
 & 0 & 0 & 0 \\
\hline
 & 0 & 2 & 1 \\
 & 1 & 1 & 0 \\
 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
\hline
\end{array}
$$

$(\boldsymbol{d}, \bar{\boldsymbol{d}})$

$$\downarrow$$

$$
\begin{array}{c|ccccc|}
 & & & & 0 & 0 \\
\hline
 & 0 & 1 & 0 & 1 & 1 \\
 & 1 & 0 & 1 & 0 & 1 \\
 & 0 & 1 & 0 & 1 & 0 \\
0 & 1 & 0 & 1 & & \\
0 & 1 & 1 & 0 & & \\
\hline
\end{array}
$$

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$$\begin{array}{c|ccc|}
 & 0 & 0 & 0 \\ \hline
 & 0 & 2 & 1 \\
 & 1 & 1 & 0 \\
 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\ \hline
\end{array}$$

$(\boldsymbol{d}, \bar{\boldsymbol{d}})$

$$\downarrow$$

$$\begin{array}{c|ccccc|}
 & & & & 0 & 0 \\ \hline
 & 0 & 1 & 0 & 1 & 1 \\
 & 1 & 0 & 1 & 0 & 1 \\
 & 0 & 1 & 0 & 1 & 0 \\
0 & 1 & 0 & 1 & 0 & 0 \\
0 & 1 & 1 & 0 & 0 & 0 \\ \hline
\end{array}$$

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$$\begin{array}{ccc} 0 & 0 & 0 \\ \end{array}$$
$$\begin{array}{|ccc|} \hline 0 & 2 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ \hline \end{array}$$

$(\boldsymbol{d}, \bar{\boldsymbol{d}})$

$$\downarrow$$

$$\begin{array}{|ccccc|} \hline 0 & 1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ \hline \end{array}$$

Binary Matrix

1 Initialize $(\boldsymbol{u}, \overline{\boldsymbol{v}})$ with $(\boldsymbol{d}, \overline{\boldsymbol{d}})$

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6 Return to the step (2).

Applications

Enumeration of Graphs with Prescribed Degree Sequences

n	k-regular	Importance Sampling	Proposed Method
4	3-regular	1.0 ± 0.0	1
6	3-regular	$70{,}625 \pm 0.895$	70
8	4-regular	$19.133{,}298 \pm 325{,}706$	19.355
10	4-regular	$(6{,}6373 \pm 0{,}1149) \times 10^7$	66.462.606
14	9-regular	$(6{,}4632 \pm 0{,}2664) \times 10^{15}$	6.551.246.596.501.035

Degree Sequence	Importance Sampling	Proposed Method
(4,2,5,2,2,3)	3.0039 ± 0.0095	3
(2,4,2,4,5,4,1)	11.9892 ± 0.0570	12
(2,2,3,1,7,2,5,3,5)	212.5956 ± 5.1241	215
(4,6,6,5,2,1,3,8,4,1,4)	$(1, 17523 \pm 0, 02909) \times 10^5$	117.697

Hypothesis Testing

	A. diemensis	Leiolopisma delicata	L. entrecasteauxii	L. metallica	L. ocellata	L. pretiosa	L. trilineata	L. sp. nov.	Lerista bougainwillii	Pseudemoia sp. nov.	S. tympanum	Egernia whitei	Tiliqua casuarinae	T. nigrolutea	A. superbus	Drysdalia coronoides	Notechis ater
Pedra Branca Island	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
Maatsuyker Island	0	0	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0
Tasmania	1	1	1	1	1	1	1	1	1	0	0	1	1	1	1	1	1
Albatros Island	0	0	1	1	0	1	1	0	0	0	0	1	0	1	1	1	1
Furneaux Group	0	0	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0
Curis Island	1	0	1	1	1	1	1	0	1	0	0	1	0	1	1	1	1
Kent Group	0	0	0	1	0	0	0	0	1	0	0	1	0	0	0	1	0
Hogan Group	0	0	0	1	0	0	1	0	1	0	0	1	0	1	0	1	0
Rodondo Island	0	0	1	1	0	0	1	0	0	0	0	1	0	1	0	0	0
Brisbane-Adelaide	0	0	0	1	0	0	0	0	0	0	1	1	0	0	0	0	0

Distribution of Island Reptile Species In Southern Australia

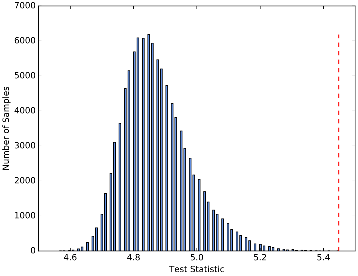
- The table indicates the presence or absence of 17 reptiles species in the Tasmania and the Bass Strait area.

- For testing whether there is competition between species, Robert and Stone(1990) proposed a test statistic which is given by

$$\bar{S}^2 = \frac{1}{n(n-1)} \sum_{i \neq j} s_{ij}^2$$

  where m is the number of species, and $S = (s_{ij}) = M^T M$.

- The statistic can be used to test the null hypothesis that the pattern of reptile species on the islands is the result of chance rather than the interactions between species on the islands.



- The p-value was estimated to be 0.02×10^{-3} with 100.000 samples.
- The results shows that the observed statistic is not consistent with the null hypothesis and there is enough evidence to reject the null hypothesis in favor of the alternative hypothesis.

- The proposed method allows one to exactly compute the number of simple graphs satisfying the degree sequence.
- The Monte Carlo methods generally run faster than the proposed method, especially when the size of the problem increases[1].
- The appeal of the proposed method stems from its exactness.
- There is no guarantee for the estimates coming from Monte Carlo methods to adequately converge.

[1] For example, Miller Harrison algorithm runs in $\mathcal{O}(m(ab+c)(a+b)^{b-1}(b+c)^{b-1}(logc)^3)$ time where $a = \max_i p_i$, $b = \max_j q_j$ and $c = \sum_i p_i = \sum_j q_j$

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J. W. Miller and M. T. Harrison (2013)
Exact sampling and counting for fixed-margin matrices
The Annals of Statistics 41, 1569 – 1592.

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Island-sharing by archipelago species
Oecologia 83, 560–567.

The End

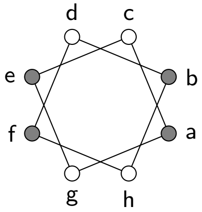
Sequential Importance Sampling

- A problem in importance sampling is to choose a good proposal distribution $q(x)$, especially, in high dimensional problems.
- The proposal distribution $q(x)$ can be written by

$$q(x) = q(x_1)q(x_2|x_1)\cdots q(x_n|x_1, ..., x_n)$$

- This factorization property can be used as a good strategy in order to generate samples from $q(x)$.

- Every bipartite graph can be represented by a binary matrix.
- For instance,



	c	d	g	h
a	1	0	1	0
b	0	1	0	1
e	1	0	1	0
f	0	1	0	1

- Chen et al.[1] proposed a sequential importance sampling algorithm for the generation of (0,1)-matrices satisfying given row and column sums.

- Let $\mathcal{M}^{\boldsymbol{p},\boldsymbol{q}}$ be the set of all possible $(0,1)$-matrices satisfying the row sum $\boldsymbol{p}$ and column sum $\boldsymbol{q}$.

- A binary matrix can be generated by sequentially constructing its column vectors.

- A simple way to construct column vectors is to choose q_j places from m possible positions.

$$
\begin{array}{c|ccc|}
 & 2 & 1 & 2 \\ \hline
1 & & & \\
2 & & & \\
1 & & & \\
1 & & & \\ \hline
\end{array}
\quad
\begin{array}{c|ccc|}
 & 2 & 1 & 2 \\ \hline
1 & 0 & & \\
2 & 1 & & \\
1 & 0 & & \\
1 & 1 & & \\ \hline
\end{array}
\quad
\begin{array}{c|ccc|}
 & 2 & 1 & 2 \\ \hline
1 & 0 & 1 & \\
2 & 1 & 0 & \\
1 & 0 & 0 & \\
1 & 1 & 0 & \\ \hline
\end{array}
\quad
\begin{array}{c|ccc|}
 & 2 & 1 & 2 \\ \hline
1 & 0 & 1 & 0 \\
2 & 1 & 0 & 1 \\
1 & 0 & 0 & 1 \\
1 & 1 & 0 & 0 \\ \hline
\end{array}
$$

Sequential construction of a binary matrix

- However, this naive approach is very inefficient, which generates lots of invalid matrices.

- *Chen et al*[1] proposed to draw column vectors from the Conditional-Poisson distribution.
- Let $R_1, ..., R_n$ be random variables where $R_i \sim \text{Bern}\,(\pi_i)$ and $S_R = R_1 + \cdots + R_n$. Then the random variable S_R is said to follow *Poisson-binomial distribution*.
- The conditional distribution of $R = (R_1, ..., R_n)$ given S_Z is called *CP distribution*, and

$$\mathbb{P}(R_1 = r_1, ..., R_n = r_n | S_R = k) \propto \prod_{i=1}^{n} w_i^{r_i}$$

where $w_i = \frac{p_i}{1-p_i}$

- Using the CP distribution is more desirable for drawing column vectors by the following. theorem.

Theorem

For the uniform distribution over all $n \times m$ binary matrices with given row sums $p_1, \ldots, p_n$ and first column sum q_1, the marginal distribution of the first column is the same as the conditional distribution of S_R given $S_R = q_1$ with $\pi = p_i/m$.

Edge-switching Markov Chain

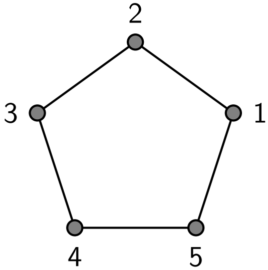
Edge-switching Markov Chain

- There are many variants of edge-switching Markov chains for sampling from a set of graphs with a given degree sequence.
- In this section, a natural Markov chain will be described.

Edge-switching Markov chain

Input: A graph G^0 satisfying the degree sequence $\boldsymbol{d}$

for $k = 1$ to K **do**
    $r \sim \mathcal{U}(0,1)$
    if $r > \frac{1}{2}$ **then**
        Uniformly choose two random non-adjacent edges $\{v, u\}$ and $\{x, y\}$.
        Choose a perfect matching M of $\{v, u, x, y\}$
        if $M \cap E(G) = \emptyset$ **then**
            Construct G^{k+1} by removing the edges $\{v, u\}$, $\{x, y\}$ and adding the edges of M
        end if
    end if
end for

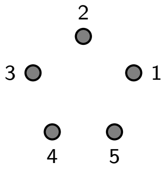


Simulation of edge-switching Markov chain

- For the Markov chain, initially a graph satisfying the degree sequence $\boldsymbol{d}$ is needed, and the Havel-Hakimi algorithm can be used to obtain a graph.

Theorem (Havel-Hakimi)

Let $\tilde{\boldsymbol{d}} = (\tilde{d}_1, ..., \tilde{d}_n) \in \mathbb{N}^n$ be a degree sequence obtained from $\boldsymbol{d}$ by subtracting 1 from d_i highest elements (other than i) in $\boldsymbol{d}$, and by letting $\widetilde{d}_i = 0$ for some $i \in \{1, .., n\}$. Then $\boldsymbol{d}$ is a graphical if and only if $\widetilde{\boldsymbol{d}}$ is graphical.



(3,2,3,2,2)

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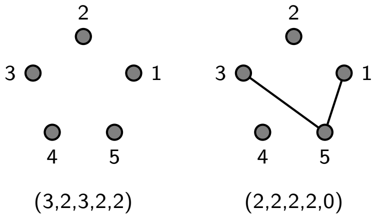

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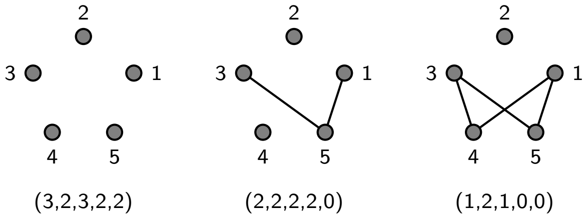

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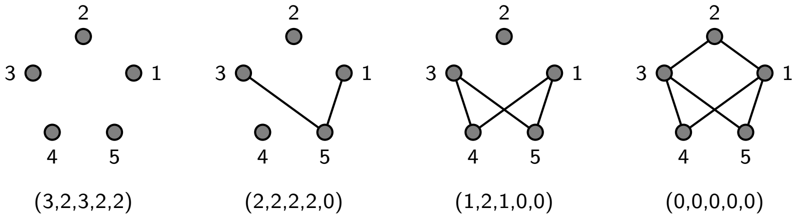
Theorem (Havel-Hakimi)

Let $\tilde{\boldsymbol{d}} = (\tilde{d}_1, ..., \tilde{d}_n) \in \mathbb{N}^n$ be a degree sequence obtained from $\boldsymbol{d}$ by subtracting 1 from d_i highest elements (other than i) in $\boldsymbol{d}$, and by letting $\widetilde{d}_i = 0$ for some $i \in \{1, .., n\}$. Then $\boldsymbol{d}$ is a graphical if and only if $\widetilde{\boldsymbol{d}}$ is graphical.



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- Since K is symmetric matrix, $\pi K^T = \pi$, and so π is uniform distribution over $\mathcal{G}^{\boldsymbol{d}}$.