Random generation of capacities

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- Important issue in machine learning: How to randomly generate capacities in a uniform way?
- Problem theoretically solved but intractable as soon as $n = 5$.
- $\hookrightarrow$ approximation methods are needed: Random Node Generator, Markov chains, two-layer approximation (our proposal), etc.
- Another problem: How to measure the performance of a capacity generator?

Outline

1. The problem of uniform random generation
2. The 2-layer approximation method
3. Measure of performance

Order polytopes

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- The *order polytope* (Stanley, 1986) associated to $(P, \preccurlyeq)$, denoted by $\mathcal{O}(P)$, is the set

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- $\mathcal{O}(P)$ is a polytope of dimension $p := |P|$.

Linear extensions

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- Vertices of R_σ are the $p+1$ functions given by

$$0 = f(x_{\sigma(1)}) = \cdots = f(x_{\sigma(k)}),\ f(x_{\sigma(k+1)}) = \cdots = f(x_{\sigma(p)}) = 1,$$

$k = 1, \ldots, p-1$, and the two constant functions 0 and 1.

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  3. Put $f(x_{\sigma(1)}) = z_1, \ldots, f(x_{\sigma(p)}) = z_p$.

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This is sequence A046873 in the *Online Encyclopedia of Integer Sequences*. $e(2^N)$ is not known beyond $n = 7$. Some bounds are known (Brightwell and Winkler, 1991).

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  - 2-additive capacities (Miranda and Garcia-Segador, 2020a)

The Random Node Generator

Algorithm:

1. $\mathcal{L} \leftarrow \{\varnothing, N\}$; $\mu(N) = 1$; $\mu(\varnothing) = 0$
2. Pick $S \in 2^N \setminus \mathcal{L}$
3. Compute $\mu_{\min}(S) = \max_{T \in \mathcal{L}, T \subseteq S} \mu(T)$,
   $\mu_{\max}(S) = \min_{T \in \mathcal{L}, T \supseteq S} \mu(T)$
4. Draw uniformly a number t in $[\mu_{\min}(S), \mu_{\max}(S)]$; $\mu(S) \leftarrow t$
5. $\mathcal{L} \leftarrow \mathcal{L} \cup \{S\}$
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Advantages: very simple and fast

Drawbacks: yields very biased distribution

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- Two linear extensions σ, τ are *neighbors* if they differ only by a single transposition of neighbor elements:

$$\begin{aligned} \sigma: &\quad x_{\sigma(1)}, \ldots, x_{\sigma(k)}, x_{\sigma(k+1)}, \ldots, x_{\sigma(p)} \\ \tau: &\quad x_{\sigma(1)}, \ldots, x_{\sigma(k+1)}, x_{\sigma(k)}, \ldots, x_{\sigma(p)} \end{aligned}$$

  for some $k \in [1, p-1]$. Denote by $n(\sigma)$ the number of neighbors of σ (at most $p - 1$).

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- The *order Markov chain M* is defined on the set of states $E(P)$ with transition probabilities:

$$P(\sigma, \tau) = \begin{cases} 1/(2p-2) & \text{if } \sigma, \tau \text{ are neighbors} \\ 1 - n(\sigma)/(2p-2) & \text{if } \sigma = \tau \\ 0 & \text{otherwise.} \end{cases}$$

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- The order Markov chain M is ergodic time-reversible and converges to the uniform distribution on $E(P)$.

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2. Find a linear extension σ on P
3. For $i = 1$ to T do:
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Estimation of T to get almost uniformity: $T = O(p^5 \log(e(P)))$.

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- As this probability directly depends on $e(P)$, the computation can be exact only when P becomes small enough.

Basic idea

- Let $(P, \preccurlyeq)$ with $P = \{x_1, \ldots, x_p\}$.
- Any linear extension $x_{\sigma(1)}, \ldots, x_{\sigma(p)}$ satisfies $x_{\sigma(1)} \in \mathrm{Min}(P)$ and $x_{\sigma(p)} \in \mathrm{Max}(P)$.
- Similarly, $x_{\sigma(2)} \in \mathrm{Min}(P \setminus \{x_{\sigma(1)}\})$, and $x_{\sigma(p-1)} \in \mathrm{Max}(P \setminus \{x_{\sigma(p)}\})$.
- Based on this observation, the probability that a linear extension of P starts with $m \in \mathrm{Min}(P)$ (resp., ends with $M \in \mathrm{Max}(P)$) is

$$\Pr(m \mid P) = \frac{e(P \setminus \{m\})}{e(P)}; \quad \Pr(M \mid P) = \frac{e(P \setminus \{M\})}{e(P)}$$

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- As this probability directly depends on $e(P)$, the computation can be exact only when P becomes small enough.
- Idea: take the lower part of the poset for choosing minimal elements, and the upper part for choosing maximal elements, thus neglecting minimal and maximal elements which are outside these two subparts.

The approximation method

- We take $P = 2^N \setminus \{\varnothing, N\}$ and delete step by step minimal and maximal elements. Generically, we call $(H, \subseteq)$ the current poset.

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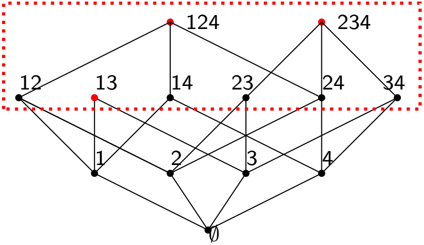

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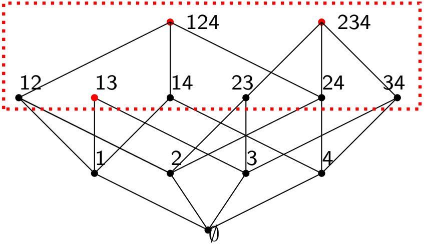

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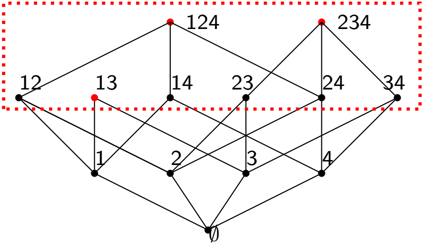

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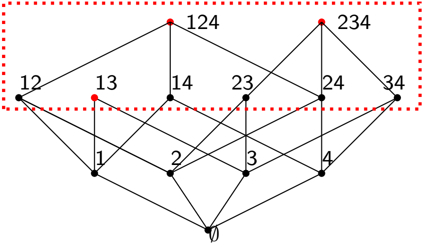

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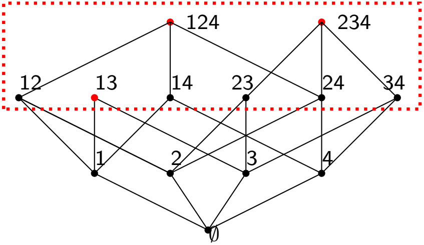

- For y in the 2nd layer, pred(y) is the set of its predecessors in the 1st layer (similarly with succ(x), x in the 1st layer)

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- Consider a maximal element M of H belonging to T_H, and a minimal element m of H belonging to B_H. We put

$$\Pr(M \mid H) \approx \frac{e(T_H \setminus \{M\})}{e(T_H)} = \Pr(M \mid T_H)$$

$$\Pr(m \mid H) \approx \frac{e(B_H \setminus \{m\})}{e(B_H)} = \Pr(m \mid B_H)$$

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- Rationale: If in average a node has ℓ predecessors in the layer just above, a node in layer k has therefore $O(\ell^{k-1})$ predecessors in H. Hence, a node in the 3d layer has very little probability to become maximal, since all its predecessors must be eliminated first, *without eliminating all nodes of the 1st layer*

The algorithm

generate-linext(P, l)
Input: a poset P subset of $2^N \setminus \{\varnothing, N\}$
Output: a linear extension l of P generated with a uniform distribution
$H \leftarrow P$; $lmin \leftarrow \varnothing$; $lmax \leftarrow \varnothing$
While height of $H > 2$ **do**

Compute the basic parameters of T_H: $k, h, |I|$
Select $M \in T_H[h, k, |I|]$ with probability $\Pr(M \mid T_H[h, k, |I|])$
Add M at the beginning of $lmax$
Compute the basic parameters of B_H: $k', h', |I'|$
Select $m \in B_H[h', k', |I'|]$ with probability $\Pr(m \mid B_H[h', k', |I'|])$
Add m at the end of $lmin$

$H \leftarrow H \setminus \{M, m\}$
end while

% Now H is reduced to two layers: B_H and T_H coincide

While height of $H = 2$ **do**

If number of nodes in the upper layer $\leqslant$ number of nodes in the lower layer **then**

Select $M \in T_H[h, k, |I|]$ with probability $\mathrm{Pr}(M \mid T_H[h, k, |I|])$

Add M at the beginning of *lmax*

$H \leftarrow H \setminus \{M\}$

otherwise

Select $m \in B_H[h', k', |I'|]$ with probability $\mathrm{Pr}(m \mid B_H[h', k', |I'|])$

Add m at the end of *lmin*

$H \leftarrow H \setminus \{m\}$

end if

end while

% Now H is reduced to one layer, which is an antichain whose elements have
% the same probability

While $H \neq \varnothing$ **do**

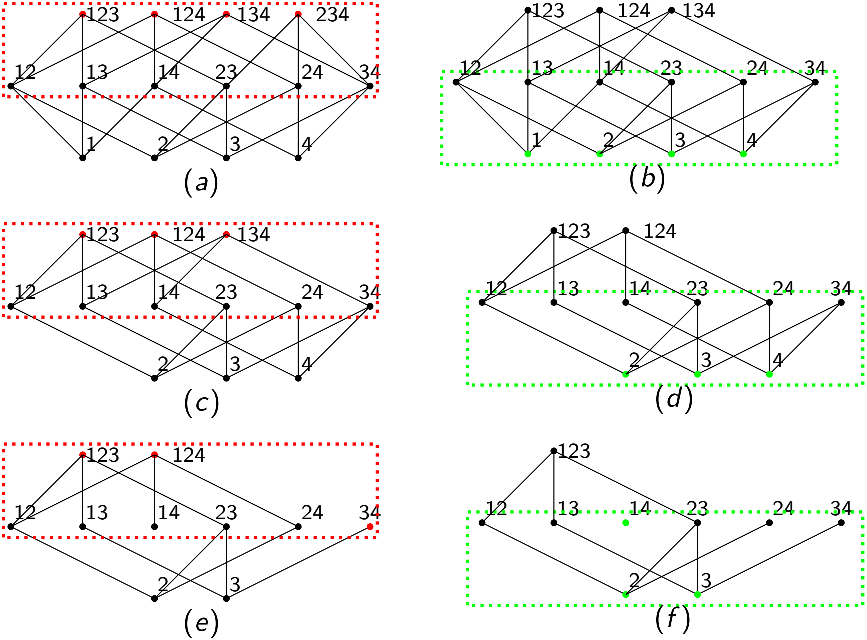
Select uniformly at random an element $x \in H$

Add x at the end of *lmin*

$H \leftarrow H \setminus \{x\}$

end while

$l \leftarrow lmin$; concatenate *lmax* to the end of l


123 124 134 234
12 13 14 23 24 34
1 2 3 4
(a)
123 124 134
12 13 14 23 24 34
1 2 3 4
(b)
123 124 134
12 13 14 23 24 34
2 3 4
(c)
123 124
12 13 14 23 24 34
2 3 4
(d)
123 124
12 13 14 23 24 34
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(e)
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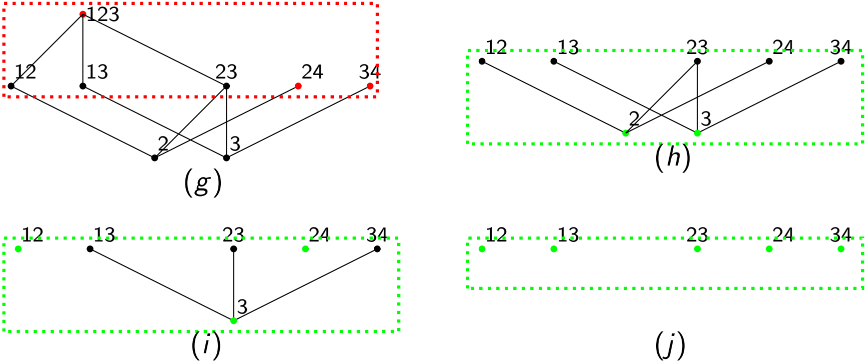
12 13 14 23 24 34
2 3
(f)



Resulting linear extension: 1, 4, 14, 2, 3, 12, 34, 24, 23, 13, 123, 124, 134, 234

Computation of the probabilities

It remains to compute $\Pr(M \mid T_H)$ and $\Pr(m \mid B_H)$. This is made possible through a simplifying assumption.

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Definition

Let x be a node of the upper layer of T_H.

1. The function f_x assigns to every node y of the lower layer an integer as follows:

$$f_x(y) = \begin{cases} |\text{pred}(y)|, & y \in \text{succ}(x) \\ 0, & \text{otherwise.} \end{cases}$$

2. The function $n_x : \mathbb{N} \to \mathbb{N}$ is defined from f_x as follows: $n_x(r)$ is the number of occurences of $f_x(y) = r$, i.e., $n_x(r) = |f_x^{-1}(r)|$. When $r > 0$, it is the number of successors of x having r predecessors, otherwise when $r = 0$ it is the number of nodes in the lower layer which are not successors of x.

Computation of the probabilities

Definition

We say that T_H is *regular* if n_x is invariant with x, i.e., $n_x(r) = n_{x'}(r)$ for every r and every two nodes x, x' in the upper layer.

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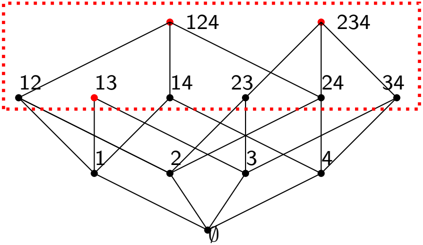

$n_{124}(0) = 3 = n_{234}(0)$, $n_{124}(1) = 2 = n_{234}(1)$, $n_{124}(2) = 1 = n_{234}(2)$, hence the above T_H is regular. Every T_H closed under intersection and balanced is regular.

Dual definitions exist for B_H.

Computation of the probabilities

Proposition

Consider the poset $T_H[h,k,|I|]$ and suppose that it is regular. Then the probabilities $\mathbb{P}_u(T_H[h,k,|I|])$ that node x of the upper layer terminates a linear extension, and $\mathbb{P}_l(T_H[h,k,|I|])$ that isolated node y of the lower layer terminates a linear extension are given by

$$\mathbb{P}_u(T_H[h,k,|I|]) = \frac{1}{h}\frac{\prod_{i=1}^{|I'|}(h-1+k-|I'|+i)}{\prod_{i=1}^{|I'|}(h-1+k-|I'|+i) + |I| \times \prod_{i=1}^{|I''|}(h-1+k-|I'|+i)\prod_{i=1}^{|I|-1}(h+k-|I|+i)}$$

$$\mathbb{P}_l(T_H[h,k,|I|]) = \frac{\prod_{i=1}^{|I''|}(h-1+k-|I'|+i)\prod_{i=1}^{|I|-1}(h+k-|I|+i)}{\prod_{i=1}^{|I'|}(h-1+k-|I'|+i) + |I| \times \prod_{i=1}^{|I''|}(h-1+k-|I'|+i)\prod_{i=1}^{|I|-1}(h+k-|I|+i)},$$

where I' is the set of isolated nodes in the poset $T_{H\setminus\{x\}}$, and $I \cup I'' = I'$.

Outline

Distribution of $\mu(S)$

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- Denote by $\boldsymbol{\mu}$ the r.v. with uniform distribution on $\mathcal{C}(N)$. Take a linear extension σ and consider the associated region $R_\sigma \subseteq \mathcal{C}(N)$.
- Given that $\boldsymbol{\mu} \in R_\sigma$, we know that $\boldsymbol{\mu}(S_{\sigma(k)})$ follows the distribution of the kth order statistics on $[0,1]$. It is known that the probability density function $f_{(k)}$ of the kth order statistics on $[0,1]$ when the underlying $2^n - 2$ random variables are i.i.d. and uniform is a Beta distribution:

$$f_{(k)}(u) = (2^n - 2)\binom{2^n - 3}{k - 1}(1-u)^{2^n-2-k}u^{k-1} = \mathrm{Beta}(k, 2^n + k - 1)$$

Distribution of $\mu(S)$

Denoting by OS_k the corresponding cumulative distribution function, it follows that for any $S \in 2^N \setminus \{\varnothing, N\}$, the distribution $F_{\boldsymbol{\mu}(S)}(\alpha)$ is given by

$$\begin{aligned}
F_{\boldsymbol{\mu}(S)}(\alpha) = \mathrm{Pr}(\boldsymbol{\mu}(S) \leqslant \alpha) &= \sum_{\sigma \in E(2^N \setminus \{\varnothing, N\})} \mathrm{Pr}(\boldsymbol{\mu}(S) \leqslant \alpha \mid \boldsymbol{\mu} \in R_\sigma)\mathrm{Pr}(\boldsymbol{\mu} \in R_\sigma) \\
&= \frac{1}{e(2^N)} \sum_{\sigma \in E(2^N \setminus \{\varnothing, N\})} \mathrm{Pr}(\boldsymbol{\mu}(S) \leqslant \alpha \mid \boldsymbol{\mu} \in R_\sigma) \\
&= \frac{1}{e(2^N)} \sum_{\sigma \in E(2^N \setminus \{\varnothing, N\})} \mathrm{OS}_{k(S,\sigma)}(\alpha), \qquad (1)
\end{aligned}$$

where $E(2^N \setminus \{\varnothing, N\})$ is the set of permutations corresponding to linear extensions, and $k(S, \sigma)$ is such that $S = S_{\sigma(k)}$.

Distribution of $\mu(S)$

Lemma

Assume $\boldsymbol{\mu}$ *is uniformly distributed and take* $\varnothing \neq S, S' \subset N$. *Then*

1. $\boldsymbol{\mu}(S)$ *and* $\boldsymbol{\mu}(S')$ *for* $|S| = |S'|$ *are identically distributed.*
2. $\boldsymbol{\mu}(S)$ *and* $1 - \boldsymbol{\mu}(N \setminus S)$ *are identically distributed.*

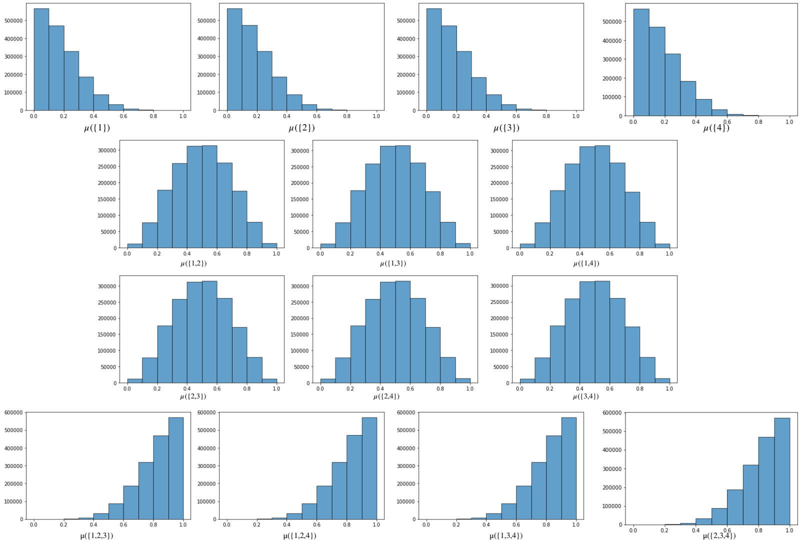

Figure: Histograms of $\mu(S)$ for $n = 4$ and the exact method

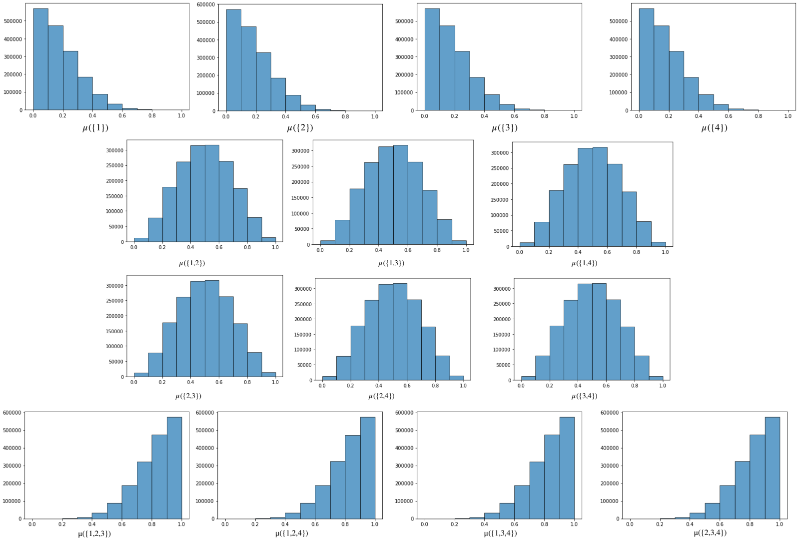

Figure: Histograms of $\mu(S)$ for $n = 4$ and the 2-layer approximation method

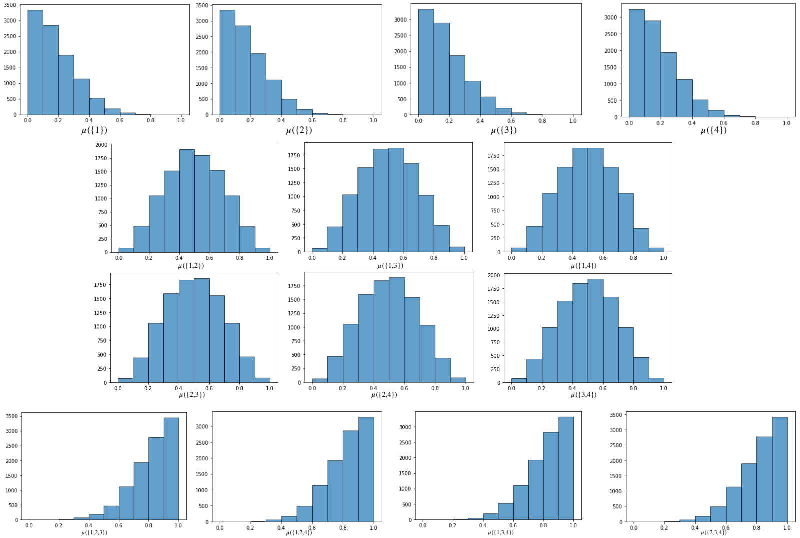

Figure: Histograms of $\mu(S)$ for $n = 4$ and the Markov chain method

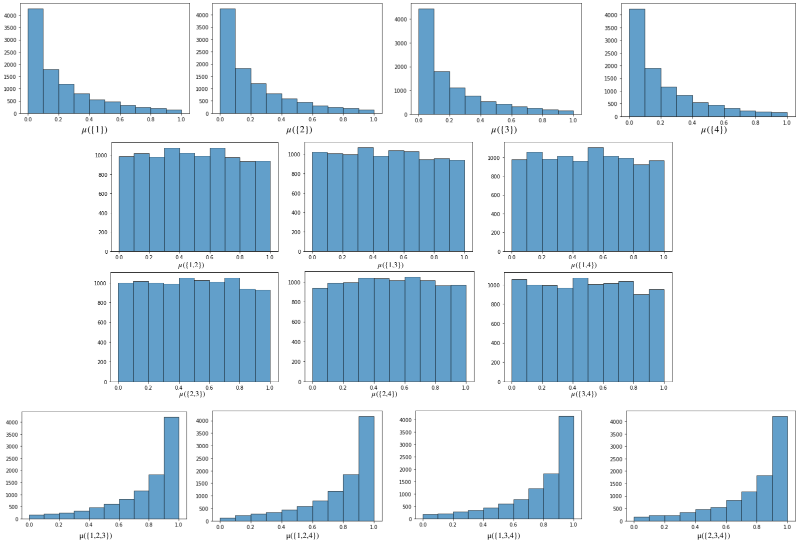

Figure: Histograms of $\mu(S)$ for $n = 4$ and the Random Node Generator

The centroid of $\mathcal{C}(N)$

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- centroid for $n = 4$:

$$c = (0.1810, 0.1810, 0.1810, 0.1810, 0.5000, 0.5000, 0.5000, 0.5000, 0.5000, 0.5000, 0.8190, 0.8190, 0.8190, 0.8190).$$

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- When $n \leqslant 4$, we take as performance the L_1 distance between the theoretical centroid and the obtained centroid. We obtain $T = 1170$.
- When $n > 4$, we use the symmetry properties of the centroid ($c(S)$ depends only on $|S|$). The performance is measured by the standard deviation of $c(S)$ when $|S|$ is constant. We obtain $T = 9000$ for $n = 5$.

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  The smaller the value, the closer are the two distributions.
- Distributions of $\boldsymbol{\mu}(S)$ are discretized with $\delta = 0.01$ on $[0, 1]$. We call $\mu_{MC}(S), \mu_{2L}(S)$ the discrete distributions obtained by the Markov chain method and the 2-layer approximation, respectively.

Experimental results: Comparison of distributions

- With $n \leqslant 4$, q is the exact distribution and p is the distribution to be tested. We compute

$$S^4_{KL}(\mu_{MC}) = \sum_{S \in 2^N} \mathbb{D}_{KL}(\mu_{MC}(S)||\boldsymbol{\mu}(S))$$
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$$S^N_{KL}(\mu_{MC}) = \sum_{S,S' \in 2^N \text{ s.t. } |S|=|S'|} \mathbb{D}_{KL}(\mu_{MC}(S)||\mu_{MC}(S'))$$
$$S^N_{KL}(\mu_{2L}) = \sum_{S,S' \in 2^N \text{ s.t. } |S|=|S'|} \mathbb{D}_{KL}(\mu_{2L}(S)||\mu_{2L}(S'))$$

- Results

$S^4_{KL}(\mu_{MC})$	$S^4_{KL}(\mu_{2L})$	$S^5_{KL}(\mu_{MC})$	$S^5_{KL}(\mu_{2L})$
0.061	0.059	2.41	2.24

Experimental results: Computation time

Comparison of CPU time (s) for generating 10,000 capacities (3.2 GHz PC with 16 GB of RAM)

Method		$n = 4$	$n = 5$	$n = 6$	$n = 7$
2 layer approximation		2.58	11.51	60.06	330.17
Markov Chain	CPU time	20.46	161.33	$\approx$ 1500	$\approx$ 9000
	T	1170	9000	80,000	500,000

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- The 2-layer approximation method is much faster.

Thank you for your attention!